15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Elastoplasticity with Linear Tetrahedral Elements: A Variational Multiscale Method

Author(s): *Nabil Abboud, *Duke University*; Guglielmo Scovazzi, *Duke University*;

We present a computational framework for the simulation of J2-elastic/plastic materials in complex geometries based on simple piecewise linear finite elements on tetrahedral grids. We avoid spurious numerical instabilities by means of a specific stabilization method of the variational multiscale kind. Specifically, we introduce the concept of subgrid-scale displacements, velocities, and pressures, approximated as functions of the governing equation residuals. The subgrid-scale displacements/velocities are scaled using an effective (tangent) elastoplastic shear modulus, and we demonstrate the beneficial effects of introducing a subgrid-scale pressure in the plastic regime. We provide proofs of stability and convergence of the proposed algorithms. These methods are initially presented in the context of static computations and then extended to the case of dynamics, where we demonstrate that, in general, naïve extensions of stabilized methods developed initially for static computations seem not effective. We conclude by proposing a dynamic version of the stabilizing mechanisms, which obviates this problematic issue. In its final form, the proposed approach is simple and efficient, as it requires only minimal additional computational and storage cost with respect to a standard finite element relying on a piecewise linear approximation of the displacement field.

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Title: Effects of Mesoscale Material Inhomogeneity on Macroscopic Dynamic Fracture Response

Author(s): *Reza Abedi, *University of Tennessee*; Philip Clarke, *University of Tennesee*; Bahador Bahmani, *University of Tennessee*; Justin Garrard, *University of Tennessee*; Katherine Acton, *University of Saint Thomas*; Robert Haber, *University of Illinois at Urbana-Champaign*;

We consider two different material models to study the effect of inhomogeneity at the mesoscale on macroscopic fracture response. First, we assume the material is homogeneous. Second, we use a Voronoi-tessellation partition to form Statistical Volume Elements (SVEs). We analyse these SVEs under three loading conditions to determine the normal and shear fracture strengths of the SVEs. After deriving the statistical properties of the SVEs, such as their probability distributions of fracture strength and two-point correlation functions, we use the Karhunen-Loeve method to derive statistically consistent fracture strength fields at the mesoscale. We compare the fracture response of the two models under uniform tensile loading. We show that the concept of dynamic fragmentation of homogeneous materials is not physical in that fractures would form instantaneously across the entire domain when the load reaches the material strength. In contrast, cracks nucleate at discrete weak points in inhomogeneous material models. The propagation of these initial cracks would generate a highly nonuniform stress field that, along with the inhomogeneous fracture strength field, would produce more realistic fracture patterns. We obtain commonly observed features of dynamic fracture, such as crack-path oscillation, microcracking, and crack bifurcation, in simulations based on the inhomogeneous model. We study the effects of certain loading and material parameters on macroscopic fracture patterns using an interfacial damage model [2]. For loading, we consider parameters related to loading rate and load biaxiality. We also study the influence of a mesoscopic fracture-energy parameter that depends on a relaxation time in the interfacial damage model. We obtain distinct fracture patterns and homogenized macroscopic stress–strain responses for different loading and material combinations. Finally, we explore the influence of the finite element discretization on fracture response. We demonstrate that the degree of mesh refinement, the mesh type (structured versus unstructured), and whether the mesh is fixed or adaptive affects the macroscopic fracture pattern, ultimate load, and dissipated energy. One of our interesting findings is that macroscopic dissipated fracture energy is relatively insensitive to increasing mesh refinement beyond a certain level of refinement. References: [1] K.A. Acton, S.C. Baxter, B. Bahmani, P.L. Clarke, R Abedi. “Voronoi tessellation based statistical volume element characterization for use in fracture modeling”, Computer Methods in Applied Mechanics and Engineering 336, 135-155, 2018. [2] R. Abedi, R.B. Haber, and P.L. Clarke. "Effect of random defects on dynamic fracture in quasi-brittle materials." International Journal of Fracture 208.1-2 (2017): 241-268.

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Title: Uncertainty Quantification for Microstructural Features of Additively Manufactured Materials

Author(s): *Pinar Acar, *Virginia Tech*;

The present work addresses a stochastic solution methodology to understand the propagation of microstructural variations to the multi-scale evolution and response of additively manufactured materials. Given small-scale experimental information of the microstructure, we discuss building a stochastic computational framework for characterizing microstructural uncertainties across larger spatial domains. The evolution of the microstructure is modeled by a stochastic process, Markov Random Field (MRF), which is utilized as a reconstruction algorithm. In this approach, the microstructures are grown layer-by-layer from a small seed image taken randomly from the input data. The MRF algorithm is capable of predicting the evolution of microstructures in larger spatial and temporal domains, and in this work, it is used to understand the large-scale evolution of the additively manufactured materials using small-scale experimental data. In the case of additive manufacturing techniques, small variations are introduced to the microstructures during thermomechanical processing of the material. Our goal is to quantify these uncertainties and model their propagation to the material response by utilizing the MRF based microstructure reconstruction technique. We will use the available electron backscatter diffraction (EBSD) data for a Titanium-Aluminum alloy (Ti-7wt%Al) which demonstrates measurements in different specimens. Even though the EBSD measurements are taken from the same material, but from different specimens, they show variations in the orientation data which are associated with the natural randomness observed in microstructures. First, we utilize the MRF algorithm to achieve the large-scale prediction of the microstructural texture using the EBSD input. Next, an analytical uncertainty quantification (UQ) methodology is addressed to model the uncertainties arising from the microstructural variations that are observed during the additive manufacturing process of the material. The analytical UQ technique is based on a Gaussian process model, which uses the transformation feature of the Gaussian distribution to explore the propagation of microstructural uncertainties to the volume-averaged material properties. Using the analytical UQ algorithm and the microstructure samples generated with the MRF approach, we model the propagation of the uncertainties to the large-scale microstructural features and analyze the effects of natural variations to the expected material response.

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Title: High Order Surface Radiation Conditions for Exterior Wave Fields

Author(s): *Sebastian Acosta, *Texas Children's Hospital and BCM*;

We present a new family of high order on-surface radiation conditions to approximate the solution to the Helmholtz equation in exterior domains. Motivated by the pseudo-differential expansion of the Dirichlet-to-Neumann map, we design a systematic procedure to apply pseudo-differential symbols of arbitrarily high order. Numerical results are presented for solving both the Dirichlet and the Neumann boundary value problems. Possible improvements, extensions and use as preconditioner will be discussed.

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Title: Adjoint-enabled Robust Radiation Shield Design

Author(s): *Brian Adams, *Sandia National Laboratories*; Shawn Pautz, *Sandia National Laboratories*; Donald Bruss, *Sandia National Laboratories*; Brian Franke, *Sandia National Laboratories*; Ethan Blansett, *Sandia National Laboratories*; Laura Swiler, *Sandia National Laboratories*;

Radiation shields make commodity microelectronics practical for use in satellite and other space systems. Shield designers wish to take advantage of new materials and manufacturing processes to meet strict weight limits while protecting electronics from naturally occurring proton and electron radiation environments. Our work couples Sandia National Laboratories' Dakota software (http://dakota.sandia.gov) with its SCEPTRE radiation transport code to automate the design exploration and reliability analysis process, enabling analysts to evaluate prospective shield materials and geometries. This talk highlights efficiency gains from pairing gradient-based optimization and uncertainty quantification algorithms in Dakota with newly implemented adjoint sensitivities in SCEPTRE. It will survey optimization, UQ, and design under uncertainty studies conducted with 1-D and 2-D transport analyses for satellite shield performance.

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Title: Modeling 3-D Grain Boundary Evolution Driven by the Five-dimensional Grain Boundary Energy Landscape

Author(s): *Nikhil Chandra Admal, *University of Illinois Urbana-Champaign*; Javier Segurado, *IMDEA, Madrid, Spain*; Matt Jacobs, *University of California Los Angeles*; Stanley Osher, *University of California Los Angeles*; Jaime Marian, *University of California Los Angeles*;

Grain boundary (GB) evolution plays an extremely important role in the mechanical, thermal and electronic properties of micro/nano-crystalline materials. In this talk, we present a three-dimensional generalization of the Kobayashi--Warren--Carter (KWC) grain boundary evolution model governed by a fully-anisotropic GB energy density that depends on the misorientation and inclination of the grain boundary (Admal et al. [2018]). The model is parameterized using grain boundary energy data from atomistic simulations making it truly predictive. Computing gradient flows of the KWC energy is highly nontrivial due to its singular diffusive nature. Inspired by the thresholding method of Merriman, Bence and Osher (mer [1992]), we present a new computational approach for the time evolution of the KWC model that results in a decisive improvement in the computation compared to existing implementations. References: Nikhil Chandra Admal, Javier Segurado, and Jaime Marian. A three-dimensional misorientation axis- and inclination-dependent Kobayashi–Warren–Carter grain boundary model. Journal of Mechanics and Physics of Solids, 2018. In review. Barry Merriman, James Kenyard Bence, and Stanley Osher. Diffusion generated motion by mean curvature. Proceedings of the Computational Crystal Growers Workshop, 1992.

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Title: Multigrid Preconditioners for Higher Order Enriched Finite Element Methods

Author(s): *Konstantinos Agathos, *ETH Zurich*; Eleni Chatzi, *ETH Zurich*;

The introduction of the stable GFEM [1] has provided a means of mitigating conditioning issues in enriched finite element methods by removing linear dependencies between the enriched and standard part of the approximation. However, for the case where multiple enrichment functions are used, conditioning problems might still be present as a result of linear dependencies between the different enrichment functions. In the present work, we combine the stable GFEM to enrichment quasi-orthogonalization [2], allowing the simultaneous use of multiple polynomial, discontinuous and singular enrichment functions. The resulting scheme, possesses a series of desirable features, the most important among which can be identified as high order convergence rates in the presence of discontinuities and singularities, hierarchical structure and close to optimal growth rates for the scaled condition number, which in turn facilitates the use of iterative solvers. To fully exploit the hierarchical structure of the system matrices produced by the method, the use of a multigrid preconditioner is proposed in combination to an iterative solver. Within the preconditioner, typical techniques employed in multigrid methods such as pre and post smoothing are utilized, while different levels correspond to different degrees of polynomial enrichment. Due to this special structure, the initialization of the preconditioner becomes straightforward, provided however, that information regarding the polynomial degree associated with each node is supplied. The proposed scheme is tested through a series of numerical examples, involving different degrees of polynomial enrichment, and its performance is compared to alternative linear solvers. [1] I. Babuška, U. Banerjee, Stable generalized finite element method (SGFEM), Computer Methods in Applied Mechanics and Engineering 201 (2012): 91-111. [2] K. Agathos, S.P.A. Bordas, E. Chatzi, Improving the conditioning of XFEM/GFEM for fracture mechanics problems through enrichment quasi-orthogonalization, Computer Methods in Applied Mechanics and Engineering (2018).

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Title: Phase Field Damage Modeling of Mechanical Degradation in Polymers under Hydro-thermomechanical Loading Conditions

Author(s): *Vinamra Agrawal, *Auburn University*; Brandon Runnels, *University of Colorado at Colorado Springs*; Asha-Dee Celestine, *Auburn University*;

In this work, we model the mechanical degradation in Nylon when subjected to hydro-thermomechanical loading using a phase field continuum damage mechanics modeling. As the water diffuses within the polymer, strength and moduli of the material degrade. This is a result of underlying chemical reactions between water molecules and polymer chains that lead of breakdown of polymer chains. While most studies have focused on studying degradation due to mass loss, this work studies the loss of mechanical properties which occurs much before any observable mass loss. This is especially important when studying polymer composites that are being used for their structural properties. This work uses ideas from continuum damage mechanics and phase field modeling to model the degradation of strength and moduli at the continuum level. The work uses a computational framework, Alamo, that features multilevel, multigrid explicit solver for phase field modeling and a multilevel, multigrid implicit solver for elasticity problems. The framework is also capable of block structured adaptive mesh refinement with distributed and shared memory parallelism. The framework has been tested for phase field problems such as grain boundary motion. The current work uses Alamo to model polymer degradation using a phase field damage model. The damage evolution model depends on the water concentration, temperature, time history and the stress states at every point. As the first step, the damage evolution model is chosen as a combination of Arrhenius type exponential terms, each contributing to a certain amount of degradation based on prescribed half-lives. This model finds its basis in chemical reaction kinetics between water and polymer chains. The model parameters are calibrated from experimental studies. The experimental studies were conducted on Nylon and Nylon blend specimens with ASTM prescribed geometries at different temperatures. Water diffusion and mass gain was studied by weighing the specimen at different intervals of time. The mechanical properties were using standard tensile tests and three-point bend tests. These tests provided evolution of mechanical properties over time. Using the phase field modeling, the specimen was degraded at different temperatures. A standard Fick’s law was used for water diffusion. The effect of temperature was incorporated by changing the diffusion coefficients. Next, using Alamo’s implicit solver, tensile tests were recreated, and effective modulus was obtained to compare against experimental observation. In the future, the model will be extended for polymer composites where anisotropic effects will be studied.

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Title: Different Reduction Techniques Based on Physical Reduced Order Modeling and Deep Learning for Geometrical Exploration of Turbulent and Incompressible Fluid Flows

Author(s): *Nissrine Akkari, *Safran Tech - Modeling and Simulation*; Fabien Casenave, *Safran Tech - Modeling and Simulation*; Vincent Moureau, *CORIA - CNRS*;

In the following work we provide recent researches and developments in model reduction technologies applied to fluid dynamics problems, in particular for design exploration purposes of gaz turbines and fuel injectors of aircraft engines. We present first a new physics based POD (Proper Orthogonal Decomposition)-Galerkin projection of the turbulent and incompressible Navier-Stokes equations. This reduced order model stabilization is based on an a priori enrichment by scales separation of the POD basis with dissipative modes of the velocity fields [2]. This a priori enrichment with space scales seperation, enables a stable dynamic reduced order model that could be used for very long time integration even for temporal extrapolation. We show that the temporal weights of the reduced modes which are solutions of the enriched reduced model are very stable. Then, we present a physics based geometrical model order reduction of the unsteady and incompressible Navier-Stokes equations, that we solve efficiently with respect to a collection of a priori designs for an injector. This framework is based on a prediction step of the global aerodynamic field using the Gappy-POD approach [4] on a local high-fidelity solution associated with a new design and a correction step by extrapolation using the Galerkin projection of the governing Navier-Stokes equations upon global and local POD modes obtained in a particular fashion. This combination between data reconstruction techniques and physics-based ROM enables a good prediction of the geometrical aerodynamic field [3]. The accuracy of this prediction is quantified by computing the error on different quantities of interest with respect to the high-fidelity LES (Large Eddy Simulations). These quantities of interest are the recirculation zones which drive the flame stabilization. Finally, we present a very recent work concerning the use of deep learning approaches for improving fluid mechanics simulations. Due to the statistical nature of the unsteady and turbulent fluid flows, data driven algorithms could potentially reduce the computational cost through reduced trained models. Among the novel paradigms emerging from the deep learning community, Generative Adversarial Networks (GAN) [1] are particularly relevant for our task. GANs aim to capture the data distribution such that they can then easily generate new realistic samples similar to the real ones. We present a study concerning the requirements for a deep neural network to learn a LES. To conclude, we illustrate the ability of the GAN to predict fluid flows in a variable domain. [1] Goodfellow, I. et al., Generative Adversarial Networks. NIPS, 2014. [2] Akkari, N. and Mercier, R. and Moureau, V. and Lartigue, G., Stable POD-Galerkin Reduced Order Models for unsteady turbulent incompressible flows. 55th AIAA Aerospace Sciences Meetings, AIAA Scitech Forum, (AIAA 2017-1000), 2017. [3] Akkari, N. and Mercier, R. and Moureau, V., Geometrical Reduced Order Modeling (ROM) by Proper Orthogonal Decomposition (POD) for the incompressible Navier-Stokes équations. AIAA Aerospace Sciences Meeting, AIAA Scitech Forum, (AIAA 2018-1827), 2018. [4] Everson, R. and Sirovich, L., Karhunen-Loève procedure for Gappy data. J. Opt. Soc. Am. A, Vol. 12, No. 8, 1995.

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Title: Local Displacement and Strain Boundary Conditions in Nonlocal Problems

Author(s): *Burak Aksoylu, *U.S. Army Research Laboratory & Wayne State University*; George Gazonas, *U.S. Army Research Laboratory*;

We provide a comprehensive treatment on how to enforce inhomogeneous local boundary conditions (BC) in nonlocal problems in 1D. In prior work [1, 2, 3], we have presented novel governing operators with homogeneous BC. Here, we extend the construction to inhomogeneous BC. The construction of the operators is inspired by peridynamics. The operators agree with the original peridynamic operator in the bulk of the domain and simultaneously enforce local Dirichlet and Neumann BC. The main tool we use to define the novel governing operators is functional calculus, in which we replace the classical governing operator by a suitable function of it. We present how to apply functional calculus to general nonlocal problems in a methodical way. We reveal a close connection between the classical and nonlocal wave equations. Namely, the combination of the function piece (even and odd parts) and the extension type used in d'Alembert's formula is identical to that in the construction of our nonlocal operators. We explain methodically how to construct forcing functions to enforce local BC and their relationship to initial values. We present exact solutions with both homogeneous and inhomogeneous BC and utilize the resulting error to verify numerical experiments. For the Neumann BC, we prescribe an interpolation strategy to find the appropriate value of the forcing function from its derivative. We also present numerical experiments with unknown solution and report the computed displacement and strain fields. [1] B. Aksoylu and F. Celiker, Nonlocal problems with local Dirichlet and Neumann boundary conditions, Journal of Mechanics of Materials and Structures, 12(4) (2017), pp. 425-437. [2] B. Aksoylu, H.R. Beyer, and F. Celiker, Application and implementation of incorporating local boundary conditions into nonlocal problems, Numerical Functional Analysis and Optimization, 38(9) (2017), pp. 1077-1114. [3] B. Aksoylu, H.R. Beyer, and F. Celiker, Theoretical foundations of incorporating local boundary conditions into nonlocal problems, Reports on Mathematical Physics, 80(1) (2017), pp. 39-71.

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Title: Fourier Multipliers for Nonlocal Operators

Author(s): *Bacim Alali, *Kansas State University*; Nathan Albin, *Kansas State University*;

Fourier multiplier analysis is developed for peridynamic Laplace operators, which are defined for scalar fields in Rn. The Fourier multipliers are given through an integral representation. We show that the integral representation of the Fourier multipliers is recognized explicitly through a unified and general formula in terms of the hypergeometric function _2F_3 in any spatial dimension n. Asymptotic analysis of _2F_3 is utilized to identify the asymptotic behavior of the Fourier multipliers m(v) as |v| goes to infinity. We show that the multipliers are bounded when the peridynamic Laplacian has an integrable kernel, and diverge to negative infinity when the kernel is singular. The bounds and decay rates are presented explicitly in terms of the dimension n, the integral kernel, and the peridynamic Laplacian nonlocality. The asymptotic analysis is applied in the periodic setting to prove a regularity result for the peridynamic Poisson equation.

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Title: Anisotropic Continuum Damage Models in Multi-layer Isogeometric Kirchhoff-Love Shell Composites

Author(s): *Mert Alaydin, *Brown University*; Yuri Bazilevs, *Brown University*; David Kamensky, *Brown University*; Marco Simone Pigazzini, *Livermore Software Technology Corporation*;

The focus of this talk will be on anisotropic continuum damage models predicting ultimate load capacity of multi-layer laminated composites where each lamina is modeled as an isogeometric Kirchhoff-Love shell. Numerical difficulties arising from local damage models will be discussed. Then it will be shown that stacking up laminas in certain layup configurations alleviates damage localization issue, which leads to non-objective results upon h-refinement. Close attention will be paid to computation of tangent stiffness and related numerical aspects. Further, capabilities of recently introduced gradient-enhanced damage model for general manifolds are briefly presented and compared with the local counterpart.

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Title: On the Connection between Optimal Uncertainty Quantification and the Mean Objective Cost of Uncertainty

Author(s): *Francis Alexander, *Brookhaven National Laboratory*; Kristofer Reyes, *University at Buffalo*; Michael McKerns, *Los Alamos National Laboratory*; Byung-Jun Yoon, *Texas A&M University*;

Accurately assessing the uncertainty, and ultimately reducing its associated effects in science and in both natural and engineered systems is crucial. For complex systems such as climate, cancer, and turbulence such an assesment and control of uncertainty and its can be quite challenging. In addition to quantifying the quality of a scientific prediction and/or controlling an engineering process, uncertainty also plays a vital role in the optimal design of experiments in order to make the best use of limited resources. Over recent years several frameworks have emerged to carry out this assessment and control of uncertainty. In this paper, we will focus on two such frameworks. These frameworks include optimal uncertainty quantification (OUQ) and the mean objective cost of uncertainty (MOCU) with its special case of knowledge gradient. MOCU is an objective-driven uncertainty quantification (UQ) framework, in which one integrates scientific prior knowledge on both the system and the available data and quantifies the uncertainty relative to the objective. Likewise, OUQ integrates the knowledge available for both mathematical models and any knowledge that constrains outcomes of the system, but then casts the problem as a constrained global optimization problem in a space of probability measures. This optimization is made tractable by reducing the problem to a finite-dimensional effective search space of discrete, parameterized probability distributions. We detail the connections between these frameworks, limiting cases and describe the advantages and problems for which they ideally suited. We will close proposing new directions for these frameworks, especially in the context of optimal experimental design.

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Title: Large-Scale Bayesian Uncertainty Quantification of Heterogeneous Aquifer Properties from Surface Deformation Data and Poroelastic Subsurface Models

Author(s): *Amal Alghamdi, *University of Texas at Austin*; Marc Hesse, *University of Texas at Austin*; Jingyi Chen, *University of Texas at Austin*; Omar Ghattas, *University of Texas at Austin*;

Rapid groundwater extraction leads in numerous cases to significant permanent reduction of aquifer capacity in addition to triggering seismic events and causing infrastructure damage. Quantifying the uncertainty of subsurface parameters in groundwater aquifers is essential for predicting the aquifer system response and optimally controlling groundwater production. We employ a scalable Bayesian framework to infer heterogeneous aquifer hydromechanical properties from surface deformation data and a poroelasticity model. The deformation data include both InSAR maps and GPS displacements, and the model is given by 3D quasi-static linear poroelasticity (Biot), which couples fluid flow in a saturated porous medium and the accompanying elastic deformation of the solid skeleton. We adopt a three-field formulation of the Biot system and use a fully coupled discretization in which a mixed method is used to approximate fluid flow in the lowest order Raviart--Thomas space. This discretization ensures local mass conservation and has a significant damping effect on the numerical (unphysical) oscillations that arises in the finite element method solution of the Biot system. Bayesian solution of this inverse problem results in a posterior probability density quantifying uncertainties in the aquifer parameters fields (in our examples, the permeability, but the framework is more general). These uncertainties stem from uncertainties in the data, model, and prior information on the parameters, along with insensitivity of observables to parameters. We explore the posterior distribution using both the Laplace approximation and discretization-invariant MCMC sampling techniques. To address the prohibitive nature of Bayesian inversion, we incorporate adjoint-based gradients and Hessians of the negative log posterior. We carry out the implementation using the FEniCS library for finite element discretization in space and hIPPYlib library for scalable Bayesian PDE-constrained inversion. Specifically, we employ an inexact Newton--conjugate gradient method to find the maximum a posteriori (MAP) point, randomized generalized eigensolvers to extract a low rank approximation of the (preconditioned) data misfit Hessian, and discretization-invariant MCMC sampling techniques. We apply the proposed methodology on a test case for a municipal well in Mesquite, Nevada, in which GPS and InSAR surface deformation data are available. We solve problems with up to 320K state variables and 16.8K parameters. This represents the first application of scalable MCMC methods to Bayesian inverse problems with high-dimensional parameters, coupled multiphysics forward problems, and multi-modal observational data.

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Title: Energy Release Rate Approximation for Surface Cracks in Three-Dimensional Domains Using the Topological Derivative

Author(s): *Kazem Alidoost, *University of Illinois at Urbana-Champaign*; Philippe Geubelle, *University of Illinois at Urbana-Champaign*; Daniel Tortorelli, *University of Illinois at Urbana-Champaign*; Meng Feng, *University of Illinois at Urbana-Champaign*;

Topological derivatives provide the variation of a functional when an infinitesimal hole is introduced into the domain. In this three-dimensional fracture mechanics work, we develop an approximation of the energy release rate field associated with a small surface crack of any boundary location, direction, and orientation combination using the topological derivative. This study builds on the work of Silva et al., in which the authors developed a similar approximation of the energy release rate field for two-dimensional domains [1]. This method offers significant computational advantages over other methods because (i) it requires only a single analysis while other methods require an analysis for each crack size-location-orientation combination, and (ii) it is performed on the non-cracked domain, removing the need for highly refined meshes in the neighborhood of the crack. In Alidoost et al., a higher-order approximation of the energy release rate was developed using higher-order topological derivatives [2]. In addition to the stress state at the crack initiation point, this higher-order approximation incorporates the derivatives of the stress state computed on the uncracked domain in the expected direction of crack propagation. The derivatives of the stress state are computed using an asymptotic expansion for the tractions along the crack surface as the crack length approaches zero. Higher-order approximations allow the analyst to accurately treat longer cracks and determine for which crack lengths the first-order approximation is accurate. In this presentation, we begin by reviewing the two-dimensional approximations of the energy release rate. These two-dimensional approximations are combined with Abaqus FEA so that by simply supplying an ODB file the energy release rate is approximated for a crack at any boundary location and any orientation. In this way, we promptly identify the critical combinations of boundary locations and orientations that reach the critical energy release rate at the smallest crack lengths. Subsequently, we introduce the three-dimensional approximation of the energy release rate and explore the significant computational advantages of the three-dimensional approximation over other methods. We conclude by presenting our current work on fracture-based shape optimization using this approximation of the energy release rate. [1] Silva, Geubelle, Tortorelli, Energy release rate approximation for small surface-breaking cracks using the topological derivative, J. Mech. Phys. Solids, 59(5) (2011), pp.925–939. [2] Alidoost, Geubelle, Tortorelli, Energy release rate approximation for edge cracks using higher-order topological derivatives, International Journal of Fracture, 210(1-2) (2018), pp.187-205.

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Title: ARIMA-GMDH: A low order integrated modelling approach for predicting and optimizing the additive manufacturing process parameters

Author(s): *Osama Aljarrah, *University of Massachusetts Dartmouth*; Wenzhen Huang, *University of Massachusetts Dartmouth*; Jun Li, *University of Massachusetts Dartmouth*; Alfa Heryudono, *University of Massachusetts Dartmouth*; Jing Bi, *Dassault System*;

This paper proposes a novel integrated inductive approach for predicting and optimizing the additive manufacturing process parameters. The integrated scheme consists of three popular algorithms: (1) group method for data handling (GMDH) as the engine of neural networks, (2) autoregressive integrated moving average (ARIMA) for characterizing spatial collinearity of residual stresses in multiple layers, and (3) indirect optimization method by self-organization (IOSO) to adopt the emerged multi-response correlated optimization problem. As a numerical case study: A computer-generated fused deposition modeling (FDM) simulation data tested the introduced algorithms. The FE models consist the multi-layer residual stresses as targets, with respect to printing speeds as process parameters. The residual stresses predicted by the low order ARIMA-GMDH variant correlate well with the cuboid FE simulations. The printing speeds and their experimental simulation results were submitted into four analytical stages: the initial phase, transient phase, steady-state phase, and terminal phase, where each stage was analyzed through a low order integrated ARIMA-GMDH variants. The results in predicted output found to have a high correlation with the simulated values. This approach provides a viable alternative for computationally-based rapid prototyping and additive manufacturing processes. Limitations of the techniques were discussed.

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Title: Variability in Apparent Properties of Polycrystalline Materials and its Effects on Uncertainty in Engineering Analysis

Author(s): *Coleman Alleman, *Sandia National Laboratories*;

The effective properties of polycrystalline materials are derived from the aggregate behavior of a collection of constituent grains. Many researchers have studied bounds and homogenization techniques to predict the behavior of polycrystalline aggregates from information about the individual grains. The simplest models use only grain orientation and volume fraction to derive, for example, effective elastic modulus from known single crystal moduli. Here, we examine the performance of some of these well-known models to assess accuracy and uncertainty in predictions of apparent modulus. We quantify the variability in predicted apparent properties and examine trends as a function of volume-element size. For engineering analysis, this variability is typically assumed to be negligible due to a separation of scales between component geometry and grain morphology. However, the degree to which this assumption is satisfied depends upon the material, the component geometry, and the imposed loading. Thus, there exists an unknown amount of uncertainty in most finite element simulations for engineering analysis. For some representative simulations, we examine how the epistemic uncertainty related to subscale variability implicit in material-point calculations impacts the uncertainty in predicted responses at the component scale. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

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Title: Non Intrusive and Non-Conforming Interface Coupling for the Global-Local Analysis of Heterogeneous Structures

Author(s): Maxence Wangermez, *ENS Paris-Saclay/Safrantech*; *Olivier Allix, *ENS Paris-Saclay*; Pierre-Alain Guidault, *ENS Paris-Saclay*; Oana Ciobanu, *Safrantech*; Christian Rey, *Safrantech*;

The new Safran Engine makes use of 3D-weaved composite fan blades. The manufacturing process is controlled by tomography. This allows comparing a given blade to a reference one. In case where locally some differences of weaving are detected, the raised question is: are those differences acceptable? The full 3D computation at the tomographic scale is prohibited. Therefore we wish to be able inserting the local tomographic details within a predefined finite elements macro-model of the reference blade. For this a non-conforming interface coupling technique allowing to reduce the incompatibility error between the heterogeneous microscopic (local) model and a first order homogenized (global) model, representative of the macroscopic behavior of a structure is defined. Its non-intrusive implementation leads to specific difficulties that will be analyzed in details. First applications are presented

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Title: Biomechanics of Intestinal Crypt Morphogenesis

Author(s): *Axel Almet, *University of Oxford*; Helen Byrne, *University of Oxford*; Philip Maini, *University of Oxford*; Derek Moulton, *University of Oxford*;

The intestinal epithelium exhibits remarkable rates of self-renewal to protect the small intestine and colon during digestion and facilitate nutrient absorption. This monolayer is maintained by the crypts of Liehberkühn, test-tube-shaped glands that are robust in morphology and structure, undergoing significantly large deformations, despite comprising a heterogeneous composition of cells with varying proliferative capacities and mechanical properties. While the genetic and molecular processes governing crypt morphogenesis have been studied in detail, there is a lack of understanding regarding the evident contribution of biomechanical factors, leading to a poor understanding of crypt morphogenesis as a whole. In this talk, I present a mathematical model of a growing intestinal crypt, using the framework of morphoelastic rods, which extends the classical Kirchhoff rod theory to account for local tissue growth. I will show how morphogenesis can be modelled through the buckling and subsequent large deformation of an elastic rod (a line of proliferating epithelial cells) tethered to an underlying foundation, representing the crypt and the supporting extracellular matrix and stroma. We then consider how to best incorporate various mechanical, chemical, and biological processes, from the subcellular to the tissue scale. Simulation results demonstrate the relative importance of each modelled component to the morphology and properties of the crypt, and how different assumptions can lead to significantly different emergent behaviours.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Summation-by-Parts Methods for Inverse Problems in Exploration Seismology

Author(s): *Martin Almquist, *Stanford University*; Eric Dunham, *Stanford University*; Joseph Jennings, *Stanford University*;

We consider the inverse problem of estimating parameters of the elastic wave equation. To use seismic data from ocean-bottom networks, we must be able to place sources and receivers at boundaries and material interfaces. Given seismograms at point locations, we set up a misfit functional that measures the difference between simulated and recorded data. The gradient of the misfit functional with respect to the large number of parameters can be efficiently computed by solving the adjoint PDE, which involves the adjoint of the elastic differential operator. Here, the restriction operator that localizes the solution to the seismometer point in the misfit functional gives rise to a singular point source term. Ideally, the discrete equations should be adjoint-consistent in the sense that their adjoint approximate the adjoint PDE to high order. We show that for adjoint consistency the restriction operators in the discrete misfit functional must be chosen so that they also approximate singular point sources. We use the summation-by-parts (SBP) framework, which provides a rigorous approach for sources at boundaries and interfaces. It also provides a recipe for constructing a difference operator whose adjoint approximates the adjoint differential operator stably. Combining such SBP operators with proper restriction operators yields adjoint-consistent discretizations. This guarantees that the computed gradient is both the exact gradient of the discrete misfit and a high-order approximation of the continuous gradient.

15th U.S. National Congress on Computational Mechanics
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Title: Design of Non-Newtonian 2D Swirl Flow Devices by Using the Topology Optimization Method

Author(s): *Diego Alonso, *Polytechnic School of the University of São Paulo*; Juan Romero, *Federal University of Esp??rito Santo*; Emílio Silva, *Polytechnic School of the University of São Paulo*;

The performance of fluid devices, such as channels, valves, nozzles and pumps, may be improved by designing them through the Topology Optimization Method. There are various fluid flow problems that can be elaborated in order to design fluid devices and among them there is a specific type which comprises axisymmetric flow with a rotation (swirl flow) around an axis. This specific type of problem allows the simplification of the computationally more expensive 3D fluid flow model to a computationally less expensive 2D swirl flow model. The Topology Optimization Method applied to a Newtonian fluid in 2D swirl flow has already been analyzed before, however not all fluids feature Newtonian (linear) properties, and can exhibit non-Newtonian (nonlinear) effects, such as shear-thinning, which means that the fluid should feature a higher viscosity when under lower shear stresses. Some fluids that exhibit such behavior are, for example, blood, activated sludge and ketchup. In this work, the effect of a non-Newtonian fluid flow is considered for the design of 2D swirl flow devices by using the Topology Optimization Method. The non-Newtonian fluid is modeled by the Carreau-Yasuda model, which is known to be able to accurately predict velocity distributions for blood flow. The design comprises the minimization of the relative energy dissipation considering the viscous and porous effects, and is solved by using the Finite Element Method. The traditional pseudo-density material model for Topology Optimization is adopted with a nodal design variable. The optimization is performed with IPOPT (Interior Point Optimization algorithm). Numerical examples are presented for some 2D swirl flow problems, comparing the non-Newtonian with the Newtonian fluid designs.

15th U.S. National Congress on Computational Mechanics
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Title: Applications of Phase-Field Modeling of Hydraulic Fracture

Author(s): *Talal Alotaibi, *The University of Texas at Austin*; Chad Landis, *The University of Texas at Austin*;

Understanding the mechanisms behind the nucleation and propagation of cracks has been a major interest in many engineering application and design decisions. In many applications in the oil industry, complicated fracture geometries and propagation behaviors are encountered. As a result, the development of modeling approaches that can capture the physics of non-planar crack evolution as well as being computationally tractable is a critical challenge. The phase-field approach to fracture has been shown to be a powerful tool for stimulating very complex fracture topologies including the turning, splitting, and merging of cracks. In contrast to fracture models that explicitly track the crack surfaces, crack propagation and the evolution thereof arise out of the solution to a partial differential equation governing the evolution of a phase-field damage parameter. As such, the crack growth emerges naturally from solving the set of coupled differential equations linking the phase-field to other field quantities that can drive the fracture process. In the present model, the physics of flow through porous media and cracks is coupled with the mechanics of fracture. Darcy-type flow is modeled in the intact porous medium, which transitions to a Stokes-type flow regime within open cracks. This phase-field model is implemented to gain insight into to the propagation behavior of fluid-injected cracks. Four general types of problems are simulated; a) interactions of fluid-driven, natural, and proppant-filled cracks, b) fluid-driven crack growth under the influence of in-situ far-field stresses, c) crack interactions with inclusions, and d) crack growth through different material layers. The simulations show the capabilities of the phase-field model for capturing interesting complex-crack growth phenomena.

15th U.S. National Congress on Computational Mechanics
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Title: Atomistic Insights into Proton Conduction Based Solid Oxide Materials

Author(s): Yuhang Jing, *University of Illinois at Urbana-Champaign*; *N. R. Aluru, *University of Illinois at Urbana-Champaign*;

Many conventional fast proton conducting materials have crystal structures of the perovskite type, ABO3. Although the stability and the crystal structure are dependent on the ratio of the ionic radii and the nature of the A and B atoms, the role of A-site ion on proton diffusion in a perovskite oxide is not clear. We investigate the effect of A ion vacancy on proton diffusion in Y-doped BaZrO3 by performing detailed density functional theory (DFT) calculations. We found that the existence of A ions facilitates proton diffusion with a lower barrier in a perovskite oxide, demonstrating the significance of perovskite structures for proton conductors. We show that the hydroxide ion rotation and proton transfer from one oxygen to another govern proton movement in a perovskite oxide. Both these motions are strongly coupled to lattice deformations. Based on NEB calculations, the key physical mechanisms and the energy barriers associated with both hydroxide ion rotation and proton transfer are revealed.

15th U.S. National Congress on Computational Mechanics
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Title: A Generalized FEM for Three-Dimensional Fractures in Fiber Reinforced Composites

Author(s): *Phillipe Alves, *University of Illinois at Urbana-Champaign*; C. Armando Duarte, *University of Illinois at Urbana-Champaign*;

Fiber reinforcements are used in a broad variety of materials in engineering. They increase the strength, stiffness, ductility, and resistance to fatigue of the unreinforced material. Computational simulations can reduce the cost of designing these materials, and improve the understanding of their failure mechanisms. However, modeling of damage evolution and the multiscale interactions in composite materials using the Finite Element Method (FEM) face significant barriers in terms of model generation and problem size. This work reports on recent advances of the Generalized Finite Element Method (GFEM) for multiscale three-dimensional modeling and simulation of crack propagation in fiber reinforced composites. Fibers are discretely modeled using a formulation of the Embedded Reinforcement with bond Slip (ERS) that allows its combination with the GFEM where fractures are represented thought enrichment functions instead of meshes fitting the crack surface. Matrix cracks are described using discontinuous and singular functions as in the GFEM for homogeneous materials. This procedure can address some of the limitations of existing FEMs by describing both cracks and fibers independently of the underlying FEM mesh. Examples illustrating the capabilities and robustness of the method are presented. Crack propagation simulations are compared to physical tests showing that the method can successfully reproduce the failure behavior of fiber reinforced composites. The results show that several failure mechanisms of the composite can be reproduced by the model, including matrix crack propagation, and fiber debonding, and failure. Keywords: Generalized/eXtended Finite Element Method (GFEM/XFEM); Embedded Reinforcement with bond Slip (ERS); Fiber Reinforced Composites (FRC); Fracture Mechanics

15th U.S. National Congress on Computational Mechanics
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Title: Spatially Local Reduced-Order Bases for Accelerating Nonlinear PROM Simulations

Author(s): *Spenser Anderson, *Stanford University*; Charbel Farhat, *Stanford University*;

Projection-based Model Order Reduction (PMOR) techniques rely on the precomputation of an approximation subspace that, despite having a dimension much smaller than that of its underlying High-Dimensional Model (HDM), exhibits the ability to capture its dominant features. It is common to construct a basis for this approximation subspace by collecting many solution snapshots from the HDM, and compressing a matrix of these snapshots using the Singular Value Decomposition (SVD) method. However, for highly nonlinear problems characterized by multiple distinct scales or regimes, a single, global Reduced-Order Basis (ROB) often needs to be prohibitively large in order to deliver a sufficient accuracy. An existing approach addresses this issue by introducing local ROBs [1], where the concept of locality refers to the region of the manifold where the solution lies. There, the solution space is first partitioned into subregions using a clustering algorithm applied to the columns of the snapshot matrix. Local ROBs are then constructed by compressing the clustered snapshots, and assigned to the various subregions. Here, a complementary method is presented where locality refers to the physical computational domain. This domain is partitioned into subregions by clustering the rows of the snapshots matrix, thereby identifying subregions of the computational mesh that exhibit similar behavior in the snapshots. Local ROBs are then constructed and assigned to each of these spatial subregions. Because each of these ROBs has local support, the assembled global ROB exhibits sparsity that can be exploited to accelerate the performance of a nonlinear Projection-based Reduced-Order Model (PROM). This approach for constructing local ROBs can be combined with the counterpart approach for clustering on the solution manifold [1], thereby achieving locality in both the solution space and the spatial domain. Algorithms for clustering the spatial domain and constructing spatially local ROBs are presented, and techniques for exploiting the resulting sparsity in PROM simulations are discussed. The overall performance of this local ROB approach for model reduction is demonstrated for several CFD applications using the Least-Squares-Petrov-Galerkin PMOR method proposed first in [2]. References [1] D. Amsallem, M. Zahr and C. Farhat, Nonlinear Model Order Reduction Based on Local Reduced-Order Bases, International Journal for Numerical Methods in Engineering, vol. 92, pp. 891-916 (2012) [2] K. Carlberg, C. Bou-Mosleh and C. Farhat, Efficient Nonlinear Model Reduction via a Least-Squares Petrov-Galerkin Projection and Compressive Tensor Approximations, International Journal for Numerical Methods in Engineering, Vol. 86, pp 155-181 (2011)

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Three Field Mixed Finite Element Method for Nonlinear Elasticity

Author(s): *Arzhang Angoshtari, *George Washington University*; Ali Gerami Matin, *George Washington University*;

We introduce a new class of three-field mixed finite element methods for nonlinear elasticity called CSFEMs. CSFEMs are conformal finite element methods and the independent unknowns include displacement, displacement gradient, and the first Piola-Kirchhoff stress. The so-called edge finite elements of the curl operator are used to discretize the trial space of displacement gradients. This choice guarantees that the Hadamard jump condition for the strain compatibility will be satisfied on the discrete level as well. We study the convergence of CSFEMs near regular solutions by employing suitable inf-sup conditions and show that certain selections of finite elements fail to yield convergent CSFEMs as they do not satisfy these inf-sup conditions.

15th U.S. National Congress on Computational Mechanics
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Title: Methods Based on Artificial Neural Networks for the Solution of Partial Differential Equations on Domains with Complex Geometries

Author(s): *Cosmin Anitescu, *Bauhaus-Universität Weimar*; Elena Atroshchenko, *University of New South Wales*; Somdatta Goswami, *Bauhaus-Universität Weimar*; Timon Rabczuk, *Bauhaus-Universität Weimar*;

Machine learning and methods based on artificial neural networks have become increasingly applied to a variety of topics in areas such as image processing, voice recognition, and object detection. In this work, we present a set of algorithms for solving partial differential equations using the approximation properties of deep neural networks (DNN). The proposed procedure is designed to solve partial differential equations on complex geometries, such as the ones obtained from spline description and can alleviate the problems encountered due to gaps in geometry description or other boundary parameterization issues. We will consider and compare algorithms based on collocation (as in [1]), as well as those based on energy minimization [2] which require evaluating an interior integral from scattered points in the domain. The relation between the standard spline-based approximation spaces and DNNs with different activation functions will be examined in in detail. The method proposed has been tested on benchmark problems with known solutions, which allows for a better understanding of the approximation and convergence properties of DNNs. References: [1] M. Raissi, P. Perdikaris, G.E. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics, Volume 378, 2019, Pages 686-707 [2] Weinan E, Bing Yu, The Deep Ritz Method: A Deep Learning-Based Numerical Algorithm for Solving Variational Problems, Communications in Mathematics and Statistics, Volume 6, 2018, Pages 1-12

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Stable Discontinuity-Enriched Finite Element Method with Strong Enforcement of Dirichlet Boundary Conditions

Author(s): *Alejandro Aragón, *Delft University of Technology*; Sanne van den Boom, *Delft University of Technology*; Jian Zhang, *Delft University of Technology*; Fred van Keulen, *Delft University of Technology*;

Enriched finite element discretization methods can be used to decouple the geometric features of a problem from the underlying finite element discretization. Such methods have fundamentally changed the modeling of problems containing material interfaces and cracks, i.e., weak and strong discontinuities, respectively. Recently, the Discontinuity-Enriched Finite Element Method was introduced to model problems containing both types of discontinuities within a unified formulation [1]. In this presentation we demonstrate DE-FEM as an unfitted discretization methodology, whereby enriched degrees of freedom are collocated to nodes created along the immersed boundary [2]. We show, through numerical examples, that the method is not only optimally convergent but also stable, i.e., that the condition number grows at the same rate as that of standard FEM. Most importantly, we showcase that Dirichlet boundary conditions can be prescribed strongly. As an application, the method is demonstrated in the mesh-independent analysis of phononic crystals. [1] Aragón A.M. and Simone A. The Discontinuity-Enriched Finite Element Method. International Journal for Numerical Methods in Engineering. 2017; 112(11):1589-1613. [2] van den Boom S. et al. A Stable Interface-Enriched Formulation for Immersed Domains with Strong Enforcement of Essential Boundary Conditions. International Journal for Numerical Methods in Engineering. 2018 (Submitted for publication).

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Novel General Higher-order Shell Theory for Compressible and Incompressible Hyperelastic Materials Using Orthonormal Moving Frame

Author(s): *Archana Arbind, *J. Mike Walker ’66 Department of Mechanical Engineering, Texas A&M University, College Station, TX.*; J N Reddy, *J. Mike Walker ’66 Department of Mechanical Engineering, Texas A&M University, College Station, TX.*; Arun Srinivasa, *J. Mike Walker ’66 Department of Mechanical Engineering, Texas A&M University, College Station, TX.*;

In this study, a novel general higher-order shell theory is presented to analyze the large deformation of thick or thin shell structures made of hyperelastic materials. The displacement field of the line normal to the shell reference surface is approximated by Legendre polynomials. The formulation uses the non-coordinate orthonormal moving frame as the vector coordinate bases in contrast to classical co-variant bases, which could be non-orthogonal. The kinematics of motion in this coordinate system is derived using the tools of exterior calculus. The use of orthonormal moving frame makes it possible to represent kinematic quantities, e.g., the determinant of the deformation gradient, far more efficiently than the in the classical tensorial representation with covariant basis. In the general surface coordinate system, the finite element formulation of the shell theory is presented and then specialized to pipe like surfaces with general cross-sections along with commonly used surfaces of revolution as well as to spherical surfaces. The methodology developed herein is very much algorithmic and hence it can also be applied for any arbitrary interpolated surfaces with equal ease. The higher-order nature of the approximation of the displacement field makes the theory suitable for analyzing thick and thin shell structures. As far as the constitutive relation of the material is concerned, the derivation is carried out for general compressible or incompressible hyperelastic material and can be specialized for various nonlinear constitutive models suitable for use in biomechanics and other soft-material problems (e.g., neo-Hookean material, Mooney-Rivlin material, Generalized power-law neo-Hookean material, and so on). Numerical examples are presented to verify and validate the formulation presented in this study.

15th U.S. National Congress on Computational Mechanics
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Title: Implicit WENO Schemes for Two-Phase Flow in Porous Media

Author(s): *Todd Arbogast, *University of Texas at Austin, USA,*; Chieh-Sen Huang, *National Sun Yat-sen University, Kaohsiung, Taiwan*; Xikai Zhao, *University of Texas at Austin, USA,*;

Simulation of flow and transport in petroleum reservoirs and groundwater aquifers involves solving coupled systems of advection- diffusion-reaction equations with nonlinear flux functions, diffusion coefficients, and reactions/wells. It is important to develop numerical schemes that can approximate all three processes at once, and to high order, so that the physics can be well resolved. In this paper, we propose an approach based on high order, finite volume, implicit, Weighted Essentially NonOscillatory (iWENO) schemes. The resulting schemes are locally mass conservative and, being implicit, suited to systems of advection-diffusion- reaction equations. Moreover, our approach gives unconditionally L-stable schemes for smooth solutions to the linear advection-diffusion-reaction equation in the sense of a von Neumann stability analysis. To illustrate our approach, we develop a third order iWENO scheme for the saturation equation of two-phase flow in porous media in two space dimensions. The keys to high order accuracy are to use WENO reconstruction in space (which handles shocks and steep fronts) combined with a two-stage Radau-IIA Runge-Kutta time integrator, which itself may be limited to backward Euler when a shock is detected. The saturation is approximated by its averages over the mesh elements at the current time level and at two future time levels; therefore, the scheme uses two unknowns per grid element per variable, independent of the spatial dimension. This makes the scheme fairly computationally efficient, both because reconstructions make use of local information that can fit in cache memory, and because the global system has about as small a number of degrees of freedom as possible. The scheme is relatively simple to implement, high order accurate, maintains local mass conservation, applies to general computational meshes, and appears to be robust. Preliminary computational tests show the potential of the scheme to handle advection-diffusion-reaction processes on meshes of quadrilateral elements, and to do so to high order accuracy using relatively long time steps.

15th U.S. National Congress on Computational Mechanics
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Title: Automatic Techniques for Determining Boundary Condition Parameters in Computational Haemodynamics

Author(s): *Christopher Arthurs, *King's College London*; Alberto Figueroa, *University of Michigan*;

In the field of 3D computational haemodyanics (CH), in which we strive for image-derived 3D Navier-Stokes modelling of pathophysiological blood flow in individual patients, data can be obtained on a range of different aspects of the individual in question, in various modalities. It is essential that this data is assimilated into the CH models to ensure these models are patient-specific. We discuss some methods for data assimilation which can be applied to CH models, in order to determine appropriate parameters for the model's boundary conditions, which are determined by zero-dimensional lumped parameter network (LPN) electric-circuit-analogous models. Finding the parameters of these LPNs fundamentally amounts to making patient-specific estimates of the properties of distal vascular beds. We developed a novel Kalman filtering based approach for determining the LPN parameters which, for the first time, supports an arbitrary class of LPN designs, extending the reduced order unscented Kalman filter applied previously to this problem to the complex LPN circuits that modern CH necessitates [1,2]. The requirement for a novel mathematical approach as part of this is due to the arbitrary nature of the LPN models. Unlike classical three-element Windkessel models, which have been determined using Kalman filtering previously [2], an arbitrary LPN model will have internal, time-dependent pressure states which are not directly determinable from the instantaneous pressure and flow state at the 3D model's boundary. These internal states must therefore be handled carefully, in such a way that the underlying mathematical model remains satisfied throughout the filtering procedure. We introduce the method, and demonstrate its efficacy by creating a CH model geometry, choosing some physiologically-appropriate LPN boundary condition parameters, and performing a "forward" simulation in order to generate some target pressure and velocity waveforms within the domain. We then reset the model boundary condition LPN parameters to some generic, incorrect values, and demonstrate that the method can recover the known parameters. All simulations were performed using the software package CRIMSON [3] Acknowledgements. This work was supported by the European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013) [ERC Grant Agreement No. 307532] References. [1] Moireau, P et al., D, ESAIM: Contr Opt Var, 17:380-405, 2010. [2] Xiao, N PhD Thesis, Stanford University. December 2013. [3] CRIMSON website. www.crimson.software

15th U.S. National Congress on Computational Mechanics
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Title: An Automated Computational Framework to Model Shear Stress Driven Atherosclerosis Growth

Author(s): *Amirhossein Arzani, *Northern Arizona University*;

Atherosclerosis growth involves complex interaction between hemodynamics, biological transport processes, and mechanical forces exerted on endothelial cells (ECs). Wall shear stress (WSS) is a prominent hemodynamic parameter that is known to influence these processes. Generally, it is believed that low WSS promotes atherosclerotic plaque growth, which in turn influences the blood flow and WSS patterns. Therefore, a two-way coupled interaction exists between WSS and atherosclerosis growth. Herein, a computational framework is presented to study the two-way interaction between WSS and plaque growth in coronary arteries. A segment of the vessel wall representing an injured EC layer is considered. An automated software framework is developed using the open-source finite element solver FEniCS. Computational fluid dynamics (CFD) simulation is performed to quantify WSS distribution. Computational nodes in the injured segment are moved in the inward normal direction according to a growth function based on WSS and a predefined injury model. Subsequently, the CFD simulation is repeated based on the new geometry to quantify updated WSS values and continue the growth process. Node movement is done using built-in arbitrary Lagrangian Eulerian (ALE) features in FEniCS. To avoid deteriorated elements, 3D diffusion-based smoothing with a variable diffusivity is implemented. To overcome potential surface mesh deterioration, surface mesh smoothing is done using visualization toolkit (VTK) libraries by relaxing the surface mesh. The entire process is completely automated in FEniCS where all components of the model are implemented. Results will be presented for an idealized tube and image-based coronary artery models. Our results demonstrate the coupled interaction between coronary stenosis growth and changes in WSS topology and magnitude. The plaque growth occurs biased towards the downstream direction in accordance with clinical observations. [1] Mortensen, M., & Valen-Sendstad, K. (2015). Oasis: A high-level/high-performance open source Navier–Stokes solver. Computer Physics Communications, 188, 177-188. [2] Farghadan, A., & Arzani, A. (2019). The combined effect of wall shear stress topology and magnitude on cardiovascular mass transport. International Journal of Heat and Mass Transfer, 131, 252-260. [3] Smedby, O. (1997). Do plaques grow upstream or downstream? An angiographic study in the femoral artery. Arteriosclerosis, Thrombosis, and Vascular Biology, 17(5), 912-918.

15th U.S. National Congress on Computational Mechanics
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Title: Numerical Modeling of Coupled Thermo-Mechanical Behavior of Ni-Ti Shape Memory Alloys for Large Deformations

Author(s): *Ozgur Aslan, *Atilim University*; Vahid Rezazadeh, *Eindhoven University of Technology*;

Shape memory alloys (SMAs) play an increasingly important role in different areas of engineering such as aeronautics, adaptive structures, oil/gas down-hole, and high-temperature applications of automobile industry and there is a growing effort to produce mathematical models in order to imitate the related behaviors in a precise manner. This work utilizes a numerical model based on the finite strain framework of continuum mechanics to establish a thermodynamically consistent theory for SMAs. With the martensitic volume fraction as the internal variable evolving with phase transformation, the thermo-mechanically coupled theory both captures the rate and temperature dependency. The model is implemented in a commercial finite element program by writing a user-material subroutine and both isothermal and coupled simulations conducted on different 2-D and 3-D model problems are shown to demonstrate the high capability in capturing various qualitative behavior of Ni-Ti SMA such as pseudoelasticity, one-way shape memory effect and thermomechanical behavior under cyclic thermal loading together with their good agreement with the experimental findings.

15th U.S. National Congress on Computational Mechanics
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Title: The Shifted Boundary Method for Embedded Domain Computations: Application to Solid Mechanics

Author(s): *Nabil Atallah, *Duke University*; Guglielmo Scovazzi, *Duke University*;

Embedded/immersed boundary methods circumvent the challenge of representing complex geometries through their ease in mesh generation. On the other hand, with such a decision arises the need to integrate over the cut elements. To counter this dilemma and maximize on the advantages of embedded methods, we propose a novel approach, named ''shifted boundary method''. The proposed method obviates the need to integrate over the cut boundary elements by weakly imposing an equivalent boundary condition on its surrogate (formed of un-cut elements) counterpart. We illustrate the SB method for the Darcy equations before proceeding to solid mechanics applications. All the while, we highlight SB's robustness with various numerical tests under different combinations of boundary conditions and FE approximation spaces.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Dislocation Dynamics Simulations of Materials with Complex Physics

Author(s): *Sylvie Aubry, *Lawrence Livermore National Laboratory*; Jaehyun Cho, *Lawrence Livermore National Laboratory*;

Discrete dislocation dynamics (DDD) simulations provide a technique for examining the effects of fundamental dislocation physics on the plastic response of crystalline solids. Many DDD simulations focus on relatively simple materials and loading conditions, such as glide-motion-dominated plasticity of pure face-centered and body-centered cubic crystals. In this presentation, we provide an overview of the more complex physical aspects of dislocation-mediated plasticity in the context of DDD. We consider both physics that are intrinsic to the crystal lattice (elastic anisotropy, nonlinear drag, and low crystallographic symmetry) and extrinsic physics that are due to defects other than dislocations (solutes, vacancies, precipitates, and grain boundaries). For each of these classes of physics, we first discuss the conditions under which they are relevant, followed by an examination of the fundamental ways in which the behaviors of dislocations are affected by the physics, and finally a presentation of the methods that have been developed for incorporating the physics in DDD. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

15th U.S. National Congress on Computational Mechanics
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Title: A Diffuse Interface Framework for Modelling the Evolution of Multi-cell Aggregates as a Soft Packing Problem Driven by the Growth and Division of Cells

Author(s): *Debabrata Auddya, *University of Wisconsin-Madison*; Jiahao Jiang, *University of Michigan, Ann Arbor*; Krishna Garikipati, *University of Michigan, Ann Arbor*; Shiva Rudraraju, *University of Wisconsin-Madison*;

Formation of multi-cell aggregates is a foundational process in the evolution of multicellular organisms. Beginning with a single cell or a small cluster, the growth of aggregates is driven by cell division, differentiation, migration and cell-cell interactions. Understanding the processes underlying the formation of these aggregates is central to many phenomena in cellular biology and physiology, including embryogenesis, regeneration, wound healing, tissue engineering, and the growth and metastasis of cancerous tumors. In this work, we present a model for cell growth, division and packing under soft constraints that arise from the deformability of the cells as well as of a membrane that encloses them. We consider a phase field-based representation of cells in a finite element framework and model the resulting soft packing dynamics of cell aggregates. Our treatment falls within the framework of diffuse interface methods, under which each cell is represented by a scalar phase field and the zero level set of the phase field represents the cell membrane. One crucial element in the treatment is the definition of a free energy density function that penalizes cell overlap, thus giving rise to a simple model of cell-cell contact. In order to properly represent cell packing and the associated free energy, we include a simplified representation of the anisotropic mechanical response of the underlying cytoskeleton and cell membrane through appropriate penalization of the cell shape change. Numerical examples are presented to demonstrate the evolution of multi-cell clusters, and the total free energy of the clusters as a consequence of growth, division and packing.

15th U.S. National Congress on Computational Mechanics
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Title: A Multiscale Model of Cardiac Remodeling under Hypertension: From Organ to Titin

Author(s): *Reza Avaz, *UT-Austin*; Emilio Mendiola, *UT-Austin*; Richard Dixon, *Texas Heart Institute*; Michael Sacks, *Ut-Austin*;

Right ventricular (RV) function is the primary determinant of pulmonary arterial hypertension (PAH) patients survival. PAH imposes a pressure overload on the RV free wall (RVFW), triggering a cascade of remodeling events at multiple length scales in the RV [1,2]. Here, our objective was to improve our understanding of the relationships between intra-cellular remodeling mechanisms and the adaptation of the RV function at the organ level. Our recent studies [1,2] suggest that, in response to pressure overload, the RV first exhausts its capacity to increase the RVFW intrinsic and hypertrophic contractility before it succumbs to a maladaptive dilation. Our results led us to a burning question: Can we identify the intracellular events that result in the changes in the contractility? We hypothesized that the alterations in the protein titin play a major role in this change and our modeling platform provides a robust tool to explore the efficacy of modulating titin characteristics as a new therapeutic target. We developed finite-element rodent heart models using data from normal and monocrotaline-injected rat hearts at control (n=4) and post-PAH time-points (n=4). A small block from the RVFW was re-constructed separating myofibers from the collagenous matrix. The contractile behavior of the fibers was characterized by an activation-contraction model that separates the forces sustained by actin and titin filaments during contraction. A substantial increase in titin stiffness and a decrease in unbinding rate of Ca2+ from TnC constituted %80 of the increase in the contractile force. Interestingly, the Hill coefficient remained nearly unchanged suggesting that the cooperative binding of Ca2+ to TnC was unaffected by hypertension. Rodent-based multiscale models provide detailed descriptions of remodeling patterns that can replace the traditional measures of RV dimensions that often leads to mis- or under-diagnosis of PAH. Ultimately, our platform could facilitate the optimal diagnosis of PAH and the investigation of RV-based therapeutic targets. References [1] Avaz, R. et al, Ann Biomed Eng, 47 138-153, 2019. [2] Avaz, R. et al, J Biomed Eng, Accepted, 2019.

15th U.S. National Congress on Computational Mechanics
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Title: Spacecraft Parachute Flow Computations with the Space–Time IGA

Author(s): *Reha Avsar, *Rice University*; Kenji Takizawa, *Waseda University*; Tayfun E. Tezduyar, *Rice University*;

Orion spacecraft landing parachutes are constructed with hundreds of gaps and slits that the flow goes through, and also some wider gaps and “windows.” This “geometric porosity” makes FSI computations challenging. The geometric porosity created by the gaps and slits needs to be modeled, as resolving that would be exceedingly difficult. The geometric porosity created by the wider gaps and windows, on the other hand, needs to be resolved. The Homogenized Modeling of Geometric Porosity (HMGP-FG) [1], used with the stabilized space–time FSI (SSTFSI) method [1], enabled successful FSI analysis with finite elements [1]. Here we present structural and fluid mechanics computations with isogeometric discretization, which serve as the early stages of FSI analysis. Starting from an unstressed shape of a quarter of a sphere, we first perform a structure computation to obtain a settled parachute shape. In representing the structure, we use cubic NURBS basis functions. In the fluid mechanics computations following that, the key components of the method are the HMGP-FG, ST Variational Multiscale (ST-VMS) method [2], ST Isogeometric Analysis (ST-IGA) [3], and the ST Slip-Interface (ST-SI) method [4]. The ST-VMS serves as a turbulence model. The ST-IGA with quadratic NURBS basis functions gives smoother parachute surface and lowers the number of unknowns necessary to represent the geometry. The ST-SI is used not only for modeling the porous parachute canopy but also for mesh generation convenience. The integration of the ST-SI and ST-IGA was applied in [5] to incompressible flow around a ram-air parachute. Here, we integrate these methods with the HMGP-FG. The computations show the effectiveness of the integrated method. REFERENCES [1] K. Takizawa and T.E. Tezduyar, “Computational methods for parachute fluid–structure interactions”, Arch Comput Meth E, 19 (2012) 125–169 [2] K. Takizawa and T.E. Tezduyar, “Multiscale space–time fluid–structure interaction techniques”, Comput Mech, 48 (2011) 247–267 [3] K. Takizawa, T.E. Tezduyar, Y. Otoguro, T. Terahara, T. Kuraishi and H. Hattori, “Turbocharger flow computations with the space–time isogeometric analysis (ST-IGA)”, Comput Fluids, 142 (2017) 15–20 [4] K. Takizawa, T.E. Tezduyar, H. Mochizuki, H. Hattori, S. Mei, L. Pan, et al., “Space–time VMS method for flow computations with slip interfaces (ST-SI)”, Math Models Meth Appl Sci, 25 (2015) 2377–2406 [5] K. Takizawa, T. E. Tezduyar and T. Terahara, “Ram-air parachute structural and fluid mechanics computations with the space–time isogeometric analysis (ST-IGA)”, Comput Fluids, 141 (2016) 191–200

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Moving Grid Thermal Modelling for Metal Additive Manufacturing

Author(s): *Can Ayas, *Delft University of Technology*;

Additive manufacturing is revolutionising industry by allowing an immense amount of form freedom This enables fabrication of topology optimised cutting edge components typically having complicated geometries. The layer-by-layer nature of the AM process is key for the near net shape realisation of a geometrically complex design at high resolution. However, layers only tens of microns thick, when fused in a powder bed by laser beam, leads to heating-cooling cycles throughout the component. The thermal cycles are the main culprit for defects, distortions, residual stresses and microstructural inhomogeneity. Consequently, modelling the thermal phenomena and investigating the relation between the design features and thermal transients are of paramount importance. The challenge therein comes from the multi-scale nature of the additive manufacturing process. The mismatch between the spatial/temporal scales of the laser beam and the part being printed is typically few orders of magnitude. Therefore, modelling the AM process using conventional numerical methods is deemed computationally intractable. In order for AM modelling to be useful mitigating above mentioned problems of metal AM, computational demands should be reduced while the desired level of accuracy should be maintained. For that purpose, a moving boundary problem is formulated for the evolution of the component geometry and thermal history. The advantage to be exploited is to keep the number of degrees of freedom fixed during the build process. A thermal load is applied to the top of a growing thermal domain and thermal history is analysed. The design features are investigated by means of quantifying the resulting ratio of time scales between the growth and thermal conduction.

15th U.S. National Congress on Computational Mechanics
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Title: The Effect of the Choice of Heterogeneous Material Mapping Method to Accurately Model Pelvic Reconstruction Using FEM

Author(s): *Ata Babazadeh, *Rice University*; Nicholas Dunbar, *Rice University*; Andrew Baines, *Rice University*; John Akin, *Rice University*; C. Fred Higgs III, *Rice University*; Benjamin Fregly, *Rice University*;

Endoprosthetic reconstruction after tumor resection provides load-bearing ability and functional gait for individuals with pelvic sarcoma. Long-term fixation of pelvic implants can be significantly improved by stimulating bone in-growth and avoiding stress shielding. Thus, accurate prediction of the stress and strain distribution in implanted bone is crucial for the long-term stability of the implants. Trabecular bone's heterogeneous material properties can be extracted from the spatial distribution of the bone density, as captured by a patient's high-resolution computed-tomography (CT) images. However, assigning these CT-derived material properties to a patient's finite element (FE) model requires a mapping step for which different node- and element-based methods have been proposed1. Previous research has shown that the choice of material mapping method (MMM) affects FE results2, which is especially important for the design of pelvic implants. In this research, high-resolution CT images from three pelvic sarcoma patients are used to extract sample fields of heterogeneous material properties based on each patient's trabecular bone density. Additionally, artificial heterogeneous materials, resembling the trabecular bone structure, are generated using random fields. FE analyses are performed to evaluate the sensitivity of the stress and strain energy density distributions within the continuum heterogeneous solid to the selected MMM. To perform these analyses, we used different methods for extracting, mapping, and assigning material properties from CT images to the FE model of each heterogeneous material. The models are subjected to axial and bending loading conditions, stress along with the strain energy density is extracted from the FE analyses, and error measures are calculated. In addition, the sensitivity of each MMM as a function of the ratio between FE mesh-size and CT voxel-size is evaluated by varying the FE mesh from a coarser to a finer mesh. Overall, node-based MMMs demonstrated a superior performance to element-based MMMs by achieving higher accuracy and requiring lower pre-processing computation time. Mesh sensitivity analyses also showed that node-based methods quickly converged, whereas element-based methods exhibited a substantial variation in the accuracy with varying mesh size. References 1Chen, G., Schmutz, B., Epari, D., et al. (2010). "A new approach for assigning bone material properties from CT images into finite element models." Journal of Biomechanics, 43(5), 1011-5. 2Helgason, B., Gilchrist, S., Ariza, O., et al. (2016). "The influence of the modulus–density relationship and the material mapping method on the simulated mechanical response of the proximal femur in side-ways fall loading configuration." Medical Engineering & Physics, 38(7), 679-89.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Mechanical Behavior of Polymer Nanocomposites with Nanoparticulate Agglomerations: A Multiscale Analysis

Author(s): *Kyungmin Baek, *Seoul National University*; Hyunseong Shin, *Yeungnam University*; Maenghyo Cho, *Seoul National University*;

Mechanical Behavior of Polymer nanocomposites with Nanoparticulate Agglomerations: A Multiscale Analysis Kyungmin Baek1 / Hyunseong Shin2 / Maenghyo Cho3 1 Seoul National University / myminvva@snu.ac.kr 2 Yeungnam University / shs1106@yu.ac.kr 3 Seoul National University / mhcho@snu.ac.kr (corresponding author) Polymer nanocomposites, filled by layered silicates, nanotube, or ultrafine particles are one of the most potential engineering material in many industry fields. For multiphase materials, the interaction level between different phases plays an important role in determining macroscopic properties of the materials. As it is well known, some factors such as filler particles agglomeration and polymer matrix structure change affects the physical behavior of the nanoparticle-reinforced polymers as well as interfacial adhesion level [1]. Our group developed an interphase percolation model to describe variation of interaction level between polymer matrix and nano-scale silicon carbide particle for inter-particular distance with multiscale approach [2]. In this study, we investigate the effect of nanoparticulate agglomeration on the mechanical behavior of epoxy-based nanocomposites with multiscale approach. According to matching between molecular dynamics (MD) simulation results and finite element homogenization analysis results, we understand interphase characteristic and propose two interphase property model to describe the effect of interphase overlap phenomenon. While the first model decreases the elastic modulus of overall interphase region, the second model only decreases the elastic modulus of overlapped interphase region. Using the different interphase property model, parametric studies for various agglomeration situations are conducted. Although similar tendency of reinforcing effect is observed, there are quantitative differences. Additionally, we apply Christensen's yield/failure criteria to investigate damage initiation and evolution of interphase and matrix phase [3]. We represents micro void nucleation, disentanglement and breakage of polymer chains through the criteria-based damage model. Like reinforcing effect results, same multi-cluster model results to different non-linear behavior of the composites because of different interphase model. We can conclude that although two different interphase models are derived from same MD simulation results, they show different mechanical behavior of the polymer nanocomposite with multi clusters. Acknowledgements This work was supported by a grant from the National Research Foundation of Korea (NRF) funded by the Korea government (MSIP) (Grant No. 2012R1A3A2048841). References [1] A. Mikitaev, G. Kozlov, G. Zaikov, Polymer Nanocomposites: Variety of Structural Forms and Application, 2008, Nova Science Publishers. [2] H. Shin, S. Yang, J. Choi, S. Chang, M. Cho, Chem. Phys. Lett. 2015, 635, 80-85. [3] R. M. Christensen, Proc. R. Soc. Lond. A. 1997, 453, 1473-1491.

15th U.S. National Congress on Computational Mechanics
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Title: Computational Modeling of Biological Cells and Cell Migration

Author(s): *Jie Bai, *University of Texas at San Antonio*; Liqiang Lin, *University of Texas at San Antonio*; Xiaowei Zeng, *University of Texas at San Antonio*;

To accomplish certain physiological tasks, cell migration must occur in a defined direction. The failure of cells to migrate or migration to inappropriate locations can result in abnormities and diseases, e.g. tumor formation and metastasis. To explain such biological and biophysical phenomenon has been the focus of cell research as well as cell mechanics research. In this study, we will present our latest results on computational modeling of biological cells and cell migration. In this presentation, a soft matter liquid crystal cell model is proposed to model biological cells to study the collective cellular motion on a substrate. The cell-cell adhesive interactions and the cell-matrix interaction were modeled by coarse-grained molecular adhesive potentials. We have developed and implemented a Lagrange type meshfree Galerkin formulation and related computational algorithms for the described model to investigate the collective cellular motion. From the simulation results, the push-pull behavior which is considered as the general mechanism of cell crawling was captured.

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Title: pH-Dependent Aggregation and pH-Independent Cell Membrane Adhesion of Monolayer-Protected Gold Nanoparticles

Author(s): *Will Baker, *University of Arkansas*; Ying Li, *University of Connecticut*; Zhiqiang Shen, *University of Connecticut*; Huilin Ye, *University of Connecticut*;

Design of pH-responsive monolayer-protected gold nanoparticles (AuNPs) that are mixed charged with the ability to switch its net surface charge based on the stimuli of environmental pH is a promising technique in nanomedicine. However, understandings of the pH-responsive mixed charged AuNPs behaviors in terms of their stability and cellular interaction are still limited. In this work, we study the aggregation of pH-responsive AuNPs and their interaction with model lipid bilayers by adopting the Martini coarse-grained (CG) molecular dynamics simulations. The surface of these AuNPs is decorated by the both positively and negatively charged ligands. The AuNP is positively charged at low pH values due to protonation of negatively charged ligands. Its net charge is lowered at higher pH by increasing the ratio of deprotonated negative charge ligands. We find that the AuNPs are severe aggregated at moderate pH value, where each AuNP has overall neutral charge, and they are stable and dispersed at both low and high pH values. Further free energy analysis reveals that the energy barrier before the location of hydrophobic driving force potential well plays the key role that determines the stability of monolayer-protected AuNPs at different pH values. This energy barrier is dramatically decreased at moderate pH value, leading to the severe aggregation of AuNPs. By investigating the interaction between AuNPs and model lipid bilayers, we find that all the AuNPs adhere onto the lipid bilayer, independent of the pH value. Moreover, the lipids originally in the bilayer are extracted by these AuNPs through a process of protrusion and upward climbing. The extraction of lipids can cause dehydration and disruption of bilayers, when multiple AuNPs adhered. Free energy analysis reveals that the penetration of AuNPs will induce dramatic free energy increment because of deformation of ligands with hydrophilic functional end groups. We have for the first time systematically studied the stability of pH-responsive AuNPs and their interactions with lipid bilayers in simulation, which might pave the way for the design of pH-responsive monolayer protected AuNPs for biomedical applications.

15th U.S. National Congress on Computational Mechanics
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Title: Output-based Mesh Adaptation for a Stabilized Finite-Element Flow Solver

Author(s): *Aravind Balan, *NASA Langley Research Center*; Mike Park, *NASA Langley Research Center*; Kyle Anderson, *NASA Langley Research Center*;

Output-based mesh adaptation capabilities, using adjoints, have been incorporated into the stabilized finite-element branch of the FUN3D flow solver, FUN3D-SFE, developed at NASA Langley Research Center. Mesh adaptation using adjoints can reduce the error in scalar output functionals, such as lift or drag coefficient in external aerodynamics, in a more efficient manner compared to that of feature-based or of uniform mesh refinement. For the mesh adaptation, a metric-based approach is used, where metric tensors encode information about simplicial mesh elements that can be passed to a metric-conforming mesh generator to produce the required anisotropic mesh. We follow a method where both the adjoint and the primal solutions are used to construct the metric field. Results for inviscid and turbulent flow simulations on adaptive meshes will be compared with results obtained using a solution-based approach that controls the Lp norm of Mach number interpolation error to evaluate the effectiveness and efficiency of the adaptive mesh technology being developed.

15th U.S. National Congress on Computational Mechanics
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Title: Grain-Scale Modeling of Non-Newtonian Fluid-Driven Fracture Initiation in Porous Media by Coupling CFD and DEM

Author(s): Zihao Li, *University of Texas at Austin*; Zhuang Sun, *University of Texas at Austin*; *Matthew Balhoff, *University of Texas at Austin*; Nicolas Espinoza, *University of Texas at Austin*;

The injection of fluid into porous media changes the formation pressure and rock stress state, which may lead to the fracture initiation. We investigate the effect of fluid rheology on fracture initiation at the grain-scale using a resolved computational fluid dynamics-discrete element method (CFD-DEM) approach. We adopt the CFD-DEM approach that models the solid phase using a fictitious domain and captures fluid-solid interactions. The cementation between grains are modeled using bonded particles model (BPM) with predefined mechanical properties, in which the grains are treated as rigid spheres and cements are treated as breakable bonds that can transfer forces and torque. The breaking of a cluster of bonds results in fracture initiation. We simulate fluid injection tests for different fluid rheologies to investigate the impact on fracture initiation. This work aims to determine the effect of fluid rheology on fracture initiation at the grain-scale. Our results show that for a Newtonian fluid, higher fluid velocity facilitates the fracture initiation as a result of the large local drag force. High viscosity Newtonian fluid also has a positive effect on increasing the drag force, but it retards the fluid flow that makes fluid uniformly penetrate into the porous medium, which leads to a damaged zone instead of a fracture. Different gradients of fluid velocity in porous media can result in varying viscosity that have a different impact on fracture initiation compared with high viscosity Newtonian fluid.

15th U.S. National Congress on Computational Mechanics
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Title: Deep Learning for Dynamic Deformation Simulation of Bioprosthetic Heart Valves

Author(s): *Aditya Balu, *Iowa State University*; Michael CH Wu, *Brown University*; Soumik Sarkar, *Iowa State University*; Ming-Chen Hsu, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*;

Patient-specific predictive biomechanics simulations can enable surgeons and clinicians to make better and informed decisions by providing information that is not directly measurable by medical imaging. In particular, obtaining meaningful information about the deformation dynamics of heart valves from medical images is challenging. Traditionally, quantities of interest such as valve opening area, coaptation area, etc. are obtained by performing biomechanics simulations (using finite element or isogeometric analysis) with physical boundary conditions on the heart valve geometry [1]. However, such methods are computationally intensive, making them unsuitable for patient-specific design and diagnostics in a clinical setting. Deep learning based methods can complement simulations by accelerating the analysis using historical data of physical simulations [2]. In this work, we have developed a novel deep learning architecture that can learn from dynamic valve deformation data to capture the temporal dynamics of bioprosthetic heart valves (called deep learning based finite element analysis, DLFEA). We make use of isogeometric analysis that directly uses non-uniform rational B-splines (NURBS) to represent the undeformed and the deformed shapes of the valves as input training data to our deep learning framework. The temporal dynamics of the heart valve can be used to infer quantities of interest such as the effective orifice area, which can be used to assess the performance of the heart valves. We had previously developed a novel NURBS-aware convolution operation and used in a deep learning model to directly predict the deformed closed geometry of heart valves. Here we extend it to develop a NURBS-aware convolutional LSTM model that is derived from the traditional convolutional LSTM networks [3] for learning the dynamic simulations of bioprosthetic heart valves. We present results comparing the valve deformations obtained from both dynamic simulations and DLFEA. [1] F. Xu, S. Morganti, R. Zaherzadeh, D. Kamensky, D. Aurichio, A. Reali, T. J. R. Hughes, M. S. Sacks and MC. Hsu, A framework for designing patient?specific bioprosthetic heart valves using immersogeometric fluid–structure interaction analysis, International journal for numerical methods in biomedical engineering, 34, no. 4, 29-38, 2018 [2] A. Balu, S. Nallagonda, F. Xu, A. Krishnamurthy, M. Hsu, S. Sarkar, Machine Learning for Diagnostics and Patient-Specific Design of Bioprosthetic Heart Valves, Integrating Design and Analysis (IGA), (Austin, TX), 2018. [3] S.H.I. Xingjian, C. Zhourong, W. Hao, Y. Dit-Yan, W. Wai-Kin, and W. Wang-chun, "Convolutional LSTM network: A machine learning approach for precipitation nowcasting." In Advances in neural information processing systems, pp. 802-810. 2015.

15th U.S. National Congress on Computational Mechanics
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Title: Quantification of Optimal Bounds on the Probability of Failure with Application to Sheet Metal Forming of DP Steel

Author(s): *Daniel Balzani, *Ruhr University Bochum, Chair of Continuum Mechanics*; Niklas Miska, *Ruhr University Bochum, Chair of Continuum Mechanics*;

An optimal or efficient design of structures and parts is often affected by uncertainties in the input parameters of the problem including structural parameters as e.g. applied boundary conditions or material parameters, as e.g., uncertain macroscopic properties induced by microstructure variation. Depending on the level of knowledge regarding the individual uncertain parameters, they may be treated differently. If a complete probability distribution is known for the uncertain quantities the calculation of the probability of failure (POF) follows classical stochastic approaches. However, in many scenarios complete distribution functions are not known, either because they are in principle not available or due to a lack of data. Then, only bounds can be considered as given, either on the uncertain quantities themselves, on their mean or on statistical moments of higher order. In this presentation, a framework is proposed for the calculation of optimal bounds on the POF, where both, complete distribution functions of some of the uncertain quantities as well as incomplete data in terms of moment constraints are incorporated. The method combines the idea of Optimal Uncertainty Quantification [1] with the incorporation of random quantities using Monte-Carlo simulations. Thereby, the approach is able to account for epistemic as well as aleatoric uncertainties. The capacity of the framework is demonstrated for an example of a sheet metal forming of DP steel. Due to the complex microstructure governing the macroscopic response of these steels, these problems are a priori multiscale and thus, for the quantification of microstructure-related uncertainties microscopic simulations are considered [2]. By comparing the resulting bounds for the POF for different levels of knowledge of the aleatoric parameters with the bounds resulting from the incorporation of the full probability distribution functions, the minimum required level of knowledge for meaningful bounds can be deduced. [1] H. Owhadi, C. Scovel, T. Sullivan, M. McKerns, and M. Ortiz. Optimal uncertainty quantification. SIAM Rev., 55:271–345, 2012. [2] N. Miska and D. Balzani. A Method to Quantify Material Parameter Statistics Uncertainties Resulting from Microstructure Variation based on Artificial Microstructures. Proceedings in Applied Mathematics and Mechanics, 18, 2018.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Evaluation of A Posteriori Error Estimation Formulas for Multi-level Sampling Uncertainty Estimates Applied to Numerical PDEs in Fluid Mechanics

Author(s): *Timothy Barth, *NASA*;

Hydrodynamic realizations often contain numerical error arising from finite-dimensional approximation (e.g. numerical methods using grids, basis functions, particles, etc) and statistical uncertainty arising from incomplete information and/or statistical characterization of model parameters and random fields. The introduction of multi-level sampling [Mishra-Schwab2010] and multi-fidelity sampling [Ng-Wilcox2014] methods over the last decade address the efficient calculation of moment statistics when the number of sources of uncertainty is large. Using the a priori convergence theories given in [Mishra-Schwab2010] and [Peherstorfer-Gunzburger-Willcox] for multi-level sampling, we construct and numerically evaluate simple a posteriori error estimates for output quantity of interest moment statistics. These estimates include the combined effects of numerical realization error and multi-level sampling error so that moment statistics with a posteriori error bound estimates are obtained. As a practical matter, the assumptions of the a priori convergence theories are almost never satisfied in practice. To address these deficiencies, techniques for improving the quality of computed a posteriori estimates for practical problems of interest in fluid mechanics are discussed. [Mishra-Schwab2010] S. Mishra and C. Schwab, "Sparse Tensor Multi-Level Monte Carlo Finite Volume Methods for Hyperbolic Conservation Laws", ETH Zurich, SAM 2010-14, 2010. [Ng-Wilcox2014] L. Ng andK. Willcox,"Multi-fidelity Approaches for Optimization Under Uncertainty", Internat. J. Numer. Methods Engrg., 100, (2014). [Peherstorfer-Gunzburger-Willcox] "Convergence Analysis of Multi-fidelity Monte Carlo Estimation", preprint.

15th U.S. National Congress on Computational Mechanics
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Title: Realistic Simulation of Brittle Plates

Author(s): *P.K. Basu, *Vanderbilt University*;

Successful numerical simulation of problems of science and engineering with increasing difficulty has become commonplace. The need for quick realistic solution of the critical problems of the day drives this effort, without just depending upon what the suite commercial software offer. In reality, many simulation efforts make unrealistic assumptions about the physics of the problem for numerical expediency in the garb of solution elegance, which often lead to predictions that cannot stand acceptable validation tests. A simple example is the use of representative volume elements in the case of many multi-phase materials, assuming periodic properties. Realistic modeling and simulation practices also help new materials tailored for particular application. Important issues related to failure and damage processes influencing predictive modeling and simulation of brittle plates are presented.

15th U.S. National Congress on Computational Mechanics
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Title: Numerical Simulations of Transient Deformations of Water/Solid/Air System Using Ghost Fluid/Solid Method

Author(s): Ruchao Shi, *Virginia Tech*; Yegao Qu, *Virginia Tech*; *Romesh Batra, *Virginia Polytechnic Institute and State University*;

The analysis of deformations of structures immersed in water due to extreme loading is important for off-shore oil and marine applications. A challenging issue in these problems is the satisfaction of continuity conditions at the fluid/structure interface. We numerically analyze these transient problems by using the ghost fluid/solid method, and coupling the isobaric fixing technique with the real ghost fluid method. We verify accuracy of the developed algorithm by comparing predictions from it with the analytical solution for a one-dimensional problem in which a plane wave traveling in water impinges upon a water/solid interface. We show that the coupled method has first order accuracy. For a 3-dimensional problem, we transform the level set equation from rectangular Cartesian to curvilinear coordinates to track the fluid/solid interface in a Lagrangian frame. Numerical results for propagation of a spherical wave interacting with a fluid/solid interface computed with the developed method are found to compare well with those from the commercial software, ANSYS, that uses the arbitrary Eulerian-Lagrangian method. It is found that the intensity of the reflected tensile wave at a solid/water interface is less than that at a solid/air interface.

15th U.S. National Congress on Computational Mechanics
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Title: A Finite Strain Constitutive Model for Polycrystalline Shape Memory Alloys Accounting for Pseudoelasticity, One Way Shape Memory Effect, Orientation, Reorientation, ``Ferroelasticity", and Latent Heat Effects

Author(s): *Theocharis Baxevanis, *University of Houston*; Mengqian Zhang, *University of Houston*; Alexandros Solomou, *Texas A&M University*;

A finite strain, thermomechanically-coupled, constitutive description of the deformation response of polycrystalline Shape Memory Alloys (SMAs) is presented. The proposed model can describe efficiently--as depicted by detailed comparison of simulations with available experimental data--various phenomena of SMAs (pseudoelasticity, one way shape memory effect, orientation, reorientation, ``ferroelasticity", and latent heat effects) in a simple and consistent manner by introducing and defining the evolution equations of just three internal state variables. In the developed numerical implementation, all the tensorial variables are cast in a corotational configuration for finite deformation analysis, based on the framework proposed by Xiao and Brunhs (1997, 1998), to achieve frame objectivity at each loading increment.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Addressing Near Incompressibility in Meshfree and Coupled IGA-Meshfree Methods

Author(s): *Yuri Bazilevs, *Brown University*; Georgios Moutsanidis, *Brown University*; Jacob Koester, *Sandia National Labs*; Michael Tupek, *Sandia National Labs*; JS Chen, *UC San Diego*;

Nearly incompressible deformations approximated in a pure displacement framework suffer from volumetric locking. To address this issue, reduced/selective quadrature techniques, as well as more advanced B-bar and F-bar type formulations, were developed and popularized in the traditional FEM community. In Meshfree methods, however, emphasis is mainly placed on nodal integration, which is a form of uniformly reduced quadrature. As a result, volumetric locking is usually not observed. However, as in traditional FEM with reduced quadrature, the resulting formulation has zero-energy modes that need to be stabilized. The issue of volumetric locking, however, resurfaces for immersed formulations coupling Meshfree methods as the foreground, and FEM or IGA as the background, discretizations. In this work we develop a new class of formulations, inspired by B-bar and F-bar approaches, to handle traditional Meshfree methods as well as novel immersed IGA-Meshfree discretizations. Because the latter may be viewed as a new generation of material-point methods (MPMs), the proposed methodology also presents a solution for volumetric locking in MPM. * Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Large-Scale Direct Numerical Simulations of Void Growth and Coalescence and Their Implications for Ductile Failure Constitutive Models

Author(s): *Richard Becker, *US Army Research Laboratory*;

Ductile fracture from growth and coalescence of voids nucleated from second phase particles is studied by direct numerical simulation. Thousands of void nucleating particles are distributed randomly in large-scale Arbitrary-Lagrange-Eulerian finite element simulations where the particle-matrix interface is captured by the multi-material algorithms within the code, and the voids expand and coalesce naturally as the material advects through the computational mesh. Local void interactions produce deformation patterns that give way to localized deformation. Analyses of the average stress state and void fraction over windows within the simulation volume are used to plot relationships among void fraction, pressure and effective stress that can be compared with the Gurson and other models to assess the functional dependence. Results under high triaxial loading demonstrate that the pressure dependence of the Gurson model fits well with the simulation results, but the effective stress deviates significantly. Additional simulations under conditions with substantially larger strains are conducted to expand the data set for model evaluation and eventual model construction.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Modeling Nanomotor-assisted Thrombolysis

Author(s): *Matthew Becton, *University of Georgia*; Xianqiao Wang, *University of Georgia*;

Using a combination of stochastic rotation dynamics (SRD) and molecular dynamics (MD), we demonstrate how magnetically-activated nanomotors can be used to accelerate the diffusion of a thrombolytic agent (tissue plasminogen activator or t-PA) into a blood clot. SRD was used for realistic hydrodynamic behavior of the blood and t-PA, while MD was used for the modeling of the nanomotors and clot. The SRD was coupled with the MD in order to provide a faster, more accurate model than either standalone method would be capable of. We modeled the clot as a pseudorandom porous fibrin network which contains breakable "bonds", triggered by the presence of t-PA. Our results demonstrate not only how active nanomotors can enhance drug delivery in blood vessels suffering low flow due to clots, but also provide a framework for performing similar vascular studies in the future.

15th U.S. National Congress on Computational Mechanics
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Title: Redesign of a Forging Geometry Using Dakota Optimization Software

Author(s): *Lauren Beghini, *Sandia National Laboratories*; Andrew Stershic, *Sandia National Laboratories*;

Residual stresses formed during the manufacturing process for applications such as forging, machining and welding, can be detrimental to the overall performance of a manufactured part. To better understand the behavior of and design for such components, we employ a multi-physics lifecycle model, where a forging begins with furnace heating continuing on through a series of steps, including high-deformation compression and ending with quench bath cooling. Each of these manufacturing processes is highly-nonlinear and computationally expensive, including capabilities such as contact, remeshing, etc. Unfortunately, situations arise where final designs do not meet expectations and redesign efforts are required. Using the Dakota optimization software package, we redesigned a forging geometry based on yield strength criteria in a target range with constraints on the final volume per customer specifications. In this talk, we address challenges in the robustness of optimizing over a series of analyses using a variety of codes and tools for a realistic forging application. *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: New Trends in Computational Prediction of Biocompatibility

Author(s): *Marek Behr, *RWTH Aachen University*; Lutz Pauli, *RWTH Aachen University*; Stefan Hassler, *RWTH Aachen University*;

Modeling and computational analysis play an increasingly important role in bioengineering, particularly in the design of implantable ventricular assist devices (VAD) and other blood-handling devices. Numerical simulation of blood flow and associated physiological phenomena has the potential to shorten the design cycle and give the designers important insights into causes of blood damage and suboptimal performance. A set of modeling techniques is presented which are based on stabilized space-time finite element formulation of the Navier-Stokes equations. In order to obtain quantitative hemolysis prediction, cumulative tensor-based measures of strain experienced by individual blood cells have been developed; red blood cells under shear are modeled as deforming droplets, and their deformation tracked throughout the flow volume. A new log-morphology formulation and its VMS stabilized discretization helps handle strong wall-induced and internal boundary layers. The methods are applied to a simplified rotary blood pump from an inter-laboratory round-robin study, as well as to current real-life configurations.

15th U.S. National Congress on Computational Mechanics
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Title: Numerical Design of Advanced Gas Flow Channels in PEM Fuel Cells through Topology Optimization

Author(s): *Reza Behrou, *University of California San Diego*; Alberto Pizzolato, *Politecnico di Torino*; Antoni Forner-Cuenca, *Massachusetts Institute of Technology*;

Proton Exchange Membrane Fuel Cells (PEMFCs) are electrochemical devices used to directly convert the chemical energy of hydrogen into electricity. They represent a high-performance power generation solution for vehicles because of low operating temperature, low weight, and sustained performance at high current density. However, durability and cost are major obstacles to achieving large scale commercialization and utilization of their potential in green energy technologies. We present a thorough and affordable numerical framework to design the flow field of PEMFCs using topology optimization. The optimization problem is formulated to maximize both the power generation and homogeneity of current density distribution, in the spirit of reduced costs and increased durability. The evolution of the flow field geometry is computed with a gradient-based optimizer with gradients of the objective and constraints computed through the discrete adjoint method. The flow of gas in the channels and the transport of chemical species are described by the incompressible Navier-Stokes, advection-diffusion, and Butler-Volmer equations. 2D finite element model is developed to predict the flow in the channels, transport of chemical species and electrochemical reactions. The 3D transport effects are accounted in the 2D model through the state-of-the-art depth-averaging procedure. Both 2D and 3D responses are calibrated using numerical and experimental results. The results of the topology-optimized designs revealed significant power generation enhancements, an improved reactant distribution and a reduced pressure drop as compared to conventional flow fields. The developed design framework can be used to identify flow field layouts that outperform current industrial solutions, catch design trends and provide guidelines to technology practitioners.

15th U.S. National Congress on Computational Mechanics
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Title: A Semi-Lagrangian, constitutive correspondence model for peridynamics

Author(s): *Masoud Behzadinasab, *University of Texas at Austin*; John Foster, *University of Texas at Austin*;

Over the past decade, the peridynamic framework has attracted a broad interest from the computational mechanics community due to its natural capabilities in modeling crack nucleation and growth without any complicated numerical treatments at discontinuities. Most developments of peridynamics have taken place using a Lagrangian foundation, in which the degree of material point interactions depend on their positions in an undeformed reference configuration. The Lagrangian framework becomes unsuitable once very large deformations happen, e.g. shock waves and ductile fracture. We present a recently developed Semi-Lagrangian constitutive correspondence modeling framework for peridynamics that approximates the velocity gradient tensor in the current configuration using an updated (semi-Lagrangian) kernel. Material stability is discussed within the Semi-Lagrangian formulation. We demonstrate the relationship of this theory to classical hypoelastic constitutive theories. Numerical examples are provided to showcase the applications of the new theory.

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Title: Higher-Order Finite Elements for Simulations of Impact with Explicit Time Integration

Author(s): *Stephen Beissel, *Southwest Research Institute*;

Improvements in accuracy with increasing element order have been exploited for years in various fields of computational science and engineering. These fields do not, however, include solid dynamics with explicit time integration. While there are likely multiple factors that have contributed to the exclusion of higher-order finite elements from general-purpose explicit codes, primary among them is that loading in solid dynamics is typically provided by contact between parts in relative motion, and such loading is not modeled by existing contact algorithms with sufficient accuracy to exploit the benefits of higher-order elements. This presentation begins by demonstrating the increased accuracy of recently developed higher-order finite elements over industry-standard first-order elements in explicit computations of wave propagation in a solid medium. To exploit such accuracy in problems involving impact, a contact algorithm is being developed for the needs of the new higher-order elements. The formulation of this algorithm is presented next, with particular emphasis on accounting for element order and curvature of the surfaces, neither of which is addressed by the legacy contact algorithms which were developed for first-order elements. Computations of a plane compressive wave passing through a contact interface, using both the legacy and proposed contact algorithms, are then presented to demonstrate the need for explicitly accounting for element order. Computations of a projectile impacting a target are then presented to demonstrate the need for explicitly accounting for surface curvature. The presentation concludes with a discussion of further developments which would help to bring the advantages of higher-order elements to the disposal of analysts modeling impact of solids.

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Title: Learning-based Robust Stabilization for Reduced-Order Models of 3D Boussinesq Equations

Author(s): *Mouhacine Benosman, *MERL*; Jeff Borggaard, *Virginia Tech.*; Omer San, *Oklahoma State University*; Boris Kramer, *MIT*;

The stable model reduction problem is well-known in model reduction for partial differential equations (PDEs). Here we consider model reduction by performing Galerkin projection of the PDE onto a suitable low-dimensional set of modes to approximate the PDE solutions using a small system of ordinary differential equations (ODEs). However, using the low-dimensional basis necessitates the truncation of modes that contain small-scale structures, and may be responsible for retaining the main characteristics of the original PDE model, such as stability and prediction precision. Thus additional modeling terms are usually necessary. We present some results on the stabilization of reduced-order models (ROMs) for thermal fluids. We address the stable model reduction problem by adding a closure model term. This term is added to the ROM equations to ensure the stability and accuracy of solutions. Closure models have classically been introduced based on physical intuition. Thus, their applicability is limited to those applications where significant research in closure models have been performed. In this work, we propose the use of robust control theory to constructively design a new closure model that is robust to parametric uncertainties. The stabilization is achieved using robust Lyapunov control theory. Furthermore, the free parameters in the proposed ROM stabilization method are optimized using a data-driven multi-parametric extremum seeking (MES) algorithm. The 3D Boussinesq equations provide challenging numerical test cases that are used to demonstrate the advantages of the proposed method.

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Title: Recent Developments in IGA for LS-DYNA

Author(s): *David Benson, *LSTC*; Attila Nagy, *LSTC*; Liping Li, *LSTC*; Marco Pigazzini, *LSTC*; Stefan Hartmann, *Dynamore*;

As industrial use of IGA moves from exploratory testing towards production analysis, the need for better interfaces in pre- and post-processing, efficient input for large scale models, and other model building issues become increasingly important. This talk focuses on these developments within LS-DYNA and our recent work with universities and companies on providing a modern modeling environment for IGA for industrial users. Topics will include human-readable vs fast binary input, issues related to FE vs IGA terminology for users, and post-processing. In addition, technical developments regarding IGA will also be presented.

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Title: Nitsche's Method for Abstract Variational Constrained Minimization Problems with Application to Thin Plates and Shells

Author(s): *Joseph Benzaken, *Walt Disney Animation Studios*; Rasmus Tamstorf, *Walt Disney Animation Studios*; Stephen McCormick, *The University of Colorado, Boulder*; John Evans, *The University of Colorado, Boulder*;

Spline-based isogeometric discretizations are advantageous for Kirchhoff-Love type thin shell-problems for many reasons, but they can present difficulty in correct enforcement of boundary conditions. Weak enforcement of boundary conditions via Nitsche’s method has grown in popularity in recent years, especially in the isogeometric analysis community, but typically one must derive and analyze Nitsche's method for each problem of interest. In this talk, we present a framework for using Nitsche's method for an abstract variational constrained minimization problem that, with the supplement of a generalized Green's identity, trace inequality, and Cauchy-Schwarz inequality, is suitable for any partial differential equation arising from an Euler-Lagrange equation. We show our approach recovers a previously presented Nitsche formulation of the Kirchhoff-Love plate and generalizes to a new Nitsche formulation for the Kirchhoff-Love shell problem. Moreover, as our formulation is set in the context of an abstract variational constrained minimization problem, it can be readily employed to partial differential equations of a higher order such as shell formulations subject to gradient damage. We show that this approach leads to a symmetric, positive-definite linear system with variationally consistent weak-enforcement of Dirichlet- and Neumann-type boundary conditions. This is accomplished by the introduction of "ersatz forces" and their complementary "corner forces" arising from integration by parts along the domain boundary. In addition, the abstract variational framework provides lower-bound estimates for the penalty parameter, which is the culprit of parasitic ill-conditioning in classical penalty methods. These lower-bound estimates rely on trace inequality constants approximated by way of a generalized eigenproblem that ensures coercivity of the Nitsche formulation. Using this method we prove optimal convergence rates in the energy norm and lower-order Sobolev norms with respect to polynomial degree, and we present supporting numerical results for a range of shell problems.

15th U.S. National Congress on Computational Mechanics
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Title: Discrete Models to Simulate Cellular Materials

Author(s): *Igor Berinskii, *Tel Aviv University*;

Cellular materials attract the attention of researchers due to their outstanding stiffness and strength and enhanced absorption of mechanical energy at relatively small density. Artificial periodic cellular materials can be relatively easy fabricated using modern additive technologies. Computer simulations can help to choose the best cell topology, a number of cells, geometry of struts, material properties. Usually FEM is used for simulations, however, in some cases, discrete models seem to be more applicable. For instance, such problems include big deformations, buckling, and fracture of cellular materials. In this work, two discrete models are proposed. Two-parametric model is used for qualitative analysis of cellular auxetic materials. The model describes an interaction between the cells' nodes with axial and torsional linear springs. The homogenization procedure is proposed to determine the effective properties of solid material corresponding to the re-entrant and regular honeycombs. The procedure is based on a comparison of strain energies of the structures and corresponding orthotropic material. The components of the stiffness tensor and Poisson's ratio of the structures are obtained as a function of interaction parameters and the angles between the structural elements. Although the two-parametric model can accurately describe the properties of the isotropic 2D material, it lacks the accuracy in the anisotropic case. Due to this, the enhanced vector-based model or EVM [1] is used for more realistic simulations. EVM model considers solid as a set of particles connected by the potential of interaction. The parameters of the potential are related to linear elastic longitudinal, transverse (shear), bending, and torsional stiffness. As a result, every strut of cellular material is modeled with two particles with an elastic bond. In this work, EVM is used to simulate the buckling induced fracture in the specimen with rectangular cells. It is shown that the simulations results are close to the experimental data. REFERENCES [1] V.A. Kuzkin, A.M. Krivtosv. Enhanced vector-based model for elastic bonds in solids. Letters on materials 7 (4), 2017 pp. 455-458

15th U.S. National Congress on Computational Mechanics
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Title: Immersed-Boundary Framework for Level-Set-Based Topology Optimization of Elastoplastic Structures

Author(s): *Manav Bhatia, *Mississippi State University*;

This talk will present a computational framework for topology optimization of large-scale structures exhibiting material nonlinearities. The geometry is implicitly defined using a level-set parameterization on a finite-element mesh and the nodal coefficients of the level-set field are defined as design variables in a nonlinear programming statement[1]. The evolving boundary of the structure is implicitly described by the zero level-set contour and the optimizer is able to directly modify the level-set function without the need to solve the Hamilton-Jacobi equations. Through the use of a smoothing function the constitutive model is stated as a complementarity problem and solved using semi-smooth Newton method[2]. The performance of this approach is compared with the commonly used return-mapping algorithm for complex models involving rate-dependent multi- surface yield criterion. Computational analysis accounts for the immersed boundary with an approach similar to the unfitted finite element. Each element with the zero level-set boundary is partitioned into material-void domains with only the material domain contributing towards the variational statement. Adjoint sensitivity analysis is used to compute the sensitivity of relevant quantities-of-interest, such as aggregated stress or dissipated plastic energy. The sensitivity problem is formulated using the continuum-sensitivity approach where the weak form is differentiated with respect to the design parameter. Through suitable modifications the sensitivity problem is written in a form that accounts for the dependence of analysis domain on the design parameter and the design velocity is only required at the domain boundary. The numerical approach is implemented in the open-source design-oriented computational framework, MAST[3]. The computational approach will be demonstrated with multiple test cases to highlight the impact of plasticity on the optimum topology. References [1] Bhatia, M., “Immersed Boundary Framework for Stress-Constrained Topology Optimization,” Structural and Multidisciplinary Design Op- timization, under review. [2] Areias, P., Dias-da Costa, D., Pires, E. B., and Barbosa, J. I., “A new semi-implicit formulation for multiple-surface flow rules in multiplicative plasticity,” Computational Mechanics, Vol. 49, No. 5, 2012, pp. 545–564. [3] Bhatia, M. and Beran, P. S., “MAST: An Open-Source Computa- tional Framework for Design of Multiphysics Systems,” AIAA-2018- 1650, AIAA 2018 SciTech Forum.

15th U.S. National Congress on Computational Mechanics
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Title: Time-Dependent Adjoint Sensitivity Analysis for Multimaterial Topology Optimization of Shape Memory Polymer (SMP) Structures

Author(s): *Anurag Bhattacharyya, *University of Illinois at Urbana-Champaign*; Kai James, *University of Illinois at Urbana-Champaign*;

Shape Memory Polymers (SMPs) are a class of materials that are capable of undergoing significant shape change in response to non-mechanical loading. An optimization framework for designing SMP structures is developed. A finite-element analysis (FEA) model based on the additive decomposition of small-strains, is implemented to analyze and predict the temperature-dependent memory characteristics of SMPs. The finite element method consists of a viscoelastic material model combined with a temperature-dependent strain storage mechanism, giving the SMPs their characteristic shape-memory property. The thermomechanical characteristics of SMPs are exploited to actuate structural deflection to enable morphing toward a target shape. A time-dependent adjoint sensitivity formulation is implemented to calculate the gradients required for the topology optimization algorithm. Topology optimization is used to optimally distribute the active material (SMP) and passive material within the design domain. This allows us to tailor the response of the structures to design them with specific target displacements. Forward analysis and sensitivity calculations are combined in an optimization framework to optimally design multi-material structures with controlled structural deformations. Keywords: Shape memory polymers, Adjoint Sensitivity Analysis, Topology Optimization, Multimaterial optimization, multi-physics design

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Title: A Port-Reduced Reduced-Basis Component Method for Structural Health Monitoring

Author(s): *Mohamed Aziz Bhouri, *Massachusetts Institute of Technology*; Anthony Tony Patera, *Massachusetts Institute of Technology*;

We present a port-reduced reduced-basis component method (PR-RBC) for partial differential equations (PDEs). The PR-RBC method [1] incorporates several principal ingredients: component-to-system model construction, underlying "truth" FE PDE discretization, Galerkin projection, parameterized model-order reduction for both the inter-component (port) and intra-component (bubble) degrees of freedom and offline-online computational decompositions. In this work, we adapt the approach to the time-domain elastodynamics PDE. We first apply the classical PR-RBC offline stage to the Helmholtz equation. The range and the discretization considered in the definition of the frequency set are determined from the characteristic times of the excitations applied on the components. Then in the online stage, and for a particular configuration of components, we consider a frequency set defined based on the characteristic times of the excitations applied on the structure. For a fixed test parameter, we first compute the PR-RBC approximations of the frequency-domain solutions associated with the test parameter and every frequency within the online-defined set. We then perform a Proper Orthogonal Decomposition on the solutions obtained for the different frequencies to obtain the reduced-basis space for time-domain approximation of the particular configuration, as justified by the Laplace transform [2]. We also consider parameterized localized excitations with Gaussian spatial dependence treated by approximate affine expansion techniques such as Empirical Quadrature Procedure (EQP) or Empirical Interpolation Method (EIM). We demonstrate the effectiveness of our PR-RBC approach in Simulation-Based Classification for Structural Health Monitoring based on random ambient local excitation and probabilistic nuisance parameters. Our method takes advantage of the PR-RBC approach to inexpensively form quasi-exhaustive synthetic training datasets. We consider time-domain cross-correlation based features [3] and apply several state-of-the-art machine learning algorithms to perform a damage detection on the structure. The quality of the classification task is enhanced by the sufficiently large size of the dataset and the accuracy of the numerical solution, both obtained thanks to the use of the PR-RBC approach. References [1] J Ballani, DBP Huynh, DJ Knezevic, L Nguyen and AT Patera. A component-based hybrid reduced basis/finite element method for solid mechanics with local nonlinearities. Computer Methods in Applied Mechanics and Engineering. 329. 498-531. 10.1016/j.cma.2017.09.014, 2018 [2] C Beattie, S Gugercin, Model Reduction by Rational Interpolation, arXiv:1409.2140v1 [math.NA] 7 Sep, 2014. [3] L-S Huo, X Li, Y-B Yan, and H-N Li. Damage Detection of Structures for Ambient Loading Based on Cross Correlation Function Amplitude and SVM. Shock and Vibration, Article ID 3989743, DOI 10.1155/2016/3989743, 2016.

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Title: Development of a Computationally Efficient Unstructured Finite Element Mesh for Use in Real-Time Forecasting of Hurricane Storm Surge

Author(s): *Matthew Bilskie, *Louisiana State University*; Scott Hagen, *Louisiana State University*;

Unstructured finite element meshes used in physics-based numerical modeling of astronomic tides and hurricane storm surge have increased in domain size and mesh node density as computational power and remote sensing technology has improved. Such models have been progressively used for coastal flood hazard studies, the design of flood protection infrastructure, assessing coastal impacts under future climates and real-time storm surge forecasts during an imminent hurricane event. In a real-time modeling, simulations and post-processing must rapidly occur in order to provide useful and usable information to emergency personnel and local officials prior to the actual threat. Therefore, a balance must be met between a model's mesh resolution (including time-step criteria) and the available high-performance computing (HPC) resources. This project address the issue by employing two a posteriori methods to compute local target element sizes and resourcefully arrange mesh nodes and elements, localized truncation error analysis (LTEA) and mesh simplification/decimation Specifically, LTEA will be used in the offshore (always wetted) regions of the model domain and mesh simplification will be employed across the coastal landscape, where local topographic elevations are gradients are high. LTEA and mesh simplification techniques were performed on a previously developed high-resolution, research-grade, unstructured finite element mesh that contains 5.5 million nodes and spans the western North Atlantic Ocean, Caribbean Sea, and the Gulf of Mexico with focus on the Mississippi, Alabama, and Florida panhandle coastal floodplain. The resulting forecast-grade mesh contains 2.1 million nodes and runs in 10.84 minutes/day of surge simulation as compared to 26.71 minutes/day of surge simulation across 1,020 computational cores. The 60% reduction in simulation time allows a typical 5-day surge forecast to be run in less than 60 minutes as compared to over 120 minutes with the original research-grade model. Furthermore, the resulting peak water levels and timing of peak surge from the forecast-grade model closely match those of the research-grade model. Lastly, the developed model was successfully implemented to provide real-time hurricane storm surge guidance during Hurricane Irma (2017) and Hurricane Michael (2018).

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Title: Locking-free Collocation for Thin-walled Structures

Author(s): Bastian Oesterle, *University of Stuttgart*; Simon Bieber, *University of Stuttgart*; *Manfred Bischoff, *University of Stuttgart*;

Collocation methods are known since the beginning of computational mechanics. For most applications in solid and structural mechanics, however, through the years the finite element method and other discretization methods based on weak forms have prevailed. With the recent developments of alternative discretization strategies, above all isogeometric analysis, collocation has returned into the focus of the computational mechanics community. The potential benefits of collocation methods in comparison to standard finite element solutions are point-wise exact solution of the underlying differential equation and the fact that no integration is needed. On the other hand, the drawbacks of collocation are the tendency to oscillating solutions and stronger continuity requirements. When using splines as shape functions, the second problem is somewhat relieved. The notorious problem of locking in the numerical analysis of thin-walled structures, namely transverse shear locking and membrane locking, has to be addressed in both strategies. Recently, a vivid publication activity in the area of collocation for problems in structural mechanics can be observed, often using splines and NURBS in the context of so-called isogeometric collocation. Here, one of the issues is the optimal choice of collocation points, which typlically has to be adjusted to the polynomial order of the function spaces used for discretization. For mixed methods, different rules may apply for the different involved physical fields. In some situations it is hard to obtain a convergent method at all. The overall situation seems to be rather complex and not fully satisfactory yet. We present a family of collocation methods for beams and plates that is based on our previous works on the so-called Mixed Displacement (MD) Method. It is a variational formulation that avoids locking prior to discretization already on the theory level. It uses equal order interpolation of displacement-like nodal quantities for approximation of displacements and strains. The latter are obtained via particularly chosen differential operators within a mixed variational framework. It turns out that collocation on the basis of the MD method yields excellent behavior for one unique choice of collocation points, regardless of the polynomial order and other parameters. Absence of locking and optimal convergence of displacements and stress resultants is demonstrated in various numerical examples.

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Title: Polyhedral Discretizations Using Tetrahedral Subdivisions, Aggregation, and Optimization-based Shape Functions for Applications in Nonlinear Solid Mechanics

Author(s): *Joseph Bishop, *Sandia National Laboratories*;

For geometrically complex parts and systems, the time required to develop an analysis capable finite element mesh can still take days to months to develop, despite vast increases in computing power. Advanced tetrahedral meshing tools can alleviate this burden, but the development of robust and efficient tetrahedral finite-element formulations for applications in large-deformation solid-mechanics is still an active area of research. The recent development of general polyhedral formulations for solid mechanics offers an opportunity to ease this meshing burden. Starting with an existing tetrahedral mesh, we first subdivide each tetrahedron using standard rectification techniques. Two types of polyhedra are formed from the tetrahedral subdivisions: (1) an aggregation of subtetrahedra attached to the original nodes, and (2) either an octahedron with 6 vertices or a polyhedron with 12 vertices and 8 faces, depending on the degree of rectification. Several approaches may then be used to define the shape functions (e.g. using harmonic or maximum entropy coordinates) and quadrature schemes for the new polyhedra to obtain a consistent and stable finite element formulation. Verification problems and examples are presented.

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Title: Numerical Prediction of Orthotropic Elastic Properties of 3D-Printed Materials Using Representative Volume Element

Author(s): *Prosenjit Biswas, *University of Massachusetts Dartmouth*; Sofiane Guessasma, *INRA French National Institute for Agricultural Research*; Jun Li, *University of Massachusetts Dartmouth*;

The mechanical property of 3D printed components often shows anisotropic behavior and strong dependence on printing orientations and process parameters. In this presentation, various computational models are developed using the representative volume element (RVE) to investigate the orthotropic elastic properties of 3D printed ABS polymers. Two finite element (FE) models, based on Micro-CT or periodic CAD geometry, with different raster angles, 0/90, 45/-45, 30/-30, and 60/-60 among layers are considered in this study. The Micro-CT model used the realistic geometry of a 3D printed cube reconstructed from Micro-CT scans. The periodic CAD model was specified according to the dimensional statistics from the Micro-CT model, including inter and intra layer porosity, bond width, layer height and filament width. All models are subjected to six independent load cases of macroscopically uniform boundary conditions (kinematic and mixed-orthogonal) admitted by Hill-Mandel condition to obtain full orthotropic elastic stiffness matrix. In addition, the size-dependent bounds from those BCs for periodic CAD model were investigated and verified with periodic BC. More anisotropy was found in the periodic CAD model than in the Micro-CT model. The numerical results are consistent with experiments and able to capture the dependence on raster angles. Finally, parametric studies were performed by varying the filament shapes, bond width, layer height and porosity to investigate the effect of those parameters in the determination of effective mechanical properties.

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Title: Development of a Novel Finite Element Based Strain Periodicity Implementation Approach

Author(s): *Sudipta Biswas, *Idaho National Laboratory*; Daniel Schwen, *Idaho National Laboratory*;

Mechanical properties of the materials at the engineering scale are strongly influenced by their microscopic characteristics. At lower length scale, various microstructural features and defects render a material heterogeneous. The multi-scale modeling approach is often used for transferring information between different length scales using a representative volume element (RVE) approach. In general, the RVE is selected such that duplicating it provides sufficient accuracy of demonstrating the temperament of the macroscopic material. Periodic boundary conditions (PBC) are imposed on the RVE to maintain the continuity of the material behavior across different scales. This boundary condition is essential to ensure the deformation compatibility and accurate estimation of the stress-strain response. Thus, RVE based computational approach has two primary advantages: firstly, it illustrates the material response at the modeling scale given specific geometry, initial and boundary conditions, and secondly, it provides the estimation of the homogenized effective properties of the material that can be used in evaluating material behavior at larger scales. The current work proposes a novel approach for implementation of the periodicity for the RVE based multiscale modeling. It is based on rigorous mechanics foundation that implements appropriate boundary conditions for RVE analysis and simplifies the homogenization technique. It relaxes the stress components in the periodic directions and calculates associated strains for maintaining periodicity. It ensures the stress/strain components in the RVE are periodic instead of the displacements. This approach is extremely useful for estimating the homogenized effective mechanical properties of the heterogeneous material. In addition, it predicts the appropriate volume change/shape distortion of the RVE while still maintaining periodicity at lower length scales. The finite element based multiphysics object oriented simulation environment (MOOSE: https://mooseframework.inl.gov/) is used for the implementation of the approach. The implemented model has been verified with analytical calculations and effective property estimation from various micromechanical approaches. The effective stiffness of a composite material calculated from this approach is in good agreement with other computational, as well as experimental findings.

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Title: Least-Squares Petrov-Galerkin Reduced-Order Models for Hypersonic Flight Vehicles

Author(s): *Patrick Blonigan, *Sandia National Laboratories*; Francesco Rizzi, *NexGen Analytics*; Micah Howard, *Sandia National Laboratories*; Kevin Carlberg, *Sandia National Laboratories*;

High-fidelity simulations are becoming indispensable across a range of scientific and engineering disciplines. These simulations often employ extreme-scale nonlinear dynamical system models that require substantial computational resources to simulate. Such computational costs impose a barrier to using high-fidelity simulations for many-query and real-time applications such as uncertainty propagation, design optimization, model calibration, and control. While a range of surrogate models (e.g., data fits, lower-fidelity models) could be used to mitigate this computational burden, projection-based reduced-order models (ROMs) provide a particularly promising mechanism for doing so. This is due to the fact that ROMs remain strongly ‘tied’ to the high-fidelity physics, as they achieve computational savings by executing a projection process directly on the equations governing the high-fidelity model. While a wide range of ROM techniques has been developed for myriad applications, we focus on the least-squares Petrov-Galerkin (LSPG) projection [1], due to its observed accuracy and stability on large-scale problems, and its flexible optimization-based formulation that readily admits integration of structure-preserving constraints [2]. LSPG has been demonstrated extensively on small-scale problems, but there have only been a few successful demonstrations of LSPG on large-scale applications [3]. This talk presents the application of LSPG to steady hypersonic computational fluid dynamics (CFD) simulations. To our knowledge, this is the first application of projection-based ROMs to hypersonic flight vehicle CFD simulations. The talk will start with an overview of ROM techniques, followed by our results and their implications for model reduction of hypersonic CFD and other high-fidelity simulations. This talk will also provide an overview of the novel implementation approach we employed, which corresponds to a new ROM `wrapper’ code (developed using C++ template metaprogramming) that can be coupled to existing simulation codes in a minimally intrusive manner. This approach significantly mitigates the implementation burden for new projection-based ROM techniques at scale and also enables rapid extensibility to new simulation codes. References: [1] K. Carlberg, C. Bou-Mosleh, and C. Farhat. “Efficient non-linear model reduction via a least-squares Petrov–Galerkin projection and compressive tensor approximations,” International Journal for Numerical Methods in Engineering, Vol. 86, No. 2, p. 155–181 (2011). [2] K. Carlberg, Y. Choi, and S. Sargsyan. "Conservative model reduction for finite-volume models," Journal of Computational Physics, Vol. 371, p. 280–314 (2018). [3] K. Carlberg, M. Barone, and H. Antil. “Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction,” Journal of Computational Physics, Vol. 330, p. 693–734 (2017).

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Title: Peridynamic Coupling of Dissolution and Fracture, and Growth and Fracture in Corrosion Damage Problems

Author(s): *Florin Bobaru, *University of Nebraska-Lincoln*; Siavash Jafarzadeh, *University of Nebraska-Lincoln*; Ziguang Chen, *Huazhong University of Science and Technology*; Jiangming Zhao, *University of Nebraska-Lincoln*;

Corrosion often leads to a damaged surface and stress concentration zones with an embrittled layer that makes crack initiation and propagation significantly easier. In such aggressive environments, materials can fail at strains several times smaller than under normal conditions [1]. The interplay between corrosion/dissolution and fracture is then a determining factor in understanding the material reliability. In this talk we introduce a coupled corrosion damage-fracture peridynamic model capable of simulating pitting corrosion and cracks that emanate from such pits. A staggered approach is used here, since the time-scale of the two processes vary significantly: the slow time-scale of corrosion and the fast time-scale of crack propagation. We present a validation example against experimental observations of pitting corrosion and fracture in a metal wire that is corroding and under tensile loadings. A similar approach can be considered when solving the problem of corrosion-induced fracture in reinforced concrete: due to corrosion, the embedded re-bars "expand", since corrosion products have lower density. This creates internal pressures in the concrete, locally tensile, which lead to crack initiation and propagation through the structure and its eventual failure. The peridynamic computations for this case match well the experimental data, but the results with a homogenized model for the concrete material are grid-dependent. A partially-homogenized model peridynamic model is insensitive to the particular grid used, and leads to delta-convergence. References: [1] S. Li, Z. Chen, L. Tan, F. Bobaru, "Corrosion-induced embrittlement in ZK60A Mg alloy", Materials Science and Engineering A, 713: 7-17 (2018). https://doi.org/10.1016/j.msea.2017.12.053

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Title: Adaptive Finite Element Methods for Eigenvalue Problems

Author(s): *Daniele Boffi, *University of Pavia, Italy*;

We review the a posteriori error analysis and the design of adaptive schemes for the approximation of eigenvalue problems arising from partial differential equations. We are interested in the optimal convergence of the adaptive scheme in terms of the number of degrees of freedom. It is well known that particular attention is needed in case of multiple eigenvalues and clusters of eigenvalues. Possible applications include mixed finite elements, Maxwell's equations, and non residual error estimators.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Piecewise-Global Nonlinear Projection-Based Model Reduction for Optimization Problems

Author(s): *Gabriele Boncoraglio, *Stanford University*; Charbel Farhat, *Stanford University*;

Optimization problems in Fluid-Structure Interaction (FSI) typically involve the solution of a combination of linear and nonlinear PDEs to evaluate the objective function, and/or enforce complex constraints. Most often, they involve a large number of optimization parameters. They are usually solved using a Nested Analysis and Design (NAND) approach, and therefore incur the repeated solutions of the aforementioned PDEs at different parameter points. The computational expense of these solutions can be reduced by substituting the underlying High-Dimensional fluid and/or structural Models (HDMs) with less computationally intensive surrogate models such as, for example, Projection-based Reduced-Order Models (PROMs). This defines the context of this talk, which will describe a novel computational framework for accelerating the solution of PDE-constrained shape optimization FSI problems using PROMs. Specifically, the focus will be set on those FSI shape optimization problems characterized by a high-dimensional design space and nonlinear steady-state flows. The proposed framework draws from the methodology presented in [1] for constructing a CFD PROM for the accurate prediction of steady-state flows past parametrically deformed complex geometries. To address the challenges raised by a high-dimensional parameter space however, it substitutes the concept of a global PROM with that of a piecewise-global PROM. To this end, it computes multiple snapshots of the fluid state for multiple deformed geometries, clusters them in the parameter space, compresses them within each cluster, and therefore creates a database of piecewise-global Reduced-Order Bases (ROBs). Next, it exploits these ROBs to construct locally optimal surrogate models in different regions of the parameter space. For a fixed level of desired accuracy, this approach is more computationally efficient than its counterpart approach based on a global PROM. For a fixed computational cost, it is more accurate. The proposed framework and its performance will be illustrated with the solution of several realistic, constrained, shape optimization FSI problems. Reference [1] K. Washabaugh, M. Zahr, C. Farhat, On the Use of Discrete Nonlinear Reduced-Order Models for the Prediction of Steady-State Flows Past Parametrically Deformed Complex Geometries, AIAA2016-1814, AIAA SciTech 2016, San Diego, CA, January 4-8 (2016)

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Gaussian Processes for Shock Test Modeling

Author(s): *Christophe Bonneville, *Cornell University*; Christopher Earls, *Cornell University*;

The US Navy relies on a set of standardized tests to assess the failure probability of its ships mechanical components under shocks and vibration. However, performing these tests in real conditions can be time consuming and expensive, and repeated testing may be required for obtaining a reliable probability estimation. While it is tempting to use physics-based simulations as a substitute, traditional mechanistic methods, such as finite elements can be cumbersome for uncertainty quantification involving such complex problem descriptions. As a result of the foregoing, new methods for predicting test outcomes are needed. We propose to use Gaussian processes (GP) [1], a class of non-parametric Bayesian machine learning (ML) tools. As in most ML approach, we optimize a fitting function to make new predictions. With GPs however, the fitting function is sampled from a Gaussian distribution derived using Bayesian inference and is equivalent to a regression with an infinite number of basis. Within this theoretical setting, the resulting function automatically adapts its complexity given the nature of the data available. Unlike other ML tools, GPs are particularly well suited for uncertainty quantification in engineering, as they predict a probability density (rather than a continuous value); thus making uncertainty quantification easier. Secondly, their Bayesian nature allows for introducing prior knowledges about the underlying physics within the data, yielding reasonable predictions even with sparse data and complex features. Additionally, as a non-parametric model, GPs are less likely to overfit and are robust to noise. Building on GPyTorch [2] (an add-on to the deep learning library PyTorch dedicated to large-scale GP inference), we develop a classifier to predict shock tests results (pass/fail) given the mechanical properties of the component and arbitrary test requirements, while relying on limited real-life or physics-based simulation generated data. Reference : [1] Rasmussen, C.E. and Williams, C.K.I. Gaussian Processes for Machine Learning. The MIT Press, 2005. [2] Gardner, J.R., Pleiss, G., Bindel, D., Weinberger, K.Q., and Wilson, A. GPyTorch: Blackbox matrix-matrix Gaussian process inference with GPU acceleration. NeurIPS, 2018.

15th U.S. National Congress on Computational Mechanics
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Title: Shear-induced Platelet Activation in Artificial Heart Valves

Author(s): Mohammadali Hedayat, *Texas A&M*; *Iman Borazjani, *Texas A&M*;

Thromboembolic complications are the major concern for recipients of bileaflet mechanical heart valves (BMHVs), which are believed to be initiated by platelet activation. The platelet activation in mechanical heart valves can be either due to non-physiologic shear stresses in bulk flow during systole phase or hinge/leakage flow during diastole phase. However, the contribution of each phase has yet to be quantified. In our study, the importance of the bulk flow in platelet activation during systole phase is first investigated by comparing the thrombogenic performance of a MHV and a bioprosthetic heart valves (as control) in terms of shear induced platelet activation in a straight aorta under the same physiologic flow conditions. Our results show that at end of the systole phase the platelet activation by the bulk flow for the MHV is several folds higher than the BHV. In addition, the role of bulk and hinge flows in the activation of platelets in BMHVs is compared for the first time by performing simulations of the flow through a BMHV using an overset grid method (one grid for the bulk flow and two for the hinge regions). The platelet activation through the hinge for two gap sizes (250 and 150 μm) is compared to the activation in the bulk flow using two platelet activation models to ensure the consistency of the results. Our results show that using two-way coupling interpolation is for overset grids is essential to get a more accurate results. In addition, the larger gap has a higher total activation, but a better washout ability due to higher velocities in the hinge region. Finally, our results suggest the total activation by the bulk flow is several folds higher than by the hinge/leakage flow which is mainly due to the higher flow rate of the bulk flow than the leakage flow. This work is supported by the American Heart Association Grant 13SDG17220022, and the computational resources were partly provided by the high-performance research computing (HPRC) at Texas A&M.

15th U.S. National Congress on Computational Mechanics
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Title: Gas/Surface Interaction Models for Porous Media

Author(s): *Arnaud Borner, *STC at NASA Ames Research Center*; Krihsnan Swaminathan-Gopalan, *University of Illinois at Urbana-Champaign*; Joseph Ferguson, *STC at NASA Ames Research Center*; Kelly Stephani, *University of Illinois at Urbana-Champaign*; Nagi Mansour, *NASA Ames Research Center*;

The Porous Microstructure Analysis (PuMA) software [1] and Stochastic PArallel Rarefied-gas Time-accurate Analyzer (SPARTA) direct simulation Monte Carlo (DSMC) code [2] are used to perform simulations of molecular beam scattering experiments of hyperthermal argon and atomic oxygen striking FiberForm. FiberForm is a carbon preform material used commonly as a precursor for NASA's Phenolic-Impregnated Carbon Ablator (PICA) heat shield material. The purpose of this study is to investigate the non-reactive and reactive interaction of fibrous carbon with atomic gases in a complex microstructure. Carbon oxidation is the primary source of carbon removal at lower temperatures. The detailed micro-structure of FiberForm obtained from X-ray micro-tomography is used in the numerical simulations to capture the complexity of the porous and fibrous characteristics of FiberForm. The argon beam shows a non-reactive and non-sticking scattering pattern that is mostly dominated by multiple collisions between atoms and carbon fibers. For the reactive atomic oxygen beam, a finite-rate surface chemistry model [3], recently constructed from the molecular beam scattering experiments on vitreous carbon, is applied to each carbon fiber of the FiberForm material. This model consists of detailed surface reaction mechanisms such as adsorption, desorption, and several types of Langmuir-Hinshelwood (LH) reactions to characterize the oxygen-carbon interactions at the surface. It was also found that a significantly higher amount of CO is generated when the beam interacted with FiberForm, when compared with vitreous carbon. This is postulated to be primarily a result of multiple collisions of oxygen with the fibers, resulting in a higher effective rate of CO production. Multiple collisions with the different fibers, resulting from the porous nature of FiberForm is also found to thermalize the O atoms, in addition to the adsorption/desorption process. The effect of micro-structure is concluded to be crucial in determining the final composition and energy distributions of the products. [1] J. C. Ferguson, F. Panerai, A. Borner, N. N. Mansour, "PuMA: the Porous Microstructure Analysis software", SoftwareX 7 (2018): 81-87. [2] M. A. Gallis, J. R. Torczynski, S. J. Plimpton, D. J. Rader, T. Koehler, "Direct Simulation Monte Carlo: The Quest for Speed", 29th Intl Symposium on Rarefied Gas Dynamics in Xi'an, China, AIP Conf Proc, 1628, 27 (2014). [3] K. Swaminathan-Gopalan, et al. "Development and validation of a finite-rate model for carbon oxidation by atomic oxygen." Carbon 137 (2018): 313-332.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Gradient Damage Model for Polydisperse Polymer Networks

Author(s): Bin Li, *SIbley School of Mechanical and Aerospace Engineering, Cornell University*; *Nikolaos Bouklas, *SIbley School of Mechanical and Aerospace Engineering, Cornell University*;

A common underlying assumption for the majority of constitutive models for polymer networks is that all the chains admit the same length, i.e. the same number of Kuhn segments. However, all synthetic polymers are polydisperse in that they contain polymer chains of unequal length, characterized by a chain length distribution functions. The chain length distribution originates from randomness of the polymerization process. Experiments and theoretical works have shown that the mechanical and mechanochemical properties, as well as the damage and fracture behaviors of a polymer networks depend on the distribution of the chain lengths between crosslinks. For this reason, a proper constitutive model should take into account the chain lengths distribution. Some constitutive models have been developed, in which the idealized networks of different chain lengths are assembled following an equal strain assumption corresponding to a parallel arrangement of chains having different lengths. However, such schemes result in large values of force and even diverged values of force for chains that their prescribed end-to-end length is beyond their contour length. One can try to remedy this problem either by restricting the end-to-end length to be less than the contour length, or by deactivating such chains accounting for chain rupture at some finite stretch. Another approach suggests the equal force assumption, corresponding to a series arrangement of chains where the subchains carry the same force between crosslinks. In this contribution, we adopt the assumption of equal force and derive an eight-chain model of non-Gaussian randomly jointed chain with arbitrary chain length distribution, accounting for the extension of the Kuhn segments. To simulate the rupture of polymers by scission of bonds in the chain backbone, we resort to a gradient damage model that has the capability of addressing the crack nucleation, path selection, and discontinuous propagation. The polymer networks is modeled as incompressible materials. We validate the gradient damage model through comparison of the simulated critical loading for crack nucleation of a 3D hyperelastic bar under tension and the theoretical prediction. We demonstrate the modeling capability of the proposed model to crack propagation in polymer networks at large strains through representative 3D simulations.

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Title: BPX Preconditioners for Isogeometric Methods Based on Hierarchical Spline Spaces

Author(s): *Cesare Bracco, *University of Florence*; Durkbin Cho, *Dongguk University*; Carlotta Giannelli, *University of Florence*; Rafael Vazquez, *Ecole Polytechnique Fédérale de Lausanne*;

Locally refinable spline spaces have been often combined with the Isogeometric Analysis (IgA) framework to construct adaptive methods for the numerical solution of PDEs. In particular, hierarchical spline spaces satisfy properties which lead to adaptive isogeometric methods with optimal convergence rates [2]. In the talk we will analyze the construction of multilevel BPX preconditioners for the linear systems whose solution is needed in the isogeometric methods based on hierarchical spline spaces. Such type of preconditioners has already been employed in the tensor-product case [1] and later extended to T-spline spaces [3]. The construction is based on a stable decomposition of the hierarchical spline space satisfying the strengthened Cauchy-Schwarz inequality. Numerical tests on 2D and 3D problems will be presented to highlight the features of the preconditioners. References: [1] A. Buffa, H. Harbrecht, A. Kunoth, G. Sangalli, BPX-preconditioning for isogeometric analysis, Comput. Methods Appl. Mech. Engrg. 265 (2013), 63-70. [2] A. Buffa, C. Giannelli, Adaptive isogeometric methods with hierarchical splines: Optimality and convergence rates, Math. Mod. Meth. in Appl. S., 27 (2017), 2781-2802. [3] D. Cho, R. Vázquez, BPX preconditioners for isogeometric analysis using analysis-suitable T-splines, IMA J. Numer. Anal. (2018), doi:10.1093/imanum/dry032].

15th U.S. National Congress on Computational Mechanics
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Title: Shape Optimization of Woven Composite Microstructures Using a Generalized Finite Element Method

Author(s): *David Brandyberry, *University of Illinois at Urbana-Champaign*; Philippe Geubelle, *University of Illinois at Urbana-Champaign*;

Fiber-reinforced composite materials are ubiquitous in high-performance applications such as aerospace and automotive parts where high specific stiffness and strength are required. Fibers are often bundled into tows, woven together, and then impregnated with resin. This manufacturing method combines ease of part layup as well as providing composite materials that are stiff in multiple directions. Understanding the failure processes of these woven geometries and designing them to withstand it are important steps in creating higher performance materials. The geometry of the weave microstructure plays a critical role in the initiation of failure and may be designed to delay its onset. Here, a geometric description of sinusoidal tows is constructed and a periodic unit cell (PUC) of a woven composite is modeled. A multiscale, parallel Interface-enriched Generalized FEM (IGFEM) solver is used to efficiently solve large 3D structural problems involving the complicated internal microstructures, provide homogenized macroscopic material properties, and compute analytic design sensitivities to drive a gradient-based design optimization algorithm. Generalized finite element methods such as IGFEM have much greater flexibility in representing the discretized geometry without the complicated and costly meshing process. Because IGFEM uses a fixed mesh, it also has advantages in shape optimization over regular FEM as large shape changes do not cause mesh distortion or require remeshing. To capture the behavior of the interface between a tow and the matrix, a cohesive law is introduced to govern their traction-separation behavior. Gradient-based design optimization presents a very efficient method for determining optimal microstructure shape and constituents. The optimal set of shape parameters are found to match the homogenized behavior to a given desired macroscopic nonlinear constitutive response or to delay the onset of failure. The use of IGFEM and a gradient-based optimizer allows us to find locally optimal geometries very quickly compared to other optimization or discretization methods. Several load cases and design goals are investigated to demonstrate the developed formulation.

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Title: The Thermodynamic Limit of Transition Rates of Crystalline Defects in the Harmonic Approximation

Author(s): *Julian Braun, *University of Warwick*; Christoph Ortner, *University of Warwick*; Manh Hong Duong, *University of Birmingham*;

We consider a point defect in a otherwise homogeneous crystalline solid. We look at the associated formation free energy as well as the transition rate between two stable configurations in the harmonic approximation and show that both quantities converge as the number of atoms tends to infinity. This justifies their role for large systems and gives a theoretical foundation for numerical methods. The limits are proven with sharp convergence rates based on new results on the uniform convergence of strains and a careful renormalisation analysis of the vibrational entropy difference, which is achieved by identifying an underlying spatial decomposition of the entropy.

15th U.S. National Congress on Computational Mechanics
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Title: Analysis of the Evolution of Natural Sediment Structures by the Particle Finite Element Method

Author(s): *Rafael Bravo, *University of Granada*; Pablo Ortiz, *University of Granada*; Sergio Idelsohn, *International Center for Numerical Methods in Engineering*; Pablo Becker, *International Center for Numerical Methods in Engineering*;

The numerical simulation of sediment transport coupled with evolutionary erodible bedforms is essential for the analysis of the morphodynamics of sediment structures. The erosion and evolution of a bedform is a dynamical coupled problem that must be studied with methods able to simulate the interface between the sediment flow and erodible bed. The Particle Finite Element Method (PFEM) with movable mesh was successfully applied in the past to model free surface flows problems such as the interaction of flows with boundaries, or the strong erosion of beds subjected to high velocity flows [1]. A numerical strategy based on the new version of the Particle Finite Element Method with fixed mesh (PFEM-2) is presented for the simulation of sediment flows coupled with evolutionary erodible boundaries. The present approach models in a Lagrangian frame with fixed mesh the evolution of a bedform using an advection–diffusion equation and is solved with the explicit time integration method PFEM-2 from [2], which permits to employ intermediate-large time steps and takes advantage of its easy computer parallelisation. This approach overcomes the restrictions of previous PFEM developments applied to model the erosion, see [1], that was simulated by the conversion of soil to fluid elements leading to sudden changes in the geometry. In this work flow and bedform are coupled in a staggered way. Flow is solved using an standard Finite Element fluid solver compatible with Arbitrary Lagrangian–Eulerian (ALE) techniques, which allows the deformation of the mesh at every time step. The evolution of bedform and flow is linked by the empirical sediment flux relation of Bagnold. The model is able to reproduce with good agreement the lab experiments of the evolution of subaqueous small dunes under different flow conditions from [3]. REFERENCES [1] Oñate E, Celigueta MA, Idelsohn SR (2006) Modeling bed erosion in free surface flows by the particle finite element method. Acta Geotechnica 1(4):237–252 ? [2] Bravo, R Becker P, Ortiz P (2017) Numerical simulation of evolutionary erodible bedforms using the particle finite element method. Computational Particle Mechanics 4(3):297–305. [3] Leclair S (2002) Preservation of cross-strata due to the migration of subaqueous dunes: an experi-mental investigation. Sedimentology 49(6):1157–1180.

15th U.S. National Congress on Computational Mechanics
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Title: A Second-Order Pyramid Element for High-Rate Nonlinear Solid Dynamics

Author(s): *Robert Browning, *U.S. Army Engineer Research & Development Center*; Kent Danielson, *U.S. Army Engineer Research & Development Center*; David Littlefield, *University of Alabama at Birmingham*;

Hexahedral (hex) and tetrahedral (tet) elements have long been the standard choices for volumetric meshing and will likely continue to be for the foreseeable future. However, the benefits of a pyramid element have increased as hex-dominant meshing has continued to garner more attention. This is because a pyramid affords the meshing algorithms another geometric shape that can be used to fill the volume to be meshed while also transitioning between hex and tet elements. However, for high-rate solid dynamics, it is common to use explicit time-integration, which necessitates the use of elements that can be successfully mass lumped. Recently, a compatible set of second-order elements has been demonstrated that successfully mass lumps for explicit-dynamic simulations. However, second-order shape functions for a pyramid element could not be found that would provide positive masses at all the nodes when mass lumping, and that would also provide compatibility with the other second-order elements – until now. This presentation will discuss the recent development and testing of a nineteen-node second-order pyramid that is appropriate for use in high-rate solid dynamics problems. While this nineteen-node element is not yet available in most meshing software, linear and quadratic pyramid elements are common and can be easily adapted until the nineteen-node version is implemented. For instance, the popular meshing software Cubit contains an eighteen-node pyramid that is trivial to convert as it only lacks the volumetric centroid node. For analysis, the pyramid element has been implemented into the ERDC-GSL in-house finite element software ParaAble and will eventually be added to EPIC as well. Permission to publish was granted by Director, Geotechnical & Structures Laboratory.

15th U.S. National Congress on Computational Mechanics
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Title: Progress Towards a Performance-Portable SIERRA/Aria

Author(s): *Victor Brunini, *Sandia National Laboratories*; Jonathan Clausen, *Sandia National Laboratories*; Mark Hoemmen, *Sandia National Laboratories*; Alec Kucala, *Sandia National Laboratories*;

SIERRA/Aria is a large complex finite element application supporting a variety of production capabilities for modeling heat transfer, fluid flow, and chemical reactions that has been developed over the past two decades. Evolving an existing application like this to achieve good performance on current generation supercomputing architectures that include novel hardware like Intel Knights Landing processors or Nvidia Volta GPUs is a significant challenge. We present our progress towards a performance-portable implementation that leverages the Kokkos programming model and Sierra Toolkit (STK) SIMD library to target these diverse platforms in a single-source application. We will also address some of the software-engineering challenges that must be overcome to support dynamic dispatch for handling polymorphism on heterogeneous architectures. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. SAND2019-0197 A

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Title: A Micromorphic-regularized Cam-clay-type Model for Capturing Size-dependent Anisotropy in Geological materials

Author(s): *Eric Bryant, *Columbia University*; WaiChing Sun, *Columbia University*;

We introduce a micromorphic-regularized anisotropic modified Cam-clay model which captures the size-dependent anisotropic elastoplastic responses for clay, mudstone, shales and sedimentary rock. To capture the distinctive anisotropic effect induced by the micro-structures of clay particle aggregate, clusters, peds, micro-fabric and mineral contact, we use a mapping the links the anisotropic stress state to a fictitious stress space to introduce anisotropy to the modified Cam-clay model at the material point scale. Meanwhile, the meso-scale aniostropy is captured via an anisotropic micromorphic regularization model such that the gradient-enhanced plastic flow may exhibit anisotropic responses via a diffusivity tensor. This diffusivity tensor enables the micromorphic regularized model to exhibit plastic flow non-co-axial to the stress gradient of the yield function without introducing non-associate flow rules and hence provide additional degree of freedom for modelers to capture the size-dependent ansiotropy of geological materials that exhibit different anisotropic responses across different length scales. Numerical examples are used to examine the volumetric locking and numerical stability issues that may occur at critical state where isochoric plastic flow dominates the deformation mode. In particular, we present evidence that the micromorphic regularization could also be a potential remedy to overcome the volumetric locking and the spurious checkerboard modes. The influence of the size-dependent anisotropy on the formation and propagation of shear band in the anisotropic material is demonstrated. In the future, we will explore coupling to a phase field fracture model, in order to predict the wide spectrum of brittle and ductile anisotropic responses.

15th U.S. National Congress on Computational Mechanics
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Title: The Mechanical Microenvironment of Human Osteocytes in Native and in Neoformed Bone Under Different Exercise

Author(s): Nabila Gaci, *ENS Paris-Saclay*; Samantha Sanders, *ENS Paris-Saclay*; Berttrand Cinquin, *ENS Paris-Saclay*; Patrick Tauc, *ENS Paris-Saclay*; Hugues Portier, *University d'Orleans*; *Elisa Budyn, *ENS Paris-Saclay*;

Osteocytes orchestrate healthy bone homeostasis. They coordinate bone resorption by osteoclasts and bone formation initiated by the recruitment of mesenchymal stem cells (MSCs) that will differentiate into bone lining to seal the site of bone formation and into osteoblasts laying collagen fibers that will further differentiate into osteocytes mineralizing the collagen fibers. To detect their mechanical environment, osteocytes bear numerous processes. However fundamental knowledge of human bone stromal cells in situ mechanobiology is challenging to quantify in particular as the mechanical properties of their environment changes as the mineralization process occurs. A Bone-on-chip system including one or multiple bone samples provides in situ 3D bone environment for human cells to grow, differentiate and form new bone. The mechanical and biological responses of the system can be simultaneously imaged in 3D at the cell and tissue scales to build a multi-scale numerical model subjected to controlled loading conditions and being cultured over long-term periods of time. In the bone-on-chip, Human MSCs were reseeded in decellularized human bones and were cultured for up to over 26 months. The systems were mechanically loaded to mimic human walk or run as exercise is known to influence cell differentiation and bone formation. The mechanical microenvironments of native osteocytes and stem cell derived osteocytes (SCDOs) were measured in multi-scale model based on real geometry and subjected to the experimental boundary conditions while the cell chemical responses were quantified in vitro by changes in fluorescence intensity. Changes in the cell morphology, gene expression, and secretome were characterized by 3D confocal imaging, PCR, immunohistochemistry and in situ immunofluorescence during their differentiation. The cell morphology of SCDOs exhibited long processes organized in a network at 19 months among different cells populations that were identified. The cell organized in layers of changing orientation up to 45o. The mechanobiology of stromal bone cells showed that cytoplasmic calcium concentration changes adapt to the expected in vivo mechanical load at the successive differentiation stages. The neo-formed bone displayed a strength nearly a quarter of native bone strength at 109 days and contained calcium minerals at 39 days and type I collagen at 256 days. The newly-formed matrix further characterization by immuno-fluorescence under confocal microscopy at 547 days revealed the presence of E11 and sclerostin of which the amounts were correlated to exercise and local stresses.

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Title: Eigenvector Based Materials Identification Approach

Author(s): *Gregory Bunting, *Sandia National Laboratories*; Scott Miller, *Sandia National Laboratories*; Timothy Walsh, *Sandia National Laboratories*;

We present eigenvector-based methods for model calibration and address key challenges in the implementation. A series of increasingly complex examples are constructed that represent models with rigid body modes, modes swapping order between iterations, modes with shared eigenvalues that indeterminately mixed eigenvectors, the solving of a singular system, while demonstrating parallel scalability and models with many degrees of freedom. These methods are implemented using the Sierra Structural Dynamics1 finite element package and utilize the Rapid Optimization Library (ROL). Sandia National Laboratories, P.O. Box 5800, MS 0380, Albuquerque, NM 87185-9999, USA. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525. 1 - Bunting, Gregory, et al. Sierra Structural Dynamics-Users Notes 4.50. No. SAND2018-10518. Sandia National Lab.(SNL-NM), Albuquerque, NM (United States), 2018.

15th U.S. National Congress on Computational Mechanics
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Title: Design of Symmetry-Specific Origami Mechanisms

Author(s): Andrew Gillman, *AFRL*; Gregory Wilson, *Texas A&M University*; Kazuko Fuchi, *University of Dayton Research Institute*; Alexander Pankonien, *AFRL*; Darren Hartl, *Texas A&M University*; *Philip Buskohl, *AFRL*;

The integration of actuating materials within origami-based mechanisms is a novel method to amplify the actuated motion and tune the compliance of the system for targeted stiffness applications. Origami structures provide natural flexibility given the extreme geometric difference between thickness and length, and the energetically preferred bending deformation mode can naturally be used as a form of actuation. However, origami fold patterns with specific actuation motions and mechanical loading scenarios are needed to expand the library of fold-based actuation strategies. In this study, an optimization framework is utilized to predict actuator topologies with different symmetry groups of input and output conditions with respect to the boundary conditions. A nonlinear mechanical analysis method that balances efficiency and accuracy has been developed including techniques for exploring critical points and bifurcations. The nonlinear truss model captures the geometric nonlinearities associated with large rotations and enables systematic study of how the stretch, bend and fold stiffness ratios affect the design space. Utilizing the patterns discovered through the optimization, the multistability of the actuator is further characterized through computational tracking of the bifurcating equilibrium branches and through empirical demonstration with actuator prototypes. This survey of origami mechanisms, combined with the characterization of energy requirements and multi-stability, provides a new set of origami actuators for future integration with actuating materials.

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Title: Extensions and Applications of a Data-Consistent Approach to Quantifying Uncertainties in Physical Parameters of Flow Models

Author(s): *Troy Butler, *University of Colorado Denver*; Timothy Wildey, *Sandia National Laboratories*; John Jakeman, *Sandia National Laboratories*; Michael Pilosov, *University of Colorado Denver*; Tian Yu Yen, *University of Colorado Denver*;

A new data-consistent approach to solving stochastic inverse problems has recently been developed and analyzed for deterministic maps [1,2]. In this approach, the solution is given by a probability measure on model input parameters in the form of a density function whose push-forward through the parameter-to-observable map exactly matches the observed distribution on model outputs. In other words, the solution is said to be consistent with the data. We summarize both this method as well as recent work that has extended this approach to stochastic maps to account for other sources of uncertainty in the discrepancy between model predictions and observable data. This approach is applied to flow models where the goal is to construct a data-consistent solution on physical parameters of the model in the presence of numerical errors, modeled as stochastic processes, polluting computational predictions. The presentation will be interactive using Jupyter notebook slides to build computational intuition on the methodology as well as reconstruct some of the published results in [1,2] in real-time. The slides with the embedded code will be available upon request. [1] T. Butler, J. Jakeman and T. Wildey, “Combining Push-Forward Measures and Bayes' Rule to Construct Consistent Solutions to Stochastic Inverse Problems”, SIAM J. Sci. Comput., 40(2), A984–A1011. [2] T. Butler, J. Jakeman and T. Wildey, "Convergence of Probability Densities using Approximate Models for Forward and Inverse Problems in Uncertainty Quantification", SIAM J. Sci. Comput., 40(5), A3523-A3548.

15th U.S. National Congress on Computational Mechanics
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Title: Timoshenko Beam-Vehicle Coupled Dynamic Model for Pavement Roughness Identification

Author(s): *Krishnanunni C.G., *Indian Institute of Technology, Madras*; B.N. Rao, *Indian Institute of Technology, Madras*;

Timoshenko Beam-Vehicle Coupled Dynamic Model for Pavement Roughness Identification Krishnanunni C.G 1, B. N. Rao2* 1 Indian Institute of technology, Madras, Tamil Nadu, 600036, India E-mail: researchunni@gmail.com 2 Indian Institute of technology, Madras, Tamil Nadu, 600036, India *E-mail: bnrao@iitm.ac.in Abstract The present paper deals with an efficient model for pavement roughness identification considering the dynamic interactions existing between a moving vehicle and pavement. The dynamic response of a half car vehicle model is used for roughness identification. The pavement is modeled as a finite length Timoshenko beam resting on a six-parameter foundation. The differential equations of motion for the Timoshenko beam-vehicle coupled system is derived based on Hamilton’s principle. The Galerkin method is employed to discretize the governing nonlinear differential equations. A decoupled solution method is developed to simulate the dynamic response of the coupled system. The technique is based on dividing the vehicle-pavement system into two subsystems and solving them independently until the solution has converged. The technique uses a combination of finite difference method and Newmark's method for computing the dynamic response. Gaussian white noise is added to the computed dynamic responses to simulate actual field measurements. The inverse problem is formulated by considering an objective function that computes the least square error between measured and identified vehicle responses. Dynamic programming based on Bellman’s principle of optimality is employed to minimize the objective function and compute the roughness profile of the pavement. Tikhonov regularization is employed to ensure a well-posed optimization problem. Numerical investigations show that by incorporating adequate measurements from the front and rear axle of the vehicle, the developed model is capable of estimating the roughness profile with high accuracy in spite of the presence of measurement noise. Additionally, it is shown that the results are significantly improved when one considers the dynamic interactions existing between the pavement and vehicle. Keywords: Galerkin method, Vehicle-pavement system, Dynamic analysis, Road roughness, Dynamic programming. References 1) Yang, Y., Ding, H., Chen, L.Q. “Dynamic response to a moving load of a Timoshenko beam resting on an nonlinear viscoelastic foundation”, Acta Mechanica Sinica, Vol. 29, 2013, pp. 718-727. 2) Tao, Zhu., Shou-ne, Xiao., Guang-wu, Yang. “Force identification in time domain based on dynamic programming”, Applied Mathematics and Computation, Vol. 235, 2014, pp. 226-234.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Fluid-Structure Interaction Analysis of Transcatheter Aortic Valve Replacement in a Patient with Concomitant Mitral Regurgitation

Author(s): *Andres Caballero, *Georgia Tech*; Wenbin Mao, *Georgia Tech*; Raymond McKay, *The Hartford Hospital*; Charles Primiano, *The Hartford Hospital*; Wei Sun, *Georgia Tech*;

Introduction: Transcatheter aortic valve replacement (TAVR) is now the standard-of-care treatment for inoperable, high- and intermediate-risk patients with severe aortic stenosis (AS). Mitral regurgitation (MR) frequently coexists in patients with severe AS, with about 20% of TAVR patients presenting concomitant more than mild MR. Moreover, patients with moderate to severe MR at the time of TAVR are at increased risk of future adverse events. Interestingly, some studies have reported acute improvement in MR following TAVR, which has been related to immediate post-procedural changes in left ventricular (LV) hemodynamics and improved mitral valve (MV) leaflet tethering. Some observational studies have also shown greater degree of reduction of MR in patients treated with a balloon-expandable as compared to a self-expandable transcatheter aortic valve (TAV). Whether the design of the implanted TAV influences the post-procedural course of MR needs to be further investigated. With these challenges in mind, this study seeks to shed some light on the biomechanical interaction between the TAV, the regurgitant MV and the left heart (LH) complex using a fluid-structure interaction (FSI) analysis. Methods: Full-phase cardiac multi-slice computed tomography (MSCT) images and echocardiography examination from a 71-year-old male patient with severe AS and MR were used to develop and validate a patient-specific 3D LH model. The FSI model comprises all major components of the LH (i.e. aortic root, AV, LV, MV and left atrium), and incorporates cardiac wall motion, anisotropic hyperelastic material models and human material properties. An FSI framework that combines smoothed particle hydrodynamics (SPH) and nonlinear finite element (FE) formulation is adopted. TAVR procedure is simulated based on previous work from our group. Pre- and post-TAVR FSI simulations during the full cardiac cycle are performed, and the effects on MR severity, TAV performance, LH hemodynamics, and leaflets deformation state and kinematics are investigated. Results: Pre-TAVR systolic function was severely reduced, with a LV ejection fraction of 25%. Low-flow, low-gradient AS was present with a peak aortic velocity of 3.2 m/s and a mean gradient of 22 mmHg. The LH model was validated by comparing the echo measurements and MV model with the MSCT images during valve closure. Apical displacement of the coaptation zone resulted in posteriorly-directed MR. A parametric study was performed to study the impact of TAV type and position on MR severity. This study is expected to provide mechanistic insights that can lead to the success of TAVR in these challenging cases.

15th U.S. National Congress on Computational Mechanics
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Title: Comparison of Sharp and Diffuse Interface Methods for Thermal Topology Optimization

Author(s): *Jean-Sébastien Cagnone, *National Research Council of Canada*; Bruno Blais, *École Polytechnique de Montréal*; Florin Ilinca, *National Research Council of Canada*;

Optimal design of heat-transfer systems can efficiently be tackled by topology optimization [1]. Unlike shape optimization, where design candidates are restrained by a predefined parameterization of the geometry, topology optimization avoids any assumption on the final shape. Instead, geometric configurations are generated by controlling a density-function at each finite-element node, which indicates whether material locally present or not. This freedom allows a great variety of design candidates, potentially vastly different from the initial configuration, and is particularly well suited to the design of heat-sinks and thermo-fluid cooling devices. The present work centers on the discrete representation of the material properties in topology-optimization finite-element problems, and compares two distinct approaches. The first and most commonly used approach consists of directly interpolating the density-function at the integration nodes. The local material properties are then evaluated with a power-law blending-rule, which regularizes the filled-to-void transition over a finite distance. Although simple to implement, this method leads to an inevitable smearing the material interface, and, possibly, oscillating density functions. The second approach consists of treating the material interface as an immersed-boundary problem [2]. Starting from the nodal density-function values, the interface dividing filled and void regions is reconstructed using a level-set function. Intersected finite-elements are sub-divided and integrated exactly using the properties pertaining to each side of the interface. To enable an accurate representation of the solution, the interpolation space is enriched with additional degrees of freedom, which are eliminated at the elementary system level by static condensation. This enrichment enforces the appropriate interfacial kinematic conditions, thereby enabling a sharp representation of the interface. We propose to compare the diffuse and sharp interface approaches, and highlight the merits and drawbacks of each approaches. The cases considered are standard 2D and 3D heat sink problems, tackled with a gradient-based optimization framework employing adjoint sensitivities. The sharp interface approach should allow the capture of smaller geometric features, leading to improved optimal configurations and reduced mesh dependency. Practical implementation concerns, regarding the computation of the adjoint state, application to industrial mold-cooling and extension to thermo-fluid problems will also be addressed. [1] Dbouk, T. (2017) A review about the engineering design of optimal heat transfer systems using topology optimization. Appl. Therm. Eng. 112:841-854. [2] Ilinca, F. and Hétu J-F. (2013) An immersed boundary–body conformal enrichment method for thermal flow problems. Comput. Fluids. 88:616–628.

15th U.S. National Congress on Computational Mechanics
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Title: A Parallel Monolithic Domain Decomposition Method for Fluid-structure Interaction Problems in Biomechanics

Author(s): *Xiao-Chuan Cai, *University of Colorado Boulder*;

We discuss some recent development of a highly scalable parallel domain decomposition algorithm for the simulation of blood flows in compliant arteries by solving a coupled system of nonlinear partial differential equations consisting of an elasticity equation for the artery and an incompressible Navier-Stokes system for the blood flow. The system is discretized with a fully implicit finite element method on unstructured moving meshes in 3D and solved by a Newton algorithm with an analytical Jacobian matrix preconditioned with an overlapping Schwarz method. Several mathematical, bio-mechanical, and supercomputing issues will be discussed in detail, and some numerical experiments for the cerebral and pulmonary arteries will be presented.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Automatic Variationally Stable Discretizations

Author(s): *Victor Calo, *Curtin University*; Roberto Cier, *Curtin University*; Quanling Deng, *Curtin University*; Alexandre Ern, *MINES ParisTech*; Sergio Rojas, *Curtin University*; Albert Romkes, *South Dakota School of Mines and Technology*;

The Discontinuous Petrov-Galerkin (DPG) methods, first introduced by Leszek Demkowikz and Jay Gopalakrishnan, are a family of Petrov-Galerkin methods where test space is discontinuous. The main advantages of such methods are that, by construction, they enjoy stability at the discrete level, while also a reliable representation for the error is obtained on the fly, making it a suitable method for mesh-adaptivity based numerical implementations. The Automatical Variationally Stable Finite Element Method (AVS-FEM) is a subclass of DPG methods where the trial space is continuous. Differing from the DPG Ultra weak formulations, the introduction of additional trace variables are no longer required when enough regularity for the solutions is assumed. In this talk, we will briefly introduce the treatment of AVS-FEM formulations in strong form. We will show that rather than considering an integration by parts rule, regularity constraints and boundary conditions can be weakly imposed with the help of an adequate duality identity. This methodology leads to natural and straightforwardly implementable FEM that keeps the spatial representation of the differential operators invariant. We will also discuss positivity preserving strategies that generalize Nitsche's ideas. We will also show through numerical examples the efficiency of the method in extreme scenarios where the method gives stable solutions that are comparable with those obtained with classical stabilized methods.

15th U.S. National Congress on Computational Mechanics
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Title: Multipoint Exponential Approximation for Large-Scale Optimization and Uncertainty Quantification

Author(s): *Robert Canfield, *Virginia Tech*; Michael Eldred, *Sandia National Laboratories*;

A newly derived multipoint exponential approximation (MPEA) is developed for large-scale optimization by narrowing it to a single set of intermediate variables, selected for use with all constraint and objective functions, based on Lagrangian sensitivity, to maintain a linear surrogate approximation [1]. Sequential Linear Programming (SLP) is first-order optimization method suitable for large-scale optimization that is made more effective by the MPEA transformation. A robust implementation of SLP with a trust region strategy is implemented here, using QMEA in conjunction with a large-scale QP solver. The number of SLP outer-loop iterations to converge is demonstrated to be reduced by the MPEA intermediate variable transformation for scalable benchmark optimization problems with a large number of design variables. A quadratic multipoint exponential approximation (QMEA) is derived that extends MPEA by adding quadratic terms that match previous function values with a sparse Hessian. QMEA generalizes the well- known two-point exponential approximation (TPEA) and two-point adaptive nonlinear approximation (TANA) [2], by matching function values of more than two previous points [3] using a quadratic term constructed in a reduced sub-space. Its effectiveness is demonstrated on benchmark uncertainty quantification (UA) test problems from the User's Manual for Sandia's Design Analysis Kit for Optimization and Terascale Applications (DAKOTA). [1] Canfield, R. A., and Eldred, M. S. "Quadratic Multipoint Exponential Approximation for Optimization and Uncertainty Quantification," AIAA Scitech 2019 Forum. American Institute of Aeronautics and Astronautics, 2019, doi:10.2514/6.2019-2215 [2] Choi, S.-K., Grandhi, R.V., and Canfield, R.A., Reliability-Based Structural Design, Springer, London, 2007 [3] Canfield, R.A.,“Multipoint cubic surrogate function for sequential approximate optimization, ”Structural and Multidisciplinary Optimization, Vol. 27, No. 5, 2004, pp. 326–336. doi:10.1007/s00158-004-0391-2

15th U.S. National Congress on Computational Mechanics
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Title: Numerical Analysis of Shock-Induced Damage and Fracture in Cylindrical Bodies Submerged in Water

Author(s): *Shunxiang Cao, *Virginia Tech*; Ying Zhang, *Duke University*; Defei Liao, *Duke University*; Pei Zhong, *Duke University*; Kevin Wang, *Virginia Tech*;

Understanding the response of solid materials to shock loading is important for mitigating shock-induced damages and failures, as well as advancing the beneficial use of shock waves for material modifications. In this talk, we present a numerical analysis of the causal relationship between the prescribed shock load and the resulting elastic waves, damage and fracture in the solid material. A representative brittle material, BegoStone, in the form of cylindrical bodies and submerged in water is considered. We employ a recently developed three-dimensional computational framework, referred to as FIVER (a FInite Volume method with Exact fluid-solid Riemann solvers), to solve this shock-dominated fluid-structure interaction problem. It couples a finite volume compressible fluid solver with a finite element structural dynamics solver through the construction and solution of local, one-dimensional fluid-solid Riemann problems. The material damage and fracture are modeled and simulated using a continuum damage mechanics model and an element erosion method, and the results are compared with experimental data. We first show that after calibrating the growth rate of microscopic damage and the threshold for macroscopic fracture, the computational framework is capable of capturing the location and shape of the shock-induced fracture observed in a laboratory experiment. The casual relationship among shock load, elastic wave, and crack formation is discussed. Next, we introduce a new phenomenological model of shock waveform, and present a series of parametric studies to examine the effects of shock waveform, magnitude and the size of the target material on the material damage. In particular, we vary the waveform gradually from one that features non-monotonic decay with a tensile phase to one that exhibits monotonic decay without a tensile phase. The result shows that when the length of the shock pulse is comparable to that of the target material, the former waveform may induce much more significant damage than the latter one, even if the two share the same magnitude, duration, and acoustic energy.

15th U.S. National Congress on Computational Mechanics
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Title: A Random Choice SPH Scheme with Adaptive Viscosity

Author(s): *Zhixuan Cao, *ANSYS/SUNY Buffalo*; E. Bruce Pitman, *University at Buffalo, SUNY*; Abani Patra, *University at Buffalo, SUNY*;

The classical smoothed particle hydrodynamics (SPH) method employs an artificial viscosity term to properly capture shock waves in high speed compressible flow. This artificial viscosity typically adds more dissipation than is needed to smooth shocks, smears discontinuities, and can overwhelm fluid turbulence. Several studies have proposed highly tuned versions of artificial viscosity, turning on and off near shocks or other troublesome wave features. A different kind of solver adapts Godunov's idea of solving local Riemann problems as building blocks for a numerical SPH solver without explicit numerical dissipation term. Unfortunately, a first order Godunov solver still introduces an effective numerical diffusion that can infect the entire numerical solution. We propose a novel SPH scheme that combines an approximate version of Glimm's Random Choice method (RCM) with SPH. RCM properly resolves and then samples all hydrodynamic waves. Our version approximately resolves hydrodynamic waves, and samples the approximate solution. No explicit artificial viscosity will be needed. We test this method on standard one dimensional shock tube problems and observe several attractive features. First of all, this method introduces adaptive artificial viscosity, assigning larger dissipation around discontinuities and smaller elsewhere. Secondly, it is less dissipative than classical SPH and GSPH resulting in less smearing of shock. Thirdly, as the new method can be viewed as generalized GSPH method in terms of sampling solutions of local Riemann problems, good features of GSPH are inherited, for example, ameliorating pressure "wiggle" around contact discontinuity. When applied to three dimensional jet flow, this method is demonstrated to introduce less overall-dissipation than GSPH.

15th U.S. National Congress on Computational Mechanics
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Title: Model Reduction of Dynamical Systems on Nonlinear Manifolds Using Deep Convolutional Autoencoders

Author(s): Kookjin Lee, *Sandia National Laboratories*; *Kevin Carlberg, *Sandia National Laboratories*;

Nearly all model-reduction techniques project the governing equations onto a linear subspace of the original state space. Such subspaces are typically computed using methods such as balanced truncation, rational interpolation, the reduced-basis method, and (balanced) proper orthogonal decomposition (POD). Unfortu- nately, restricting the state to evolve in a linear subspace imposes a fundamental limitation to the accuracy of the resulting reduced-order model (ROM). In particular, linear-subspace ROMs can be expected to produce low-dimensional models with high accuracy only if the problem admits a fast decaying Kolmogorov n-width (e.g., diffusion-dominated problems). Unfortunately, many problems of interest exhibit a slowly decaying Kolmogorov n-width (e.g., advection-dominated problems). To address this, we propose a novel framework for projecting dynamical systems onto nonlinear manifolds using minimum-residual formulations at the time-continuous and time-discrete levels; the former leads to manifold Galerkin projection, while the latter leads to manifold least-squares Petrov–Galerkin (LSPG) projection. We perform analyses that provide insight into the relationship between these proposed approaches and classical linear-subspace reduced-order models. We also propose a computationally practical approach for computing the nonlinear manifold, which is based on convolutional autoencoders from deep learning. Finally, we demonstrate the ability of the method to significantly outperform even the optimal linear-subspace ROM on benchmark advection-dominated problems, thereby demonstrating the method’s ability to overcome the intrinsic n-width limitations of linear subspaces.

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Title: Dynamic Behavior of Elastic Solids Using Mathematical Models Derived Based on Non-classical Continuum Mechanics Incorporating Internal Rotations

Author(s): Karan Surana, *University of Kansas*; *Celso Carranza, *University of Kansas*; J. N. Reddy, *Texas A&M University*;

The thermodynamics framework based on non-classical continuum mechanics incorporating internal rotations, hence incorporating entirety of the displacement gradient tensor in the thermodynamic framework presented in references [1,2] is considered in this work to formulate mathematical models for: (i) undamped natural dynamic response of the solid continua (ii) transient damped and undamped dynamic response using space-time decoupled methods including modal synthesis as well as (iii) transient dynamic response using space-time coupled methods. Mathematical models as well details of computational methodologies used are presented. Model problems studies are presented in R2. Numerical solutions computed using the mathematical models derived based on non-classical continuum mechanics are compared with those that are obtained using the mathematical models derived using classical continuum mechanics conservation and balance laws. Significance of the additional physics of deformation incorporated in the non-classical continuum mechanics mathematical models is discussed and illustrated. References: [1] Surana, K. S. and Powell, M. J. and Reddy, J. N. A more complete thermodynamic framework for solid continua. Journal of Thermal Engineering, 1(1):1–13, 2015. [2] Surana, K. S. and Powell, M. J. and Reddy, J. N. A polar continuum theory for solid continua. International Journal of Engineering Research and Industrial Applications, 8(2):77-106, 2015.

15th U.S. National Congress on Computational Mechanics
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Title: Error Estimation and Mesh Adaptation with Continuous and Discontinuous Finite Element Methods

Author(s): *Hugh Carson, *MIT*; Arthur Huang, *MIT*; David Darmofal, *MIT*; Marshall Galbraith, *MIT*; Steven Allmaras, *MIT*;

Yano's Mesh Optimization via Error Sampling and Synthesis (MOESS) algorithm has proven successful in a range of contexts, particularly for convection dominated problems. The MOESS algorithm was originally derived for a discontinuous Galerkin (DG) discretization and the extension to other discontinuous finite element discretizations, such as Hybridized-DG, is relatively simple. However, the extension of MOESS to continuous discretizations is less straight forward. The central feature of MOESS is the elemental sampling procedure, where solutions computed using subdivided elements are used to synthesize a model that couples changes in the mesh with changes in an error estimate. Computing solutions with this elemental subdivision is naturally suited to discontinuous discretizations where boundary conditions can be applied by freezing the solution in neighboring elements. The extension of the elemental sampling process to continuous Galerkin discretizations, and what boundary conditions to impose for these local solves, is not obvious. In this talk we present work towards a MOESS algorithm for anisotropic output-based mesh adaptation for stabilized continuous Galerkin discretizations of advective-diffusive systems. The algorithm, in particular the local sampling procedure, is outlined and comparisons of accuracy and efficiency with respect to discontinuous type discretizations are presented.

15th U.S. National Congress on Computational Mechanics
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Title: An Error Indicator-based adaptative Reduced Order Model for nonlinear structural mechanics

Author(s): *Fabien Casenave, *SafranTech, department Modelling and Simulation*; Nissrine Akkari, *SafranTech, department Modelling and Simulation*;

In the aicraft engine industry, the prediction of high-pressure turbine blades lifetime remains a challenging computational task: the finite element models involve large meshes to take into account small structures such as the internal cooling channels, and the simulation of the stabilized cycle requires computing potentially a very large number of time steps. In [1], our team has proposed a nonintrusive reduced order modeling framework for nonlinear structural mechanics, in a high-performance computing context, to accelerate such computations. The algorithmic choices rely on energy-conserving schemes originally introduced in [2] in the reduced-order community. In this work, we illustrate that even a relatively small variability in the thermal loading that was not encountered in the offline phase can lead to important errors for the reduced order model. From this observation, we propose a simple and cheaply computed heuristic error indicator. When the indicator becomes too large in the online stage, the reduced order model is updated with a snapshot computed using the high-fidelity model. The approach is illustrated on a series of academic test cases and applied on a setting of industrial complexity, where the whole procedure is computed in parallel with distributed memory [3]. [1] F. Casenave, N. Akkari, F. Bordeu, C. Rey and D. Ryckelynck, A Nonintrusive Distributed Reduced Order Modeling Framework for nonlinear structural mechanics -- application to elastoviscoplastic computations. Submitted. [2] Farhat, C.; Avery, P.; Chapman, T.; Cortial, J. Dimensional reduction of nonlinear finite element dynamic models with finite rotations and energy-based mesh sampling and weighting for computational efficiency. International Journal for Numerical Methods in Engineering 2014, 98, 625–662 [3] F. Casenave and N. Akkari, An error indicator-based adaptative reduced order model for nonlinear structural mechanics -- application to fatigue computation of high-pressure turbine blades. In preparation.

15th U.S. National Congress on Computational Mechanics
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Title: Learning Model Parameters with Uncertainty Using Statistical Inference of Hypothetical Data Sets

Author(s): *Tiernan Casey, *Sandia National Laboratories*; Habib Najm, *Sandia National Laboratories*;

Closure models employed in predictive simulations of physical systems such as fluids and solid materials often rely on comparison of model outputs to noisy experimental data to constrain parameter values. The noise and bias in these experimental data result in uncertainty in the model parameters, which must be propagated through the predictive simulations for results to be meaningful. Information on model parameters and their uncertainties is often incomplete or inconsistent with the context of the predictive model. These issues could be corrected if the original data is available for re-analysis, which is often not the case for legacy experiments. Using concepts from entropic inference and approximate Bayesian computation, we explore a space of hypothetical data consistent with the available information reported from the experiments. Analysis of this ensemble of consistent data delivers the desired joint parameter uncertainties that may have been missing from the original fitting, and also allows for the combination of information across experiments using a data centric approach.

15th U.S. National Congress on Computational Mechanics
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Title: Bridging the Gap Between the Design of Smooth Surfaces with Arbitrary Topology and Kirchhoff-Love Shell Analysis

Author(s): *Hugo Casquero, *Carnegie Mellon University*; Xiaodong Wei, *Carnegie Mellon University*; Deepesh Toshniwal, *University of Texas at Austin*; Angran Li, *Carnegie Mellon University*; Thomas JR Hughes, *University of Texas at Austin*; Josef Kiendl, *Norwegian University of Science and Technology*; Yongjie Jessica Zhang, *Carnegie Mellon University*;

Analysis-suitable T-spline (ASTS) surfaces including both extraordinary points and T-junctions are used to solve Kirchhoff-Love shell problems. T-junctions enable to locally refine the mesh where increased resolution is needed [1]. Extraordinary points are required to mesh geometries with arbitrary topology [2]. The benefits of using ASTS to define shell geometries are at least two-fold: (1) Avoids the manual and time-consuming task of building a new mesh for engineering analysis using the CAD geometry as an input and (2) C^1 or higher inter-element continuity enables to apply the Galerkin method to discretize shell formulations defined by fourth-order partial differential equations. The applicability of the proposed technology is illustrated by performing Kirchhoff-Love shell simulations of a pinched hemisphere, an oil sump, a T-shaped junction, and a B-pillar with 44 holes [3]. Building ASTS surface meshes for these examples involves using T-junctions and extraordinary points with valences 3, 5, and 6, which often suffice for the design of free-form surfaces. Our analysis results are compared with data from the literature using either Reissner-Mindlin shells or Kirchhoff-Love shells. We have also imported both finite element meshes and ASTS meshes into the commercial software LS-DYNA, used Reissner-Mindlin shells, and compared the result with our Kirchhoff-Love shell results. Excellent agreement is found in all cases. References [1] H. Casquero, L. Liu, Y. Zhang, A. Reali, J. Kiendl, H. Gomez, Arbitrary-degree T-splines for isogeometric analysis of fully nonlinear Kirchhoff-Love shells, Computer-Aided Design, 2017, 82, 140-153. [2] D. Toshniwal, H. Speleers, T. J. R. Hughes, Smooth cubic spline spaces on unstructured quadrilateral meshes with particular emphasis on extraordinary points: Geometric design and isogeometric analysis considerations, Computer Methods in Applied Mechanics and Engineering, 2017, 327, 411-458. [3] H. Casquero, X. Wei, D. Toshniwal, A. Li, T. J. R. Hughes, J. Kiendl, Y. J. Zhang, Seamless integration of design and nonlinear Kirchhoff-Love shell analysis using analysis-suitable unstructured T-splines, in preparation.

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Title: Image Processing-Based Pulmonary Functional Imaging from Non-Contrast Computed Tomography

Author(s): *Edward Castillo, *Beaumont Health Research Institute*;

Background: CT-ventilation algorithms approximate voxel volume changes induced by the respiratory motion apparent within an inhale/exhale pair of non-contrast 3D computed tomography scans. In particular, Hounsfield Units (HU) methods approximate this volume change from the measured variations in HU density between spatially corresponding inhale/exhale tissue locations, under the assumption that mass is conserved. Numerical implementations require a deformable image registration (DIR) to determine the inhale/exhale spatial correspondence (voxel mapping), a preprocessing lung volume segmentation, a preprocessing high-intensity vessel segmentation, and a post-processing smoothing applied to the raw volume change estimates obtained for each lung tissue voxel [1]. Contribution and Summary: The apparent mass of the lungs is not constant from inhale to exhale, due to the variations in pulmonary blood mass induced by changes in intra-thoracic pressure [2]. This violates the standard mass conservation assumption employed by current CT-ventilation methods. A novel method, referred to as CT-derived functional imaging (CTFI), is presented. CTFI recovers both a voxel volume change image (CT-V) and a blood mass change image (CT-P) from the HU values of spatially corresponding voxel locations within an inhale/exhale CT image pair. Thus, CTFI provides surrogates for pulmonary ventilation (CT-V) and pulmonary perfusion (CT-P) from a single pair of non-contrast CT scans. The CTFI algorithm is based on making a series of subregional volume changes estimates that 1) respect the resolution of the digital grid and 2) possess quantitatively characterized and controllable levels of uncertainty. Therefore, in contrast to existing CT-ventilation methods, CTFI images are more robust to small variations in DIR solutions and the resulting volume change and mass change images are overall more reproducible. Moreover, CTFI does not require a pre-processing lung vessel segmentation or a post-processing Gaussian smoothing. Potential applications of CTFI include the diagnosis of pulmonary embolism from non-contrast CT imaging and radiotherapy dose-response modeling. 1. Richard Castillo, Edward Castillo, Josue Martinez, and Thomas Guerrero. Ventilation from Four Dimensional Computed Tomography: Density Versus Jacobian Methods. Physics in Medicine and Biology, 55: 4661-4685, 2010. 2. Nicholas Myziuk, Thomas Guerrero, Gukan Sakthivel, David Solis, Girish Nair, Rudy Guerra, and Edward Castillo. Pulmonary Blood Mass Dynamics on 4DCT During Tidal Breathing. Physics in Medicine and Biology. In Press, 2019. 3. Edward Castillo, Richard Castillo, Yevgeniy Vinogradskiy, and Thomas Guerrero. The Numerical Stability of Transformation-Based CT Ventilation. International Journal of Computer Assisted Radiology and Surgery, 12(4): 569-580, 2017.

15th U.S. National Congress on Computational Mechanics
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Title: A Nonlinear Finite Element Formulation Based on Multiscale Approach for Solving the Incompressible Navier-Stokes Equations

Author(s): Riedson Baptista, *CEUNES/UFES*; Sérgio Bento, *CEUNES/UFES*; Leonardo Lima, *IFES*; Andrea Valli, *CT/UFES*; Isaac Santos, *CEUNES/UFES*; *Lucia Catabriga, *CT/UFES*;

In this work we present a variational multiscale (VMS) finite element method for solving the incompressible Navier-Stokes equations. The proposed method consists of a decomposition for both the velocity and the pressure fields into coarse/resolved scales and fine/unresolved scales together with the addition of a residual-based nonlinear operator to the enriched Galerkin formulation, following a similar strategy of the method presented in [1] for scalar advection-diffusion equation. This operator introduces an artificial viscosity only on the unresolved mesh scales of the discretization. This is done dynamically at element level, by imposing some constraints on the resolved scale solution, yielding a parameter-free consistent method as given in [2]. This choice of decomposition is shown to be favorable for simulating flows at high Reynolds number. In order to reduce the computational cost typical of two-scale methods, the subgrid scale space is defined using bubble functions whose degrees of freedom are locally eliminated in favor of the degrees of freedom that live on the resolved scales. The convergence of the nonlinear process is enhanced considering a dynamic damping factor presented by [3] reducing the number of iterations and, consequently, the CPU time. Accuracy comparisons with the streamline-upwind/Petrov-Galerkin (SUPG) formulation combined with the pressure stabilizing/Petrov-Galerkin (PSPG) and least-squares on incompressibility constraint method are conducted based on 2D benchmarks problems. [1] Santos, I. P. and Almeida, R. C. and Malta, S. M. C. Numerical analysis of the nonlinear subgrid scale method. Computational & Applied Mathematics, 31(3):473–503, 2012. [2] Andrea M.P. Valli and Regina C. Almeida and Isaac P. Santos and Lucia Catabriga and Sandra M.C. Malta and Alvaro L.G.A. Coutinho A parameter-free dynamic diffusion method for advection-diffusion-reaction problems. Computers & Mathematics with Applications 75: 307–321, 2018. [3] John, Volker and Knobloch, Petr On spurious oscillations at layers diminishing (SOLD) methods for convection–diffusion equations: Part II–Analysis for P1 and Q1 finite elements. Computer Methods in Applied Mechanics and Engineering 197:1997–2014, 2008.

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Title: The Effect of Dislocation Character on Dislocation Line Tension in bcc Tungsten and Its Impact on Kink-pair Enthalpy

Author(s): Sicong He, *University of California Los Angeles*; Emma Overly, *University of California Los Angeles*; Vasily Bulatov, *Lawrence Livermore National Laboratory*; Jaime Marian, *University of California Los Angeles*; *David Cereceda, *Villanova University*;

In addition to the well-characterized elastic contribution, the energy of a dislocation contains an inelastic, or ‘core’, term that reflects the loss of validity of elasticity theory at dislocation segments. While the elastic part is known to be symmetric about its maximum value for the edge orientation (minimum for screw), in bcc metals, the core energy displays an asymmetry than can be characterized using atomistic calculations. In kink-pair configurations on screw dislocations, this asymmetry leads to a difference in energy between ‘right’ and ‘left’ kinks that is not captured in elastic models. In this work, we calculate dislocation segment self-energies as a function of dislocation character in bcc tungsten and kink-pair enthalpies as a function of stress. To avoid finite-size artifacts in atomistic simulations, we develop continuum models of kink-pair configurations based on full elasticity and line tension approaches, parameterized with a substrate Peierls potential and dislocation self-energies obtained from atomistic calculations. The elastic and line tension models represent specific situations of the environment of these kink-pair configurations, and we discuss our results in terms of the range of validity of each as well as the effect of self-energy asymmetry on kink-pair enthalpy. To match the continuum results to direct atomistic simulations, we vary the core radius of elasticity theory and discuss the implications of the values obtained.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Non-intrusive Reduced Order Data Assimilation Method Applied to the Monitoring of Urban Flows

Author(s): Janelle K. Hammond, *INRIA*; *Rachida Chakir, *Université Paris Est, IFSTTAR*;

As the population increases, cities must constantly reassess their urban planning. However, this must be done in such a way to preserve the quality of life of its inhabitants. Energy saving, sustainable water and air quality are some of the important challenges associated with growing cities. In this context, the monitoring of the different urban flows (pollution, heat) is very important. For instance data assimilation approaches can be used in monitoring. These methods incorporate available measurement data and mathematical model to provide improved approximations of the physical state. The effectiveness of modeling and simulation tools is essential. Advanced physically based models could provide spatially rich small-scale solution, however the use of such models is challenging due to explosive computational times in real-world applications. Beyond computational costs, physical models are often constrained by available knowledge on the physical system. To overcome these difficulties, we resort to a new technique combining Model Order Reduction (MOR) and variational data assimilation known as PBDW state estimation and introduced in [1]. The PBDW formulation combines a Reduced Basis (RB) from the physically based model and the experimental observations, in order to provide a real-time state estimate in a non-intrusive manner. The RB is used to diminish the cost of using a high-resolution model by exploiting the parametric structure of the governing equations. In addition, variational data-assimilation techniques are used to correct the model error. In this work we extend the PBDW method previously applied to small-scale experimental problems [2] to the monitoring of urban pollution as an important test case for practical applications, but also as an example of the very generic approach that proves well suited to online monitoring of urban flows over large scales. Our focus here is a problem of pollutant dispersion at the urban scale which can provide insight on how to treat the practical problems associated to MOR and data assimilation of complex flows involved in many sophisticated methods of urban air quality modeling REFERENCES [1] Y. Maday, A. Patera, J. Penn, M.Yano, A Parameterized-Background Data-Weak Approach to Variational Data Assimilation: Formulation, Analysis, and Application to Acoustics, Int. J. Numer. Meth.Engng, vol 102, no. 5, p933-965 (2014). [2] J.K Hammond, R. Chakir, F. Bourquin, Y. Maday, PBDW: a non-intrusive Reduced Basis Data Assimilation Method and its application to outdoor Air Quality Models, (2018), HAL-01698089.

15th U.S. National Congress on Computational Mechanics
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Title: Metric-based Anisotropic Adaptation for Optimal Petrov-Galerkin Methods

Author(s): *Ankit Chakraborty, *RWTH Aachen*; Ajay Rangarajan, *RWTH Aachen*; Georg May, *RWTH Aachen*;

Certain Petrov-Galerkin schemes are inherently stable formulations of varia- tional problems on a given mesh. This stability is primarily obtained by comput- ing an optimal test basis for a given approximation space [1]. Furthermore, these Petrov-Galerkin schemes are equipped with a robust a posteriori error estimate which makes them an ideal candidate for adaptation. One could extend these Petrov-Galerkin schemes not only to have optimal test spaces but also optimal approximation spaces with respect to current estimates of the solution. These extensions, using piecewise polynomial approximation at fixed degree, are the main focus of this talk. Conventionally, adaptation entails manipulating a given discrete mesh through local processes like edge swapping and element subdivision etc. A step forward would be to globally optimize the mesh with respect to an error estimator. In this context, metric based methods have emerged as an interesting paradigm. A metric conforming mesh is a triangulation whose elements are (nearly) equilat- eral with respect to a Riemannian metric induced by a tensor valued mapping. Meshes can be generated by using a standard metric based mesh generator. Previously, we have proposed a metric based mesh adaptation technique for higher order schemes on triangular and tetrahedral meshes [2]. There the error estimator employed was based on a high order interpolation error model [3]. Here, in contrast, we propose to use the inbuilt error estimator provided by the optimal Petrov-Galerkin framework. This estimator computes the error in the energy norm, from which an optimized continuous mesh model is created. We thus obtain a scheme with nearly optimal test and approximation spaces. References: 1. Leszek Demkowicz, Jay Gopalakrishnan, A class of discontinuous Petrov{Galerkin methods. II. Optimal test functions, Numerical Methods for Partial Differential Equations., Vol. 27, pp. 70-105, 2011 2. Rangarajan, Ajay & Chakraborty, Ankit & May, Georg & Dolejsi, Vit. A continuous- mesh optimization technique for piecewise polynomial approximation on tetrahedral grids. AIAA Paper 18-3246, American Institute of Aeronautics and Astronautics, 2018. 3. Dolejsi, Vit. Anisotropic hp -adaptive method based on interpolation error estimates in the Lˆq norm. Applied Numerical Mathematics. Vol 82,pp. 80 - 114, 2014.

15th U.S. National Congress on Computational Mechanics
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Title: Structural Optimization by Unstructured Bézier Meshes with CAD-compatible Boundary Representation

Author(s): Jorge López, *Bauhaus-Universität Weimar*; *Chiu Ling Chan, *Bauhaus-Universität Weimar*; Cosmin Anitescu, *Bauhaus-Universität Weimar*; Timon Rabczuk, *Bauhaus-Universität Weimar*;

We present a method for structural optimization using Bézier meshes. In this procedure, we consider CAD-compatible boundary representations of the domain and interior meshes obtained by standard triangular or tetrahedral meshers such as Gmsh. These meshes are converted to a higher-order Bézier representation by degree elevation as in [1], while maintaining the exact geometry description at the boundary. This allows complex geometric features such a voids to be parameterized and represented exactly. The optimization procedure requires an efficient procedure to evaluate the gradients of the constraint and goal functions with respect to the design variables. Other issues to be considered are ensuring mesh quality, increasing inter-element continuity by minimal determining sets as in [2] or Lagrange multipliers [3], as well as error estimation and adaptivity. We will present a software framework which addresses the above points and allows a general treatment of optimization problems of engineering interest such as those related to wind turbines and propellers. References: [1] S. Xia, X. Qian, Generating high-quality high-order parameterization for isogeometric analysis on triangulations, Computer Methods in Applied Mechanics and Engineering, Volume 338, 2018, Pages 1-26 [2] C.L. Chan, C. Anitescu, T. Rabczuk, Isogeometric analysis with strong multipatch C1-coupling, Computer Aided Geometric Design, Volume 62, 2018, Pages 294-310 [3] N. Liu, A. E. Jeffers, A geometrically exact isogeometric Kirchhoff plate: Feature-preserving automatic meshing and C1 rational triangular Bézier spline discretizations, International Journal for Numerical Methods in Engineering, Volume 115, 2018, Pages 395-409

15th U.S. National Congress on Computational Mechanics
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Title: A Survey of Some Discretely Entropy Stable Discontinuous Galerkin Methods for the Shallow Water Equations

Author(s): *Jesse Chan, *Rice University*;

High order discontinuous Galerkin (DG) methods are known to be unstable when applied to nonlinear conservation laws with under-resolved solution features (e.g. discontinuities or turbulence), and have traditionally required additional filtering, limiting, or artificial viscosity to avoid solution blow up. Entropy stable DG schemes address this instability by ensuring that physically relevant solutions satisfy a semi-discrete entropy inequality even in the presence of under-resolved solution features and inexact quadrature. We review the construction of several entropy stable DG methods for general nonlinear conservation laws and discuss their application to the shallow water equations.

15th U.S. National Congress on Computational Mechanics
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Title: A Spectral Shape Descriptor Based Approach for Data-Driven Metamaterials Design Optimization

Author(s): *Yu-Chin Chan, *Northwestern University*; Liwei Wang, *Shanghai Jiao Tong University*; Ramin Bostanabad, *Northwestern University*; Ping Zhu, *Shanghai Jiao Tong University*; Wei Chen, *Northwestern University*;

Spurred by advancements in additive manufacturing that allow geometrically complex designs to be realized, metamaterials, which are hierarchical structures composed of smaller-scale unit cells (“building blocks”), have risen in popularity. Due to their multiscale features, they can exhibit exceptional properties, e.g., graded stiffness, negative Poisson’s ratio, and wave filtering. However, current computational design techniques for metamaterials, such as multiscale topology optimization, are hindered by the expanse of the design space, the difficulty of solving the inverse problem, and computational expenses. As such, most works simplify the problem by repeating the same unit cell throughout the structure, limiting the achievable properties. More recent methods allow the unit cells to be heterogeneous, but the disparate unit cells are often disconnected and thus not able to be manufactured. To tackle these challenges, we explore harnessing Laplace-Beltrami spectral shape descriptors as latent space representations of the metamaterial “building blocks” for data-driven design. Using a precomputed database of unit cells that cover a wide range of mechanical properties, we map the Laplace-Beltrami spectra of the unit cells to their mechanical properties using supervised learning methods such as neural networks and a globally-approximate Gaussian random process model for big data. To demonstrate the generalizability of the shape descriptor method, we test its ability to preserve the geometric and physical information of conventional representations, including topology optimized results and lattice structures. Ultimately, the database and structure-property models powered by reduced-dimension geometric representations can lead to the efficient optimization of well-connected, heterogeneous metamaterials.

15th U.S. National Congress on Computational Mechanics
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Title: Predicting Properties of Cementitious Materials by Mesoscale Modeling

Author(s): Mark Adley, *U.S. Army Engineer Research and Development Center*; *Mei Chandler, *U.S. Army Engineer Research and Development Center*; Robert Moser, *U.S.Army Engineer Research and Development Center*; William Lawrimore, *U.S. Army Engineer Research and Development Center*; Jameson Shannon, *U.S. Army Engineer Research and Development Center*; Micael Edwards, *U.S. Army Engineer Research and Development Center*;

Cementitious materials such as concrete are intrinsically heterogeneous, and include internal structures and constituents across length scales ranging from nanometers to millimeters. Mesoscale structures and constituents of cementitious materials include heterogeneities such as aggregates, sand, fibers, porosities and cracks. The properties and responses of concrete under different loading conditions are strongly dependent on the properties of the mesoscale structures and constituents. In this work, we constructed finite element models of a concrete as a three-phase composite with aggregates, mortar, and interfacial transition zone (ITZ) modeled explicitly. The aggregates were represented as spheres with volume fractions and size distributions based on the experimental characterizations. The constitutive laws of the aggregate phase and mortar phase were based on the Advanced Fundamental Concrete (AFC) model, and parameters were fitted to the experimental test data of individual aggregate and mortar phases. ITZ phase was modeled with cohesive elements using a bilinear traction-separation law. The parameters of the traction-separation law were based on the properties estimated from Virtual Cement and Concrete Testing Laboratory (VCCTL) simulations. The sizes and boundary conditions of the finite element models were based on laboratory testing of cylindrical specimens. The simulations were performed with applied loadings of unconfined compression, hydrostatic compression, triaxial compression and uniaxial strain compression. The simulation results compared well with the experimental results of the concrete, which demonstrates the suitability of the modeling methods, and provides a pathway for optimizing concrete materials at mesoscale for different applications in the future. Permission to publish was granted by the Director, ERDC Geotechnical and Structures laboratory.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Toward Plasticity without Phenomenological Assumptions

Author(s): *Sabyasachi Chatterjee, *Carnegie Mellon University*; Giacomo Po, *University of California, Los Angeles*; Xiaohan Zhang, *Carnegie Mellon University*; Amit Acharya, *Carnegie Mellon University*; Nasr Ghoniem, *University of California, Los Angeles*;

We demonstrate a concurrent multiscale strategy involving Discrete Dislocation Dynamics (DD) and Field Dislocation Mechanics (FDM) based on Practical Time Averaging (PTA). The constitutive assumptions of a pde model of dislocation based plasticity (FDM) are obtained from DD through the scheme. PTA is a scheme to understand and exploit the slow time-scale behavior of rapidly evolving microscopic dynamics. The microscopic systems considered are posed in terms of systems of non-linear ordinary differential equations, not necessarily containing an a priori split into fast and slow variables. The methodology employed involves a computational scheme based on fundamental mathematical theory that a) defines appropriate `coarse' variables corresponding to the microscopic dynamics that evolve in a stable manner on the coarse time scale; b) determines the equation of evolution for such variables; and c) defines a practically useful strategy for accurately initializing short bursts of microscopic runs for the evolution of the slow variables, without special requirements on the nature of the microscopic dynamics (like ergodicity).

15th U.S. National Congress on Computational Mechanics
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Title: Information Reuse for Importance Sampling in Reliability-Based Design Optimization

Author(s): *Anirban Chaudhuri, *Massachusetts Institute of Technology*; Boris Kramer, *Massachusetts Institute of Technology*; Karen Willcox, *University of Texas at Austin*;

This work introduces a new approach for importance-sampling-based reliability-based design optimization (RBDO) that reuses information from past optimization iterations to reduce computational effort. RBDO is a two-loop process---an uncertainty quantification loop embedded within an optimization loop---that can be computationally prohibitive due to the numerous evaluations of expensive high-fidelity models to estimate the probability of failure in each optimization iteration. In this work, we use the existing information from past optimization iterations to create efficient biasing densities for importance sampling estimates of probability of failure. The IRIS-RBDO (Information Reuse for Importance Sampling in RBDO) method involves two levels of information reuse: (1) reusing the current batch of samples to construct an a posteriori biasing density with optimal parameters, and (2) reusing the a posteriori biasing densities of the designs visited in past optimization iterations to construct the biasing density for the current design. There are several advantages of the proposed IRIS-RBDO method. First, the method is computationally efficient as it does not require building a biasing density from scratch at every iteration and can build efficient biasing densities by reusing existing information. Second, the method can overcome bad initial biasing densities by reusing samples to build (at every design iteration) a posteriori biasing densities for future reuse. Third, the method is potentially useful for building biasing densities for disconnected feasible regions or multiple failure regions because it uses a mixture of existing biasing densities. Fourth, there is no bias in the IRIS-RBDO reliability analysis. We demonstrate the efficiency of the proposed method for the RBDO of a benchmark speed reducer problem and a combustion engine problem.

15th U.S. National Congress on Computational Mechanics
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Title: A Comparison Study on Deformation Gradients in Peridynamics

Author(s): *Hailong Chen, *University of Kentucky*;

Peridynamic models that aim to incorporate a given stress-strain constitutive relationship from classical local continuum theory typically start with a nonlocal analog to the local deformation gradient as input to the given local stress-strain constitutive relationship. With a formulated nonlocal analogous deformation gradient, force density functions can then be derived in terms of stress tensor using the concept of energy conjugate. It should be noted that the formulation of this nonlocal analogous deformation gradient plays a significant role in the performance of related correspondence model. Issues such as material instability and penetration are well known in the model formulated based on the nodal average deformation gradient. In this presentation, we will present a comparative study on various deformation gradient formulations in peridynamics, namely, the nodal average deformation gradient, the bond-level deformation gradient, the bond-associated deformation gradient and nodal high-order deformation gradient. Rather than solving the mechanics problem using peridynamic model, prescribed displacements fields are used in this study to better investigate potential issues with each deformation gradient formulation. Prediction accuracy for both homogeneous and inhomogeneous deformations will be studied. Issues for different formulations will be discussed.

15th U.S. National Congress on Computational Mechanics
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Title: Physics-Informed Data-Driven Meshfree Modeling for Biomaterials

Author(s): *J. S. Chen, *UC San Diego*; Qizhi He, *UC San Diego*; Chung-Hao Lee, *The University of Oklahoma, Norman*;

Physics-informed data-driven computational mechanics is a hybrid approach that integrates universal physical laws with data-based models of experimental data to enhance traditional scientific computing. A local convexity preserved data-driven approach is developed based on manifold learning techniques and formulated under the nodal integrated Galerkin meshfree methods for nonlinear elastostatics analysis, termed the locally convex data-driven (LCDD) computing. The employment of smooth meshfree approximation functions with nodal integration of state and field variables at the set of nodes yields a better conditioned and reduced-dimension data-driven optimization system. To enhance accuracy and robustness against noise and outliers in data sets, this new approach reconstructs the local data manifold by a convex hull based on the nearest experimental points, and seeks for the optimal solution via the projection onto the associated manifold. A penalty relaxation is further introduced to recast the local learning solver in the context of non-negative least squares that can be solved effectively. Due to the inherent manifold learning properties, LCDD performs well for high-dimensional data sets that are relatively sparse in real-world engineering applications. In this work, LCDD is adopted to simulate heart valve tissues under finite deformation, where the experimental data from biaxial mechanical tests were employed in the data-driven processes.

15th U.S. National Congress on Computational Mechanics
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Title: Optimal Design of Acoustic Cloak under Uncertainty

Author(s): *Peng Chen, *University of Texas*; Michael Haberman, *University of Texas*; Omar Ghattas, *University of Texas*;

In this talk, we present simulation-based optimal design of acoustic cloak under uncertainty and scalable approximation and optimization methods to solve the optimal design problem. The design parameter is taken as an infinite-dimensional space-dependent variable that represents the material property, while the additive uncertain parameter is modeled by an infinite-dimensional random field that represents the possible variability of the material property or the manufacturing error. A faithful discretization of the optimal design problem results in high-dimensional design and uncertain parameters. To solve this problem, we develop a computational approach based on a Taylor approximation and a quasi-Newton method, which is scalable with respect to the dimension of both the design and uncertain parameters. We demonstrate that a robust design of acoustic cloak is achieved by taking the uncertainty into account by this computational approach. Moreover, we extend it for acoustic cloak design subject to from a single-direction and single-frequency incident wave to multiple-direction and multiple-frequency incident waves. Furthermore, we apply it to a more complex geometry than the classical circular obstacle surrounded by a ring-shaped cloaking region.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: An Inherent Strain Based Path Planning Optimization Method for Metal Additive Manufacturing with Experimental Validation

Author(s): *Qian Chen, *University of Pittsburgh*; Wen Dong, *University of Pittsburgh*; Kyle Johnson, *Sandia National Laboratories*; Shaun Whetten, *Sandia National Laboratories*; Albert To, *University of Pittsburgh*;

Residual stress and distortion associated with local rapid heating and cooling during metal additive manufacturing process is one of most common defects for metal AM parts, which reduces part tolerance and causes potential cracking and build failure. This work presents a novel layer-wise laser scanning path optimization method for laser engineered net shaping (LENS) processing to mitigate this issue. The scanning path of each deposition layer is represented by a level set function, from which the scanning orientation is easily obtained. The orientation-dependent inherent strain vector is employed to quantify the thermal loading in finite element analysis. Full sensitivities for the formulated compliance- and stress-minimization problems is derived, and a specific strategy called adaptive level set adjustment (ALSA) is applied in iterations to remedy the deficiency of neglecting non-implementable sensitivity terms and guaranty stable convergence. The optimized scanning paths from compliance- and stress-minimization optimization are utilized on LENS process, respectively. Through comparison with experimentally measured stress and deformation profiles of commonly used scanning patterns, the effectiveness of this proposed method is validated. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

15th U.S. National Congress on Computational Mechanics
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Title: Structural and Fatigue Modeling of a 5MW Wind Turbine Blade Under Different Wind Loads

Author(s): *Shunhua Chen, *The University of Tokyo*; Shinobu Yoshimura, *The University of Tokyo*; Kaworu Yodo, *Insight, Inc.*; Naoto Mitsume, *The University of Tokyo*; Yasunori Yusa, *Tokyo University of Science*; Tomonori Yamada, *The University of Tokyo*; Chisachi Kato, *The University of Tokyo*; Shori Orimo, *The University of Tokyo*; Yoshinobu Yamade, *Mizuho Research Institute*; Akiyoshi Iida, *Toyohashi University of Technology*;

With the pressing requirement of wind energy capacity, the wind turbine blade size has been getting larger and larger in recent decades. For such a large-size blade, it is of prime importance to accurately evaluate the mechanical response under various wind loading conditions. In this work, we present a computational framework to achieve this end. Firstly, a finite element model for a 5MW blade is established according to the well-known NREL report. A composite laminated element is adopted to describe the blade structure. The effectiveness of this model is validated by means of eigenfrequency analysis. Secondly, a one-way partitioned FSI coupling algorithm is developed to consider the wind loading condition applied on the blade surface. The coupling algorithm facilitates the use of two parallel open source codes, e.g. FrontFlow/blue and ADVENTURE. Finally, an empirical approach is adopted to estimate the fatigue life of the blade under wind loads. This approach uses the so-called rainflow counting algorithm to reduce a spectrum of varying stress to equivalent stress cycles with constant amplitude. The remaining service life of the blade is then estimated by means of the Goodman diagram and the Miner’s damage accumulation law. Several numerical cases are carried out, which validates the capacity of the proposed computational framework for structural and fatigue analysis of wind turbine blades under various wind loads.

15th U.S. National Congress on Computational Mechanics
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Title: Magnetic Field Driven Buckling in Architected Magnetoelastomers

Author(s): *Vincent Chen, *AFRL*; Artemii Goshkoderia, *Technion Institute of Technology*; Carson Willey, *AFRL*; Stephan Rudykh, *University of Wisconson-Madison*; Abigail Juhl, *AFRL*; Phiip Buskohl, *AFRL*;

Magneto-Active Elastomers (MAEs) are an important class of soft, shape-recoverable materials that exhibits a stiffness increase in response to an applied magnetic field. Using magnetic field to tune material stiffness is advantageous due to the fast, remote and reversible switching, which is relevant for applications in areas of soft actuators, adaptive vibration dampers and acoustic filters. 1D and 2D architected MAE composites, such as laminates and periodic inclusions, have been predicted to possess novel mechanical instabilities, due the spatial distribution of stiffness mismatch and the ability to dynamically tune the mismatch with magnetic field. We fabricated MAE composites using a commercial silicone as the non-responsive soft matrix and a silicone loaded with iron microparticles for the stiff, magnetoactive regions to experimentally demonstrate these concepts. The silicone matrix formulation was modified to increase the stiffness contrast between the soft encapsulating matrix and the stiff MAE regions, including tuning of the crosslinker to polymer ratio, and addition of silicone oil to further reduce crosslinking. 3D printed templates were used as molds to construct laminates and 2D periodic MAE architectures. Magnetic field induced stiffening was characterized using a custom compression test jig that was designed and 3D printed to systematically load the specimen within a 2 Tesla electromagnet. The study provides experimental feedback on the sensitivity of the buckling strain to experimental specimen sizing/edge effects and provides broader insight on the practical integration of MAE instabilities into functional devices.

15th U.S. National Congress on Computational Mechanics
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Title: A Preliminary Study on Nonlocal Mechanics via Combined MPM and SPH

Author(s): *Zhen Chen, *Dalian University of Technology / University of Missouri*;

Zhen Chen, Dalian University of Technology / University of Missouri Lisha He, Nanchang University *Email: chenzh@missouri.edu Nonlocal elastoplasticity and/or damage models in terms of gradient or integral of strain or internal state variables have been proposed to regularize softening with localization in model-based simulation of failure evolution, as reviewed by Chen and Schreyer [1]. For transient problems, the numerical oscillations due to semi-discretization in space make the evaluation of higher order terms a difficult task in avoiding numerical failure such as premature cracking. Based on the previous work [2, 3], a combined MPM (material point method) and SPH (smoothed particle hydrodynamics) numerical scheme is proposed to implement a nonlocal model via the gradient of plastic strain, with an application to a one-dimensional bar under impact. The MPM is used to discretize the region near the impact surface without the need for master/slave nodes at contact, while the SPH is adopted around the softening zone to facilitate the evaluation of strain gradient. A parametric investigation is performed to illustrate the effects of controlling parameters on the evolution of localized softening. It is demonstrated that integrating nonlocal constitutive modeling with spatial discretization might yield an effective computational procedure for predicting and evaluating failure evolution. References [1] Chen, Z., and Schreyer, H.L., "On Nonlocal Damage Models for Interface Problems," International Journal of Solids and Structures, Vol. 31(9), pp. 1241-1261, 1994. [2] Schreyer, H.L., and Chen, Z., "One Dimensional Softening with Localization," Journal of Applied Mechanics, Vol. 53(4), pp. 791-797, 1986. [3] He, L., Gan, Y., and Chen, Z., “Preliminary Effort in Developing the Smoothed Material Point Method for Impact,” Computational Particle Mechanics, Vol. 6, pp. 45-53, 2019.

15th U.S. National Congress on Computational Mechanics
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Title: An Intermediate Homogenization Approach for Electromechanical Peridynamic Modeling of Damage and Fracture in Composites

Author(s): *Ziguang Chen, *Huazhong University of Science and Technology*; Pan Wu, *Huazhong University of Science and Technology*; Yuantai Hu, *Huazhong University of Science and Technology*; Florin Bobaru, *University of Nebraska-Lincoln*;

Random networks of conductive nanofibers within a polymer matrix have been increasingly considered for use in flexible and transparent electronics, strain sensors, etc. as they offer higher sensitivity and superior electrical properties. The numerical simulation of the electromechanical response usually includes either homogenization of material properties or of explicit, high-resolution microstructural representations. The homogenization methods may not work, especially when damage and fracture are included, for example, in the case of strain and damage sensing. In this work, we introduce an intermediate (or partial) homogenization peridynamic (IH-PD) approach for electromechanical modeling of deformation, damage and consequent piezo-resistive response in the conductive nanofibers-based nanocomposite. In this model, peridynamic mechanical-bonds are superposed onto recoverable electrical-bonds. Different from the explicit heterogeneity method (which has a major limitation on the simulation size), in the IH-PD model we have two types of bonds: inter-phase and intra-phase bonds, representing properties of the distinct composite phases and of interfaces between them. For nanofibers-based nanocomposites with phases A (conductive nanofibers) and B (non-conducting polymer), we define A-A bonds (intra-phase) for the first phase, A-B bonds (inter-phase), and B-B bonds (intra-phase) for the second phase [1]. The distribution of the different bonds depends on the volume fraction of the phases in the nodes. While the specific geometry of the microstructure is not preserved, the specific volume fraction is and, in many instances, this is a critical parameter in modeling the evolution of damage [2]. We verify the IH-PD model of electrical conduction using experimental data for electrical conductivity of metal matrix composites containing high volume fractions of non-conducting inclusions. The model is then used to study damage and the piezo-resistive response under 2D uniaxial tensile tests. Comparisons with the fully homogenized model and the explicit microstructure one show that the IH model captures key deformation and damage mechanisms associated with the complex material (obtainable with an explicit model but not with the fully homogenized one), while preserving the computation efficiency of fully homogenized computations. This model can also be extended to other multi-physical problems with damage and fracture. [1] Chen, Z., Niazi, S., Zhang, G., & Bobaru, F. (2017). Peridynamic functionally graded and porous materials: Modeling fracture and damage. Handbook of Nonlocal Continuum Mechanics for Materials and Structures, 1-35. [2] Chen, Z., Niazi, S., & Bobaru, F. A peridynamic model for damage and fracture in porous materials. Submitted.

15th U.S. National Congress on Computational Mechanics
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Title: A Direct Forcing Immersed Boundary Method for Topology Optimization of Incompressible Flow

Author(s): *Lin Cheng, *University of Pittsburgh*; Hao Deng, *University of Pittsburgh*; Albert To, *University of Pittsburgh*;

In the current work, a topology optimization method employing direct forcing immersed boundary (DFIB) method for Navier-Stokes flow problems is proposed. The DFIB method has been applied to simulate complex flows around moving arbitrary bodies in a Eulerian-Lagrangian framework, in which the fluid flow is simulated in a regular Eulerian mesh while the presence of a solid boundary is represented by a set of Lagrangian markers. These markers are formulated by a level set field in this work and are iteratively updated to achieve an optimal design for fluid flow problems. Unlike the commonly used continuous forcing immersed boundary (CFIB) approach (e.g., Brinkman model) in topology optimization, the DFIB method avoids the application of artificial parameters for the implementation of rigid no-slip boundary condition. Instead, the no-slip boundary condition is imposed directly through a local interpolation between the Eulerian mesh and Lagrangian markers. The interpolation circumvents the necessity of re-meshing for the update of the sharp interface in the optimization and thus makes it desirable for level set topology optimization for fluid flow problem. Also, the proposed method does not rely on artificial parameters and has better local accuracy of the solution on the boundary. It not only mitigates the spurious pressure diffusion of the Brinkman model through solid material but also eliminates the influences of model parameters on optimization results. For comparison purpose, several numerical examples are conducted using both the DFIB method and the Brinkman model to illustrate the effectiveness of the proposed methodology for fluid flow optimization.

15th U.S. National Congress on Computational Mechanics
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Title: A Semi-Lagrangian Reproducing Kernel Approach for Simulation of Munitions Penetration into Geo-materials

Author(s): *Sheng-Wei Chi, *University of Illinois at Chicago*; Ashkan Mahdavi, *University of Illinois at Chicago*; Mohammed M. Atif, *University of Illinois at Chicago*;

In this paper, a mixed-field u-p semi-Lagrangian reproducing kernel (RK) approach is introduced for simulating munitions penetration into soils and studying the penetration depth of various projectile types into dry and fully saturated geo-materials. To describe the poromechanics of saturated materials, Biot theory is incorporated into semi-Lagrangian RK formulation and a damage model is embedded into Drucker-Prager constitutive model to represent the soil mechanical behavior during the impact and penetration process. To ensure numerical stability due to domain integration, the modified stabilized non-conforming nodal integration is introduced into semi-Lagrangian RK formulation and the kernel contact algorithm is implemented to model to contact between soil and projectile's bodies. Furthermore, an absorbing boundary layer is developed and introduced in the semi-Lagrangian RK framework to reduce the reflection waves from the model boundaries. To verify the proposed method's performance in predicting final penetration depth, several examples are solved, and numerical results are compared to those reported in the literature.

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Title: Modeling Curved Interfaces without Element-Partitioning in the Extended Finite Element Method

Author(s): *Eric Chin, *UC Davis*; N. Sukumar, *UC Davis*;

In this talk, we model holes and material interfaces (weak discontinuities) in two-dimensional linear elastic continua using the extended finite element method on higher-order (spectral) finite element meshes. Arbitrary parametric curves such as rational Bézier curves and cubic Hermite polynomials are adopted in conjunction with the level set method to represent curved interfaces. To recover explicit parameterized curves from the implicit algebraic curve that describes the level set zero isocontour, optimized approximate Bézier curves are used. For geometry described using rational Bézier curves, we use implicitization techniques to determine an exact level set function. Efficient computation of weak form integrals with polynomial integrands is realized via the homogeneous numerical integration scheme [1]—a method that uses Euler's homogeneous function theorem and Stokes's theorem to reduce integration to the boundary of the domain. Numerical integration over cut-elements require the evaluation of a one-dimensional integral over a parametric curve, and hence the need to partition curved elements is eliminated. To improve stiffness matrix conditioning, ghost penalty stabilization and the Jacobi preconditioner are used. For material interface problems, we develop an enrichment function that accurately captures weak discontinuities on spectral meshes. Taken together, we show through numerical experiments that these advances deliver optimal rates of convergence with h-refinement and exponential rates of convergence with p-refinement in the L2 norm and the strain energy for elastostatic problems with holes and material inclusions on refined, structured p-th order spectral finite element meshes. References [1] Chin EB, Lasserre JB, Sukumar N. Numerical integration of homogeneous functions on convex and nonconvex polygons and polyhedra. Comput Mech 2015; 56(6): 967—981.

15th U.S. National Congress on Computational Mechanics
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Title: Extended Virtual Element Method for the Laplace Problem with Singularities and Discontinuities

Author(s): *Andrea Chiozzi, *University of Ferrara*; Elena Benvenuti, *University of Ferrara*; Gianmarco Manzini, *Los Alamos National Laboratory*; N. Sukumar, *University of California, Davis*;

The Virtual Element Method (VEM) [1] is a stabilized Galerkin finite element formulation that is capable of dealing with very general polygonal or polytopal meshes, wherein the basis functions are implicit (virtual) — they are not known explicitly within the problem domain. Suitable projection operators are used to decompose the bilinear form on each element into two parts: a consistent term that reproduces the first-order polynomial space and a correction term that ensures stability. In this contribution, we propose a first-order extended virtual element method (X-VEM) to treat singularities and crack discontinuities that arise in the Laplace problem. The approach herein draws from the development of the extended finite element method for fracture problems [2], in which the discrete space is extended by means of additional basis functions that capture the salient features of the exact solution. A similar approach is pursued in the proposed X-VEM formulation with a few notable extensions. To suitably represent singularities and discontinuities in the discrete space, we augment the standard virtual element space with an additional contribution that consists of the product of virtual nodal basis functions with so-called enrichment functions. For discontinuities, the enrichment function is discontinuous (generalized Heaviside function) across the crack and for singularities it is a weakly singular function that satisfies the Laplace equation. For the Laplace problem with a discontinuity, we project the virtual basis functions onto affine polynomials over the two partitions of an element cut by the discontinuity. For the Laplace problem with a singularity, we devise an extended projector that maps functions that lie in the extended virtual element space onto linear polynomials and the enrichment function. The homogeneous numerical integration method is used to accurately compute integrals with integrands that are discontinuous or are weakly singular. Numerical experiments are performed on quadrilateral and polygonal meshes for the problem of an L-shaped domain with a corner singularity and the problem of a cracked membrane under mode III loading. Numerical results illustrate the accuracy and demonstrate optimal rates of convergence in both L2 norm and energy of the proposed method. References: [1] Beirao da Veiga, L., Brezzi, F., Cangiani, A., Manzini, G., Marini, L.D., Russo, A., “Basic Principles of the Virtual Element Method”, Mathematical Models and Methods in Applied Sciences, 23(1), 2013. [2] Moes, N., Dolbow, J., Belytschko, T., “A finite element method for crack growth without remeshing”, International Journal for Numerical Methods in Engineering, 46(1), 1999.

15th U.S. National Congress on Computational Mechanics
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Title: Simulations of the Fruit Fly Flight with Immersed Boundary Method

Author(s): Yen Ku, *National Tsing Hua University*; Sheng-Chiang Lin, *National Tsing Hua University*; *Tzu-Hsuan Chiu, *National Tsing Hua University*; Chao-An Lin, *National Tsing Hua University*;

Fruit fly flight is simulated with a immersed boundary method [1,2]. By simulating the force generation of a fruit-fly wing, we discovered the importance of wing deviation during hovering. It is related to the complexity of the fruit-fly hovering motion where the wing angle variations of sweeping, rotation, and deviation complement one another to maintain a high lift with a relatively low drag. The effective complexity is determined by comparing the force generation along a period and the vortex structures between different wing motions, including the realistic fruit-fly motion and the simplified symmetric rotating motion. [1] Liao, C. C., Chang, Y. W., Lin, C. A. and McDonough, J. M., 2010, "Simulating flows with moving rigid boundary using immersed boundary method," Computers and Fluids, Vol. 39 No. 1, pp. 152-167. [2] Liao, C. C., Hsiao, W. W., Lin, Y. T. and Lin, C. A., 2015, Simulations of two sedimenting-interacting spheres with different sizes and initial configurations using immersed boundary method, Computational Mechanics, Vol. 55, pp. 1191-1200.

15th U.S. National Congress on Computational Mechanics
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Title: Efficient Computational Approach to Micro-Macro Modeling via Projection-based Model-Order Reduction

Author(s): *Haeseong Cho, *Seoul National University*; Iksu Jeong, *Seoul National University*; Maenghyo Cho, *Seoul National University*;

Recent advances in computational speed have resulted in the ability to model composite materials using larger representative volume elements (RVEs) with greater numbers of inclusions than have been previously studied for the effective evaluation of material properties, failure analysis, and constitutive law development [1]. Specifically, for the materials under nonlinear history dependent behavior, fully coupled simulation between the macroscopic and microscopic structures can be used in order to obtain an accurate solution. In that sense, recursive computation for microscopic structures, modelled with the RVE, should be conducted [2]. However, direct computation of such a situation still requires significant computational costs. In this study, projection-based model-order reduction technique in conjunction with the hyper reduction approach, such as discrete empirical interpolation method [3], will be developed and applied to such a RVE for the materials at nonlinear history dependent material behavior. The resulting reduced-order model will be capable to consider parameter variation, i.e., material properties and distribution of heterogeneities. The relevant application will be accomplished for two-dimensional and three-dimensional RVE and the efficiency of the present approach will be verified. References [1] Tyrus, J.M., Gosz, M., DeSantiago, E., A local finite element implementation for imposing periodic boundary conditions on composite micromechanical models, International Journal of Solids and Structures 44, 2007, pp. 2972-2989. [2] Kouznetsova, V., Brekelmans, W.A.M., Baaijens, F.P.T., An approach to micro-macro modeling of heterogeneous materials, Computational Mechanics 27, 2001, pp.37-48. [3] Chaturantabut, S., Sorensen, D.C., Nonlinear model reduction via discrete empirical interpolation, SIAM Journal on Scientific Computing 32(5), 2010, pp. 2737-2764. Acknowledgement This work was supported by a grant from the National Research Foundation of Korea (NRF) funded by the Korea government (MSIP) (Grant No. 2012R1A3A2048841).

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Title: Data-driven Computational Hyperelastic Continuum Based on Molecular Dynamics Simulation

Author(s): *Maenghyo Cho, *Seoul National University*; Sunyoung Im, *Seoul National University*; Ingyun Chung, *Seoul National University*;

The classical dynamics simulations are based on two different types of equations. One has axiological characteristics related to balance law, and the other has phenomenological characteristics derived from experiments or observations on nature. The first type is equilibrium equation and compatibility equation which are reliable equations, and the second one is constitutive equation which is lacking in generality. Hyper-elastic material is a type of elastic material whose stress-strain relationship derived from a strain energy density function. To construct the constitutive equation, hyperelastic model assume a specific form of strain energy density function, and find the material parameter that best describes the given data set. Various models such as Mooney-Rivlin model, Neo-Hookean model, and Ogden model have been proposed to determine the constitutive equations of hyper-elastic materials. But, this approach is somewhat particular and often not be suitable for new experiments data. This study applies the stress-strain relationship directly to the continuum analysis process with machine learning, instead of using a specific form of the strain potential function to compute the hyper-elastic material behavior. The multiple stress-strain data sets are obtained by molecular dynamics simulation (MD simulation) in various loading condition such as uniaxial tension, uniaxial compression, simple shear, and biaxial tension. Machine learning is used to extract the characteristics of raw data obtained in the atomistic simulations. The MD data sets are trained with the strain as input and the stress as output, and the hypothesis function is created. During the nonlinear finite element model analysis, the element stress is determined by the given element strain and constructed hypothesis function. From assuming the locally linear tangent behavior, the components of tangent modulus are computed as the gradient of the nearest neighbors of the given strain state.

15th U.S. National Congress on Computational Mechanics
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Title: Morphologic Constructions of the Virtual Element Method

Author(s): *Habeun Choi, *Yonsei University*; Heng Chi, *Georgia Institute of Technology*; Kyoungsoo Park, *Yonsei University*; Glaucio Paulino, *Georgia Institute of Technology*;

The Virtual element method (VEM) is able to consistently handle arbitrarily shaped polygonal and polyhedral elements [1]. Because of the flexibility on element shape (convex and nonconvex), the VEM is attractive for mesh modification events (e.g., adaptive refinement and coarsening). In this study, we propose an adaptive mesh morphogenesis procedure exploring mesh coarsening. The morphogenesis procedure is simply performed by merging elements on the basis of a posteriori error estimator [2]. After merging elements, the local element connectivity is updated by means of a topology-based data structure (TopS) [3], which completes one generation of mesh adaptation. The morphogenesis procedure can be recursively conducted regardless of mesh quality and the number of generations. Computational results demonstrate that the adaptive morphogenesis with VEM can effectively handle mesh coarsening of unstructured meshes. References [1] Beirão da Veiga, L., Brezzi, F., Cangiani, A., Manzini, G., Marini, L. D., & Russo, A. (2013). Basic principles of Virtual Element Methods. Mathematical Models and Methods in Applied Sciences, 23(1), 199–214. [2] Chi, H., Beirão da Veiga, L., & Paulino, G. H. (2019). A simple and effective gradient recovery scheme and a posteriori error estimator for the Virtual Element Method (VEM). Computer Methods in Applied Mechanics and Engineering, 347, 21-58. [3] Celes, W., Paulino, G. H., & Espinha, R. (2005). A compact adjacency?based topological data structure for finite element mesh representation. International Journal for Numerical Methods in Engineering, 64(11), 1529-1556.

15th U.S. National Congress on Computational Mechanics
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Title: A Practical Space-time Reduced Order Model for Large-scale Dynamical Problems

Author(s): *Youngsoo Choi, *Lawrence Livermore National Laboratory*;

A classical reduced order model for dynamical problems involves spatial reduction of the problem size and complexity. However, temporal reduction accompanied by the spatial reduction can further reduce the problem size and complexity without losing accuracy much, which results in a considerably more speedup than the spatial reduction only. Recently, a novel space–time reduced order model for dynamical problems has been developed [1]. The space–time reduced order model shows an order of a hundred speedup with a relative error of 10?4. However, all the numerical examples presented in the paper were simple one-dimensional problems implemented in MATLAB. In order for the method to be applicable to a large-scale problem, an efficient space–time reduced basis construction algorithm needs to be developed. In this talk, we present two ways to achieve this goal: 1. incremental space– time reduced basis construction algorithm and 2. Solution-based Nonlinear Subspace (SNS) method [2]. The incremental algorithm is fully parallel and scalable. Additionally, the SNS method is applicable for nonlinear dynamical systems. These novel techniques are applied to a large-scale particle transport simulation. The numerical example shows that the algorithm is scalable and practical. Also, the space– time reduced order model via this basis achieves a size reduction of around twenty-seven million and solving time speedup of around four thousand. References [1] Youngsoo Choi and Kevin Carlberg. Space–time least-squares petrov–galerkin projection for nonlinear model reduction. SIAM Journal on Scientific Computing, 41(1):A26–A58, 2019. [2] Youngsoo Choi, Deshawn Coombs, and Robert Anderson. Sns: A solution-based nonlinear subspace method for time-dependent nonlinear model order reduction. arXiv preprint arXiv:1809.04064, 2018.

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Title: A Bond-based Peridynamic Model of Penetration Resistance Mechanism for Ceramic Composite Armor

Author(s): *Bufan Chu, *Wuhan University of Technology*; Lisheng Liu, *Wuhan University of Technology*; Qiwen Liu, *Wuhan University of Technology*;

The behavior of penetration resistance for ceramic composite armor under impact load is a hot issue in the field of armor protection. Peridynamic?PD? formulation is a new theory based on non-local hypothesis and uses integration of nodal force instead of spatial derivatives in the equations of motion, and thus it can support the discontinuity of deformation field naturally and can be well applied to the description and analysis of the dynamic mechanical behavior of brittle materials. In this work, a new method is proposed to establish the bond-based PD constitutive model describing ceramic materials subjected to high-speed bullet impact, including how to determine the relationship between material strength under the theory of continuum mechanics and the critical stretch of the bond and describe the strain rate in the peridynamic theory. Then the model is applied to analyze the dynamic responses of ceramic composite armor system with metal backing under impact loading and the development of crack in the ceramic is obtained. The numerical results obtained from the PD model are in general agreement with the those from the experiment, which verify the correctness and validity.

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Title: Stochastic Multiscale Analysis with Material Properties Defined on Complex Domains

Author(s): *Shanshan Chu, *Duke University*; Johann Guilleminot, *Duke University*;

Stochastic multiscale analysis involves the definition and simulation of random properties on complex domains. In particular, the consideration of connected phases, relevant to most composite materials, generally requires generating spatially varying (linear or nonlinear) properties on nonconvex domains. In this work, we propose a novel methodology that allows for modeling and efficiently sample non-Gaussian random fields of material parameters on such geometries. An application to a polydisperse random microstructure is provided to assess the relevance of the computational framework.

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Title: Topology Optimization of 3D Nonlinear Thermomechanical Structures Using a Level-set Method

Author(s): *Hayoung Chung, *UC San Diego*; Oded Amir, *Technion*; Sandilya Kambampati, *UC San Diego*; Hyunsun Alicia Kim, *UC San Diego*;

High temperature environments are ubiquitous in aerospace, civil, and mechanical structures. There is a rising interest in studying the optimum designs for combined thermomechanical loads. The existing topology optimization studies have predominantly focused on two-dimensional linear thermomechanical optimization. By assuming infinitesimal thermoelasticity, the formulation of the finite element method and the evaluation of state and adjoint variables are greatly simplified. However, it has been suggested that the linear assumption is inadequate even at a moderate level of mechanical and thermal loads, when combined. Furthermore, the linear optimum solutions can be far from achieving the optimum performance [1]. In this work, we present a level-set topology optimization formulation that considers geometric and material nonlinearity under thermoelastic loadings. A finite deformation hyperelastic thermoelastic model is formulated and used to analyze structural behavior with the multiplicative decomposition of mechanical and thermal deformations. Such a high-fidelity model is essential in evaluating state and adjoint variables and for computing design sensitivities. Topology optimization of high-resolution 3D structures is enabled by a fully parallel finite element method and a novel level set topology optimization method utilizing the sparse hierarchical data structure called VDB (Volumetric Dynamic Grid), VDB-LSTO. It has been demonstrated that VDB-LSTO requires a fraction of memory and computes an order of magnitude faster relative to a conventional level set topology optimization method [2]. To the best of our knowledge, this is the first paper that investigates the expanded design space of three-dimensional nonlinear thermoelastic structures. Several numerical examples are presented to demonstrate the capability of the current methodology. The effects of mechanical and thermal loads on the optimal layouts are also discussed. Reference 1. H. Chung, O. Amir, and H. A. Kim. (2019) “Nonlinear Thermoelastic Topology Optimization with the Level-Set Method”, AIAA SciTech Conference. 2. S. Kambampati, C. Jauregui, K. Museth, and H. A. Kim. (2019) "Fast level set topology optimization using a hierarchical data structure", AIAA Aviation Forum.

15th U.S. National Congress on Computational Mechanics
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Title: A Residual Minimization Based Nonlinear Penalty Method for Positivity Preserving in Convection-Dominated Problems

Author(s): V. Calo, *Curtin Univ/CSIRO*; *R. Cier, *Curtin Univ./CSIRO*; S. Rojas, *Curtin Univ.*;

The standard (Galerkin) finite element method (FEM) delivers unphysical oscillatory discrete solutions in convection-dominated regime. We present a stabilized method to enforce weakly the positivity properties in the discrete solution in order to overcome oscillations. The method combines nonlinear penalization, based on the previous result of Burman and Ern [1], the Discontinuous Galerkin (DG) based residual minimization method stated by Calo et al. [2] and, due to the nonlinearity of the penalty term, the nonlinear Discontinuous Petrov-Galerkin (DPG) methodology proposed by Carstensen et al. [3]. The resulting method is a non-conforming DPG scheme where the test space is a discontinuous polynomial space, and the trial space is a subspace of the test space. The main advantage of the residual minimization technique is that an error estimator is obtained on-the-fly to guide adaptivity. Numerical examples are presented to illustrate the performance of the method. References: [1] Burman, E., & Ern, A. (2017). A nonlinear consistent penalty method weakly enforcing positivity in the finite element approximation of the transport equation. Computer Methods in Applied Mechanics and Engineering, 320, 122-132. [2] Calo,V., Ern, A., Muga, I. & Rojas, S. (2019). An adaptive stabilized finite element method based on residual minimization. In preparation. [3] Carstensen, C., Bringmann, P., Hellwig, F., & Wriggers, P. (2018). Nonlinear discontinuous Petrov–Galerkin methods. Numerische Mathematik, 139(3), 529-561.

15th U.S. National Congress on Computational Mechanics
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Title: Interrogation of Spline Surfaces with Application to Isogeometric Design and Analysis of Lattice-skin Structures

Author(s): Xiao Xiao, *University of Cambridge*; Malcolm Sabin, *University of Cambridge*; *Fehmi Cirak, *University of Cambridge*;

A novel surface interrogation technique is proposed to compute the intersection of curves with spline surfaces in isogeometric analysis. The intersection points are determined in one-shot without resorting to a Newton-Raphson iteration or successive refinement. Surface-curve intersection is required in a wide range of applications, including contact, immersed boundary methods and lattice-skin structures, and requires usually the solution of a system of nonlinear equations. It is assumed that the surface is given in form of a spline, such as a NURBS, T-spline or Catmull-Clark subdivision surface, and is convertible into a collection of Bezier patches. First, a hierarchical bounding volume tree is used to e■ciently identify the B´ezier patches with a convex-hull intersecting the convex-hull of a given curve segment. For ease of implementation convex-hulls are approximated with k-dops (discrete orientation polytopes). Subsequently, the intersections of the identified B´ezier patches with the curve segment are determined with a matrix-based implicit representation leading to the computation of a sequence of small singular value decompositions (SVDs). As an application of the developed interrogation technique the isogeometric design and analysis of lattice-skin structures is investigated. Although such structures have been common in large-scale civil engineering, current additive manufacturing, or 3d printing, technologies make it possible to produce up to metre size parts with designed geometric features reaching down to submillimetre scale. The skin is a spline surface that is usually created in a computer-aided design (CAD) system and the periodic lattice to be fitted consists of unit cells, each containing a small number of struts. The lattice-skin structure is generated by projecting selected lattice nodes onto the surface after determining the intersection of unit cell edges with the surface. For mechanical analysis, the skin is modelled as a Kirchhoff-Love thin-shell and the lattice as a pin-jointed truss. The two types of structures are coupled with a standard Lagrange multiplier approach.

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Title: On the Stability of Term-by-Term Stabilized Finite Element Methods for Transient Incompressible Flows

Author(s): *Ramon Codina, *Universitat Politècnica de Catalunya*;

In this talk we discuss several stability issues related to term-by-term stabilized finite element methods for incompressible flows. We consider three methods of this type, namely, the local projection stabilization (LPS), the edge stabilization (ES) and a term-by-term version of the orthogonal subgrid-scale (OSS) method, referred to as Split OSS (SOSS) method. In all three cases, two crucial terms are introduced, one aiming to stabilize the pressure interpolation and the other convective-dominated flows (a term involving the velocity divergence can also be introduced). We show that the stability structure for the three methods in the stationary case is similar: while some enhanced stability with respect to the Galerkin method is trivial to obtain, it is more elaborated to obtain stability in global norms. In fact, we show that this global stability is not obtained for the pressure gradient term and the convective term independently, but for the sum of both, exactly as for residual based stabilized finite element methods. For time dependent problems, we propose an extension of the SOSS method based on two velocity subgrid scales. We state the stability results for the new method and discuss its dissipative structure, showing some advantages with respect to classical residual based stabilization. We also explain how LPS and ES methods could be extended to time dependent problems with similar stability properties to those of the SOSS method.

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Title: Parameter Identifiability in 1D-0D Coupled Subject-Specific CFD Models of the Pulmonary Circulation

Author(s): *Mitchel Colebank, *North Carolina State University*; M. Umar Qureshi, *North Carolina State University*; Mette Olufsen, *North Carolina State University*;

One-dimensional (1D) fluid dynamics model can be used to describe network dynamics in a system of branching blood vessels. This is a promising tool for clinical diagnostics, as data cannot be measured in all of the downstream vasculature. Moreover, imaging practices have limited resolution for detecting in-vivo patient geometry, thus limiting the number of vessels captured for subject-specific modeling. To combat this, researchers will employ 0D boundary conditions, such as 3 element Windkessel models, or try to capture the downstream branching properties of the network using fractal based models, such as the structured tree model put forth by Olufsen et al. [1]. Determining the parameters that describe distal vascular resistance and compliance are especially important in the case of Pulmonary Hypertension (PH), where pulmonary vessels branch rapidly to supply blood to the lungs for oxygenation and are suspected to play the largest role in disease progression. However, a lack of data distal to the proximal arteries can lead to issues with parameter identifiability, as parameters may not be uniquely informed from the data. A 1D-0D model is employed in a subject-specific geometry of the pulmonary circulation. An identifiability analysis using both a local, covariance-based method and a global MCMC sampling based algorithm are carried out. Results show that, given the limited hemodynamic data available from PH testing, some model parameters are not uniquely identifiable. Moreover, a smaller subset of parameters is found to be more influential than others in perturbing model predictions. A reduced parameter set is introduced in order to remedy the issue of parameter identifiability. In addition, we suggest the use more developed cost functions that account for physiological properties of the pulmonary circulation. Moreover, we show that the complexity of the network used in the modeling framework affects the influence of model parameters on predictions of pulmonary arterial pressure. The results from parameter estimation indicate that specimen suspected of PH have increased proximal and distal arterial stiffness in contrast to their control counterparts. [1] Olufsen et al. Numerical simulation and experimental validation of blood flow in arteries with structured-tree outflow conditions, Ann Biomed Eng, 2000.

15th U.S. National Congress on Computational Mechanics
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Title: Output Error Estimation for Projection-Based Reduced Models

Author(s): *Gary Collins, *University of Michigan, Ph.D. Candidate*; Krzysztof Fidkowski, *University of Michigan, Associate Professor*; Carlos Cesnik, *University of Michigan, Professor*;

Projection-based model reduction techniques, such as Proper Orthogonal Decomposition (POD) and the Discrete Empirical Interpolation Method (DEIM) (Chaturantabut, 2009), have garnered interest due their potential to yield high-fidelity solutions while alleviating computational costs compared to their full-order counterparts. This characteristic becomes important when the need for rapid high-fidelity solutions outpaces our technological abilities to generate them, such as in multidisciplinary design optimization and in high-fidelity aeroservoelastic controls systems. However, the errors of these models often remain unquantified. The contribution of this work is the introduction of a method for evaluating the error of a projection-based reduced-order model via adjoint-weight residual error estimation (Fidkowski, Darmofal, 2011). The presentation will begin with the derivation of these techniques for POD and DEIM models, building on existing work in adjoint-based error estimation for variational formulations. For example, adjoint-based error estimation quantifies the error between a "coarse" and a "fine" space, e.g. coarse and fine meshes. The model reduction analogs are state representations using a varying number of basis vectors. Error estimation results are then presented for a scalar transport problem and compressible flow over an airfoil. The first is meant to verify the techniques, as for a linear problem and output the error estimation should be exact, while the second example is meant to demonstrate the error estimation technique on a nonlinear model reduction problem. Finally, we demonstrate a method for online adaptation of reduced models driven by the error estimates.

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Title: Effective Properties of Woven Composites from Image-Based Mesostructures

Author(s): *Lincoln Collins, *Sandia National Laboratories*; Scott Roberts, *Sandia National Laboratories*;

Thermal, chemical, and mechanical properties of woven composites are tied directly to their constituent materials' properties and their mesoscale arrangement. Mesoscale-resolved simulations incorporate these material arrangements and constituent material properties and upscale them to macroscopic effective behaviors. While it is convenient to study these mesoscale interactions using analytical geometric descriptions, real materials have inherent geometric non-idealities and defects (e.g. voids) that can impact material performance or lead to macroscale heterogeneities. Therefore mesoscale simulations informed by as-manufactured mesoscale material parameters are crucial for predicting as-manufactured material performance and its variability. Three-dimensional images of woven composites are obtained from both X-ray computed tomography and serial-sectioned optical microscopy. The greyscale images are segmented using both commercial tools and an in-house deep learning convolutional neural network algorithm. Segmented images are used both to inform analytical descriptions of the mesostrcture and directly for meshing. To generate computational meshes for simulations, we implement the Conformal Decomposition Finite Element Method (CDFEM) to decompose a background tetrahedral mesh into conformal material domains representing each phase present in the reconstructed and simulated three-dimensional geometries. A comparison of segmentation techniques is performed along with a quantitative comparison of experimental and simulated unit cells and effective properties. Finally, an examination of the unit-cell variability in a multi-layer sample is performed. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Title: Embedded Stabilized Methods for Free Surface Flow problems

Author(s): *Oriol Colomés, *Duke University*; Guglielmo Scovazzi, *Duke University*; Léo Nouveau, *Duke University*;

The generation of Finite Element meshes on complex geometries can be a demanding and costly task, not to mention that usually it requires the assistance or support of trained personnel. The use of embedded geometries into background (structured or unstructured) meshes is very appealing in these situations since they obviate the need for continual re-meshing in many applications involving rapid prototyping and design. Unfortunately, many finite element embedded boundary methods for incompressible flow are also difficult to implement due to the need to perform complex cell cutting operations at boundaries, and the consequences that these operations may have on the overall conditioning of the ensuing algebraic problems. We present a new, stable, and simple embedded boundary method, which we call “shifted boundary method” (SBM), that eliminates the need to perform cell cutting. Boundary conditions are imposed on a surrogate discrete boundary, lying on the interior of the true boundary interface. We then construct appropriate field extension operators, with the purpose of preserving accuracy when imposing the boundary conditions. We demonstrate the SBM applied to several free surface flow problems.

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Title: Progress on Development and Evaluation of Higher-order IMEX SSP Methods with Embedded Error Estimation: Application to Plasma Continuum Physics Models

Author(s): *Sidafa Conde, *Sandia National Laboratories*; John Shadid, *Sandia National Laboratories*;

Strong-Stability-Preserving Runge-Kutta methods (SSP-RK) are popular time-stepping schemes that are widely used for evolving the numerical solution of hyperbolic conservation laws and in particular where solutions have discontinuities or sharp gradients. Compared to standard RK methods, the methods (under appropriate conditions) offer advantages such as maintaining nonlinear stability with respect to the total variation and preserving monotonicity conditions with respect to some convex functional. In the context of more general strongly coupled balance law systems with disparate timescales, we extend the SSP theory to additive problems and construct implicit-explicit (IMEX) methods. Based on sufficient conditions for an additive method to be SSP, we formulate an optimization problem to obtain optimal SSP IMEX methods. In this work, we extend the concept of varying orders of accuracy for linear and non-linear components to the class of implicit-explicit (IMEX) Runge–Kutta methods methods. Finally, we construct efficient embedded pairs for optimal explicit, implicit, and IMEX SSP methods to be used for error control. These methods are tested on sample problems to verify order of convergence and to demonstrate the sharpness of the SSP coefficient and the typical behavior of these methods on test problems.

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Title: Fast Model Reduction for Radiation Diffusion with High-order Mixed Finite Elements

Author(s): *Dylan Copeland, *Lawrence Livermore National Laboratory*; Robert Anderson, *Lawrence Livermore National Laboratory*;

We present a projection-based model reduction for nonlinear three-dimensional multi-material radiation diffusion, discretized by high-order finite elements. Using the MFEM finite element framework, we employ a mixed finite element formulation with a discontinuous finite element subspace of L^2 for approximating material and radiation energy, and an H(div) conforming finite element space for approximating radiation flux. Implicit time integration is used, to allow for large timesteps. Solution data from the full finite element approximation is used to train or construct a small proper orthogonal decomposition basis via singular value decomposition. Using reduced bases results in a much smaller system of nonlinear ODE's, and the nonlinear terms are hyper-reduced by the DEIM or GNAT methods for sparse sampling. Numerical experiments will be presented to examine the effect of the order of the finite element approximation, sampling strategy, and hyper-reduction strategies on the accuracy and robustness of the reduced model. Prepared by LLNL under Contract DE-AC52-07NA27344.

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Title: Using FEniCS for Simulating the Nonlocal Cahn-Hiiliard Equation with Spatio-Temporal Adaptivity

Author(s): Gabriel Barros, *COPPE/Federal University of Rio de Janeiro*; Adriano Cortes, *Federal University of Rio de Janeiro*; *Alvaro Coutinho, *COPPE/Federal University of Rio de Janeiro*;

In this work, we propose a spatio-temporal adaptivity scheme for the nonlocal Cahn-Hilliard equation with the Ohta-Kawasaki model. The standard splitting strategy available in FEniCs is used, where the fourth-order system is recast into a two second-order coupled nonlinear system of equations. The spatial adaptivity scheme consists of a flux-jump indicator driving the bissection method for refinement, while the temporal adaptivity scheme is recast under the linear feedback control theory. We consider an error estimation in time that extrapolates the solution obtained from an energy-stable time marching scheme, and three time step controllers: a simple integral controller, a complete Proportional-Integral-Derivative controller, and the predictive controller known as PC11. We assess the performance of the adaptive schemes for local and nonlocal Cahn-Hilliard equations, simulating different physics and time scales. We observe that the coupled space-time adaptive scheme is useful for the Cahn-Hilliard equations with constant and degenerated mobility. For the nonlocal Cahn-Hilliard equations, the time adaptivity scheme is always beneficial, while the performance of the coupled space-time adaptivity scheme depends on the parameters of the Ohta-Kawasaki model.

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Title: FFT-based Micromechanical Modelling of Precipitated SMAs

Author(s): *Aitor Cruzado, *Texas A&M University*; Jobin Joy, *Texas A&M University*; Alexandros Solomou, *Texas A&M University*; Amine Benzerga, *Texas A&M University*; Dimitris Lagoudas, *Texas A&M University*;

Precipitation in Shape Memory Alloys (SMAs), such as Ni-rich NiTi and NiTiHf, plays an important role in the actuation characteristics of the reversible martensitic transformation, including hysteresis and actuation strain. A better understanding of precipitation in the actuation response of SMAs would benefit from the development of microstructure-based computational homogenization models. A full-field Fast Fourier Transform (FFT) based micromechanical model is used in the current work. The approach is based on a recently developed variational FFT formulation, adapted to the non-linear and hysteretic thermomechanical constitutive response of SMAs. Comparison with finite element approaches has been carried out, and the efficiency of this methodology is discussed, especially for cases where periodic boundary conditions are justified. Microstructure-based models, however, require the definition of a representative volume element (RVE) of the material with the appropriate number of precipitates. The RVE needs to be sufficiently large to capture accurately the effective non-linear behavior. An extensive study is conducted to analyze appropriate RVE size ranges with respect to changes in the volume fraction, number and shape of precipitates. Statistical relations that describe the minimum number of realizations for a given RVE size and variance in the expected effective response are provided. This FFT-based full-field virtual testing approach is a step towards efficient design of SMAs, especially in cases where uncertainty quantification requires a large number of parametric studies.

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Title: The Mechanical Principles behind the Golden Ratio Distribution of Veins in Plant Leaves

Author(s): *Tianchen Cui, *State Key Laboratory of Structural Analysis for Industrial Equipment Department of Engineering Mechanics, Dalian University of Technology, Dalian, 116023, P.R. China.*; Zhi Sun, *State Key Laboratory of Structural Analysis for Industrial Equipment Department of Engineering Mechanics, Dalian University of Technology, Dalian, 116023, P.R. China.*; Guo Xu, *State Key Laboratory of Structural Analysis for Industrial Equipment Department of Engineering Mechanics, Dalian University of Technology, Dalian, 116023, P.R. China.*;

Tree leaves are commonly composed of thin mesophyll, carrying out photosynthesis under sunlight, and thick veins. Although the role of leaf veins in water transportation has been known for a long time, their role in providing structural support and guaranteeing large sunlighted area was rarely studied and remains elusive. Here, with use of a novel inverse optimization approach, we aim for uncovering the material design principle behind the unique pattern of venation. It is intriguing to observe that an almost Golden Ratio (GR) distribution of leaf veins always provides optimized structural behavior. Specifically, our research reveals, for the first time, that this unique GR distribution of relatively strong vein material is helpful for maximizing the bending stiffness and leading to a large sunlighted area which is vital for the photosynthesis process of a leaf. Moreover, the GR distribution of leaf veins is also observed in a wide class of plant leaf geometries (i.e., shape, thickness), where experimental evidence is provided for the optimized results. Therefore, our findings can not only serve to explain the mystery of veins GR distribution but also provide widely applicable guidelines on designing soft structures with exceptional mechanical performances.

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Title: New Development of Entropy Stable Solid Wall Boundary Conditions for the Compressible Navier-Stokes Equations

Author(s): *Lisandro Dalcin, *King Abdullah University of Science and Technology*; Matteo Parsani, *King Abdullah University of Science and Technology*;

We present a novel technique for the imposition of non-linear entropy conservative and entropy stable solid wall boundary conditions for the compressible Navier–Stokes equations in the presence of a wall with a prescribed heat entropy flow. The procedure relies on the formalism and on the mimetic properties of diagonal norm, summation-by-parts and simultaneous- approximation-term operators. Discontinuous spectral collocation operators on high-order unstructured grids are used for the purpose of demonstrating the robustness and accuracy of the new boundary conditions. Simulations confirm the non-linear stability and the reliability of the proposed techniques, with applications to three-dimensional subsonic and supersonic flows.

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Title: A Computational Damage Sensor Using Electromechanically Coupled Piezoelectric Materials

Author(s): *Saikat Dan, *Graduate Student, Johns Hopkins University*; Preetam Tarafder, *Graduate Student, Johns Hopkins University*; Somnath Ghosh, *Michael G Callas Chair Professor, Johns Hopkins University*;

Piezoelectric actuators and sensors are widely used in structural health monitoring applications. In this paper, a nondestructive computational damage sensor is developed using piezoelectric materials. On applying mechanical loads to a structure, an irreversible damage field evolves in the domain. The evolving damage affects the mechanical constitutive laws. The change in the mechanical constitutive parameters due to the evolving mechanical damage affects the electrical response of the structure. Therefore, the electromechanical coupling allows the damage in the structure to be indirectly sensed and quantified using the evolving electrical fields. This work requires the development of multiphysics analysis tools for solving the coupled mechanical and electrical fields and predict their evolution in a finite deformation regime. The computation of the electrical and mechanical fields requires solutions to Maxwell's equations and the equations of mechanical equilibrium respectively. In case of solids, the former is classically formulated in a Eulerian framework while the latter is formulated in a Lagrangian framework. In this paper, a Lagrangian approach has been considered for both the fields [1]. A coupled free–energy form has been used to obtain the constitutive law. A neo–Hookean material model has been considered for the mechanical fields. A thermodynamically consistent damage model [2] has been used for which the evolution is dependent only on the mechanical fields. Linear coupling between the electrical and mechanical fields have been used. Also, a linear constitutive model for the electrical fields has been considered. The evolving damage affects the subsequent mechanical constitutive parameters, which in turn affects the evolving electrical fields. Measurement of the evolving electrical fields provides a sense of the state of damage in the structure. Therefore, this work can quantify the damage in the structure by measuring the distribution of the electrical fields within the domain. Finally, this work establishes the use of piezoelectric materials not only in damage sensing but also in its quantification. The efficient and consistent computational framework and nondestructive damage quantification is the most important aspect in this work. References 1. R. Yaghmaie and S. Ghosh, "Computational modeling of finite deformation piezoelectric material behavior coupling transient electrical and mechanical fields", Comp. Physics, Vol. 373, pp. 148 – 170, November 2018 2. X. Zhang, D. J. O'Brien and S. Ghosh, "Parametrically homogenized continuum damage mechanics (PHCDM) models for composites from micromechanical analysis", Comp. Meth. in App. Mech & Engg, Vol. 346, pp. 456 – 485, April 2019

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Title: Evaluation of Higher-Order Finite Element Formulations for Lumped-Mass Explicit Modeling

Author(s): *Kent Danielson, *U.S. Army Engineer Research and Development Center*; Robert Browning, *U.S. Army Engineer Research and Development Center*;

This presentation discusses some observations of higher-order finite elements for lumped-mass explicit approaches typically needed for high-rate modeling. Various recent efforts have demonstrated the benefits of 2nd order, as well as higher orders, for intricate lumped-mass explicit simulations. The U.S. Army Engineer Research and Development Center (ERDC) developments are included in ERDC Geotechnical and Structures Laboratory's in-house meshing tools (ProMesher and PRefine), parallel FEA code (ParaAble), and visualization software (PenView), as well as implemented into popular production meshing (Cubit), parallel analysis (EPIC), and visualization (ParaView) software; similar capabilities have also appeared in so-called "Spectral-Element" and in commercial finite element software for various classes of applications. This presentation discusses subtle but important details for a range of applications from linear wave propagation to complex highly- nonlinear problems. Topics include formulations for varying element type (tetrahedral, wedge, hexahedral, and pyramid), mass lumping, numerical quadrature, nearly incompressible materials, superconvergence and variable extraction, optimal nodal spacing, and efficient explicit time solution methods. Acknowledgments: Permission to publish was granted by Director, Geotechnical and Structures Laboratory.

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Title: Linear Stability Analysis of Bilayer Wrinkling in an Infinite-Sized Homogeneous Matrix

Author(s): *Mohsen Darayi, *University of Notre dame*; Jérôme Colin, *University of Poitiers*; Maria Holland, *University of Notre dame*;

The understanding of mechanics of wrinkling in elastic materials under external loading is essential in various biological and engineering systems, with examples ranging from brain morphology to stretchable electronics and composite materials. In this study, a linear stability analysis is presented for the wrinkling of two identical layers embedded in a homogeneous matrix under compression [1]. Both layers are incompressible neo-Hookean elastic materials. We applied the variational method to minimize the free energy functional for the two-dimensional plane strain model and obtain the equations for the eigenvalue problem [2]. By means of Ridder's bracketing method, we numerically solved the governing equations for the various distances between layers and shear moduli ratio to consider the effects of stiffness ratio and layer spacing on wrinkling. The combined influences of shear moduli and layer spacing on wrinkling configurations, critical strain, and critical wavelength are observed. The investigation demonstrates that the stiffness ratio between layers and the matrix is the dominant influence on the instability of the system. For softer layers, layer spacing along with the stiffness ratio affects the unstable state of the multilayer system. On the other hand, in stiffer layers, stiffness contrast influences stability more than spacing. We identified a discontinuity in threshold wavelength when layers are softer than the matrix, at certain layer spacing. Symmetric and antisymmetric modes have been taken into account. The results indicate when the distance between layers is small, the symmetric mode dominates, while large spacing could lead to either symmetric or antisymmetric configurations. [1] J. M. Colin, M. Darayi, and M. Holland, "Stiffness contrast and separation influence wrinkling of adjacent layers in a homogeneous matrix," J. Appl. Mech., Jan. 2019. [2] J. Colin and M. A. Holland, "Layer wrinkling in an inhomogeneous matrix," Int. J. Solids Struct., vol. 156–157, pp. 119–125, Jan. 2019.

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Title: Physics Informed Machine Learning

Author(s): Kailai Xu, *Stanford*; *Eric Darve, *Stanford*; Daniel Huang, *Stanford*;

Machine learning is opening new avenues for predictive computer modeling in science and engineering. In this work, rather than developing a purely data-driven method, we propose an approach that uses DNNs to model unknown parameters (in particular functions) in PDEs, such as constitutive models, and couples the output of the DNN with mathematical models and PDE numerical solvers. Instead of directly fitting the DNN parameters using observed input/output pairs such as x -> u(x) for position and displacement, we instead minimize the "downstream" PDE residual. For example, consider a general PDE for a mechanical system of the form L(u(x),M(x,u(x))) = F(x,u(x)), where F is an external force or load, and M is an unknown constitutive law or homogenized model. The DNN, parameterized by theta, is used to represent the mapping (x,u) -> M(x,u(x); theta). However, we do not directly observe (in the training set) the output of the DNN. Instead, the PDE is considered in its discretized form (for example after a finite-element analysis) such as P(u,M(x,u;theta)) = F(x,u(x)). We assume that we are given pairs (ui,Fi) of displacements and forces. The DNN parameters are then chosen to minimize |P(u_i,M(x,u_i; theta)) - F(x,u_i)|^2, over all the observations i. This approach greatly expands the applicability of DNN techniques. It allows using DNNs in different parts of a complex modeling workflow (based on mathematical models and numerical discretization schemes) and tuning the DNN parameters based on the output of the workflow only. These techniques open new avenues in designing complex constitutive laws, homogenized models, and upscaling strategies. We will also present extensions of these ideas to uncertainty quantification. An important practical ingredient is that we use the automatic differentiation capabilities of TensorFlow, and the language Julia with its multiple dispatch and operator overloading capabilities to simplify the code development. This approach allows re-using a nearly unmodified FEM code and interfacing it seamlessly with TensorFlow using thin Julia wrappers. Thanks to our framework, relatively minimal new programming effort is required. We will demonstrate applications of these approaches to various mechanical models, including homogenized fiber reinforced models and rubber membrane models.

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Title: Large Scale Orbital-free DFT and Kohn-Sham DFT Calculations of Dislocation Energetics in Al-Mg Materials System and Their Connection to Mesoscale Models

Author(s): *Sambit Das, *University of Michigan*; Phani Motamarri, *University of Michigan*; Vikram Gavini, *University of Michigan*;

We study the dislocation core in Aluminum and Magnesium using real-space formulations of orbital-free DFT and Kohn-Sham DFT, implemented using finite-element discretization [1, 3]. In the first part of this work, we use orbital-free DFT, where the local real-space formulation coupled with bulk Dirichlet boundary conditions enables us to directly obtain the isolated dislocation core energy. Our studies on dislocations in Aluminum [2], and Magnesium, suggest that the core size—region with significant contribution of electronic effects to dislocation energetics—is around seven to ten times the magnitude of the Burgers vector. This is in stark contrast to estimates based on atomic displacements. Interestingly, our study further indicates that the core-energy of the dislocations are strongly dependent on external macroscopic strains. Next, we use this to develop a continuum energetics model for discrete dislocation networks [2], which accounts for the core energy dependence on macroscopic deformations. The variations of the core energy with respect to the nodal positions of the network results in a nodal core force, which can directly be incorporated into discrete dislocation dynamics (DDD) frameworks. The nodal core force contributions are currently not accounted for in commonly used DDD models. Using case studies of static dislocation-dislocation interactions, we demonstrate that core forces can be significant in comparison to the elastic Peach-Koehler force even up to distances of 10-15 nm between dislocations. Furthermore, we have incorporated the core force into a DDD implementation, and demonstrate the influence of core effects on elementary dislocation mechanisms in Aluminum such as structure and strength of dislocation junctions and critical stress of a Frank-Read source. Finally, in the second part of this work, we use the more quantitatively accurate Kohn-Sham DFT to study dislocation core energetics of <c+a> screw dislocations in Magnesium, and show initial results which involve large system sizes (5,000-10,000 atoms). [1] Das, S., Iyer, M, and Gavini, V., 2015, Real-space formulation of orbital-free density functional theory using finite-element discretization: The case for Al, Mg, and Al-Mg intermetallics, Phys. Rev. B 92, 014104. [2] Das, S., and Gavini, V., 2017, Electronic-structure study of a screw dislocation in Aluminum and the role of macroscopic deformations on its energetics, J. Mech. Phys. Solids 104, 115-143. [3] DFT-FE: https://github.com/dftfeDevelopers/dftfe — parallel adaptive finite-element code for material modeling using density functional theory.

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Title: Effective Temperature Based Constitutive Theories for Thermoplastics and Thermoplastic Elastomers

Author(s): *Sanhita Das, *Indian Institute of Science, Bangalore, India*; Debasish Roy, *Indian Institute of Science, Bangalore, India*;

Understanding and modelling viscoelastic deformation of amorphous polymers has been of immense interest to researchers both from scientific and industrial standpoints. Predictive models are required for efficient design of polymers under extreme environmental and loading conditions. We thus propose a unified, thermodynamically consistent, visco-elastic approach for the two widely used varieties of polymers, thermo-rheologically simple thermoplastics (homopolymers) and complex thermoplastic elastomers (copolymers). These models aim at reproducing the fundamental features of mechanical behaviour over a wide range of temperatures and strain rates across glass transition. The models draw upon micro-mechanical perspectives that take into account the intra-molecular processes of chain straightening and inter-molecular processes of localised segmental rotations. The modelling of structural relaxation is facilitated through the use of an effective temperature framework that bridges the widely separated time scales involved in the underlying micro-mechanisms. In general, we split the thermodynamic system into a kinetic-vibration (K-V) subsystem and one or more configurational sub-systems and define separate thermodynamic states (energies, entropies, temperatures and internal variables) for each subsystem. This is followed by the exploitation of the laws of thermodynamics to establish thermodynamic restrictions on the forces and the fluxes. By implementing free energies (specific to the polymer) in the constitutive forms, we define the constitutive relations for stresses and evolution equations for temperatures and internal variables explicitly. The multi-temperature framework assumes a weak interaction between each configurational subsystem and the K-V subsystem, which forms the basis of structural relaxation. For homopolymers, we define a single configurational subsystem as it proves adequate to model the single relaxation process occurring in the material. For copolymers, on the other hand, we define two configurational subsystems to model multiple relaxation mechanisms associated with the thermodynamically incompatible hard and soft phases. Both the models are validated against uniaxial compression experiments for a wide range of temperatures and strain rates. They predict the intrinsic behaviour with accuracy and also capture physical ageing. The copolymer model, in addition predicts Mullin’s softening and shape-memory effects too. Not only do our formulations provide correct predictions, but they are far more generic as they are micro-mechanically motivated. The formulation for the co-polymer does not pose any restriction on the regimes of the constituent phases, hence may be suitably modified for other two-phase polymeric systems. Our formulation utilises some crucial material parameters like the volume fraction, which makes our formulation suitable for microstructural design optimisation.

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Title: Development of a Moving Window Molecular Dynamics Framework to Model Shock Wave Interactions at Microstructural Features in Materials

Author(s): *Alexander Davis, *Auburn University*; Vinamra Agrawal, *Auburn University*;

In this work, we develop a long-time, large-domain moving window Molecular Dynamics (MD) framework to model shock wave interactions at microstructural features in materials such as grain boundaries. Research on shock wave propagation from an atomic point of view has been minimal largely because of the transient effects due to small domain sizes. To circumvent these problems, we implement ideas of control volume on a MD framework where a moving window follows a propagating shock. By tracking an individual shock wave, we simplify the problem significantly which allows us to model a shock wave's encounter with a microstructural feature. As a first step, we create a one-dimensional version of this MD moving window framework. We model wave development in a one-dimensional chain of atoms for various FCC materials as well as compare the behavior of these atoms subject to different potential functions such as Lennard-Jones and Embedded Atom Model (EAM). We validate the framework by computing the elastic modulus of the system and comparing such values with those found in literature. Then, we perform shock simulations and build the moving window structure using the one-dimensional framework. We achieve this by splitting the chain into three sections composed of copper atoms. The two outer thermostat regions represent the continuum states in front of and behind the shock wave front and incorporate a Langevin (Brownian) thermostat. The inner true dynamics region, containing the shock wave, consists of atoms where the classic MD equations are solved using the velocity Verlet algorithm. We implement the moving window by adding or removing atoms from the boundaries to the window after the shock has traveled a distance of one lattice constant. Then, we modify the parameters of the atomic chain until the shock front maintains its position at the center of the middle section throughout the simulation. To validate the moving window formulation, we compare the steady speed from our MD simulations with experimental values. Additionally, we compute the coefficients of the linear shock equation and compare these with values found in literature. Our next immediate step will be to use this framework to study shock scattering and microstructural changes upon a shock's interaction with an interface. In the future, we will expand this system to higher dimensions to capture how such phenomena would behave in the natural world. Understanding such microstructural interactions will lead to improved energy dissipation mechanisms for application in ballistics and detonations.

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Title: Using preCICE to Perform Multi-Physics Simluations

Author(s): *Kyle Davis, *University of Stuttgart*; Miriam Mehl, *University of Stuttgart*; Klaudius Scheufele, *University of Stuttgart*; Benjamin Uekermann, *Technical University of Munich*;

Fluid-structure interaction (FSI) simulations are able to provide invaluable information regarding complex multi-physics problems. However they still suffer from a multitude of issues, from the internal coupling numeric efficiency, to the usability by the end user. To solve these problems, preCICE was developed as a black-box, multi-physics coupler that has successfully been used to couple a variety of solvers for a wide range of problems. By utilizing the black-box approach, preCICE is able to perform mesh mapping, simulation coupling and control. A number of user specified settings is required by preCICE to perform the solver coupling. These settings may have a large effect on the efficiency and stability of the simulation coupling. Therefore, sophisticated and robust iterative methods for implicit coupling have been implemented in preCICE to improve stability, and lessen the impact that user specifications have on the coupling performance. The preCICE work group also provides active support to the FSI community by providing a wide range of ready-to-use adapters for many different solvers, allowing easy change of combinations of various solvers. This talk will discuss some of the main features of preCICE, including current mapping techniques and post-processing methods implemented in preCICE. A number of test cases will be presented to show the ease of use of preCICE to implement any combination of solvers in a black-box fashion. The test cases will cover a number of examples, including conjugate heat transfer (CHT) of heat exchangers and mechanical FSI of heart valves. The impact of the choice of input settings will be discussed and results showing best practices for input setting selection. Future work in preCICE will include further increasing the computational efficiency and usability of preCICE, mainly through auto-tuning methods for input settings and further best practices for FSI simulations with preCICE.

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Title: Vectorization of Discontinuous Galerkin Schemes for Shallow Water Flows

Author(s): *Clint Dawson, *University of Texas at Austin*; Maximilian Bremer, *University of Texas at Austin*;

Widening SIMD vector lengths, achieving a high degree of high degree of vectorization is increasingly important for optimizing compute resource utilization. In this talk we will outline efforts to vectorize dgswemv2, a discontinuous Galerkin finite element code for costal flows. In particular, we will emphasize programming abstractions that have allowed us to maintain readability of the code base while still achieving a high degree of vectorization. Detailed profiling results including roofline analyses will be presented on TACC's Stampede2.

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Title: Optimization under Uncertainty Using Stochastic Gradients

Author(s): *Subhayan De, *University of Colorado, Boulder*; Alireza Doostan, *University of Colorado, Boulder*; Kurt Maute, *University of Colorado, Boulder*;

Robust design of engineering structures requires the inclusion of uncertainties in the design process. A Monte Carlo approach based on random sampling in such cases, however, needs many forward and adjoint solves thus requiring significant computational resources. To reduce this computational burden, we employ stochastic gradient descent algorithms, where we approximate the design sensitivities using only a few random samples of the gradients at every optimization iteration. In practical engineering settings, often models with different levels of fidelity are used to describe the problem at hand. Lower-fidelity models (e.g., using coarser grid discretizations) can be simulated cheaply but may lead to inaccurate solutions relative to high-fidelity models (e.g., using fine grid discretizations) that are often expensive to simulate. To reduce the design optimization cost further, we incorporate these low-fidelity models in the optimization and propose bi-fidelity versions of stochastic gradient descent algorithms, e.g., stochastic average gradient descent (SAG), and stochastic variance reduced gradient descent (SVRG). We illustrate these approaches using numerical examples from shape and topology optimizations. These examples show that the use of stochastic gradients with bi-fidelity approaches can reduce the computational cost of design optimization under uncertainty significantly.

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Title: Stress-based Topology Optimization Formulation for Multi Material Problems Using a Normal Distribution Approach

Author(s): *Daniel M. De Leon, *UFRGS*; César Kiyono, *USP*; Emilio Carlos Nelli Silva, *USP*;

In this work, a stress-based topology optimization formulation is developed aiming to design structures composed of several materials. A normal distribution function is applied to deal with the optimum selection of material in the domain. A continuation scheme is applied to the functions to obtain discrete optimized designs. The goal of using a normal distribution function is to allow the algorithm to easily handle different materials properties without the need of creating several design variables. The optimization formulation is written such that each material is insured not overcome a given strength criterion. In order to catch the points where the mechanical failure is more suitable, a multi-p-norm is proposed to approximate the stress field. The advantages of using several penalization exponents to evaluate the p-norm are that the algorithm can make use of the stability provided by low coefficients for the norm and a smoother stress distribution when using larger penalization coefficients. By computing these stress points, safety factors are calculated to ensure the mechanical integrity in each material that makes part of the structure. A multi objective problem is solved out using the safety factor approach as a constraint. The Global Convergent Method of Moving Asymptotes (GCMMA) is used as the mathematical solver for the optimization problem. The proposed methodology shows that the optimization problem successfully produces designs with an efficient material distribution and structural integrity.

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Title: Resolving Immersed Thin Walls Using Discontinuous Shape Functions

Author(s): *Facundo Del Pin, *Livermore Software Technology Corporation*; Iñaki Çaldichoury, *Livermore Software Technology Corporation*; Rodrigo Paz, *Livermore Software Technology Corporation*; Chien-Jung Huang, *Livermore Software Technology Corporation*;

The pre-processing of complex geometries exported from CAD programs is a big challenge in the Finite Element analysis of fluid problems. There are many situations where a detailed high quality mesh is preferred and possible mandatory. Such is the case for problems where shear stresses are an important component of the total force, i.e. ground vehicle aerodynamics, aircraft drag prediction and some bio-mechanics applications where the stresses in the endothelium are need to predict the development of some diseases. There are many other applications though where pressure forces are enough in terms of accuracy or where rapid prototyping of engineering parts do not need the accuracy required in the final stages of engineering design. In these cases the geometry could be simplified by approximating the domain walls immersing them inside a much simpler domain. This simplification becomes even more appealing in the presence of an internal structure that interacts with the fluid which in many engineering applications are modeled as thin shell structures. In the current work the sub-element interfaces of the geometry will be approximated by level set distance functions. The walls could be part of a flexible structure or they could be rigid and they may be "wet" on both sides. The pressure discontinuity across the wall (in the case of shell structural elements) will be approximated by discontinuous shape functions as described in [1]. One of the main advantages of this approach is that it is easily adapted to an existing solver since no additional degrees of freedom need to be added. The presentation will include details of the additions that the existing solver needed such as: 1) boundary recognition; 2) level set representation; 3) sub-element splitting; 4) computation of the new interpolation functions and integration; 5) assembly and solution. [1] R.F. Ausas, F.S. Sousa, G.C. Buscaglia, An improved finite element space for discontinuous pressures, Comput. Methods Appl. Mech. Engrg. (2009), doi: 10.1016/j.cma.2009.11.011

15th U.S. National Congress on Computational Mechanics
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Title: Progress Towards Conservative and Stable Overset Methods

Author(s): Joseph Derlaga, *NASA LaRC*; *David Del Rey Fernández, *NASA LaRC and NIA*; Mark Carpenter, *NASA LaRC*;

Solving the compressible Navier-Stokes equations for external aerodynamics on complex moving/deforming geometries on high-performance computing architectures necessitates robust numerical methods. One approach to deal with complex moving/deforming geometries that has received sustained development at NASA and is widely used both in industry and academia is the overset method (e.g. overflow). In this approach, geometric complexity and moving components are elegantly handled by attaching body-fitted meshes to individual components. This has the dual benefit of simplifying meshing difficulties and resulting in high-quality near-body meshes. However, overset approaches can suffer from robustness issues and lack of strict discrete conservation. Conversely, The summation-by-parts (SBP) framework (see Refs. [1,2]) is advantageous in the construction of discrete schemes as it leads to conservative methods of arbitrary high-order that are provably linearly or non-linearly stable. While there are a number of ways of extending the SBP concept to overset technologies, our goal is to develop design-order perturbations to the base overflow software stack in a minimally invasive manner. The idea is to retain as much of the original code and hence operability as possible. In this talk, we cover progress towards attaining this goal. [1] David C. Del Rey Fernández, Jason E. Hicken, and David W. Zingg, “Review of Summation-by-Parts Operators with Simultaneous Approximation Terms for the Numerical Solution of Partial Differential Equations”, Computers & Fluids, Vol. 95, No. 22, 2014, pp. 171-196. [2] Magnus Svärd and Jan Nordström, “Review of summation-by-parts schemes for initial-boundary-value-problems”, Journal of Computational Physics, Vol.268, No.1, 2014, pp.1738.

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Title: Topology Optimization of Frequency Response Functions Using Moment Matching

Author(s): *Arnoud Delissen, *Delft University of Technology, Department of Precision and Microsystems Engineering*; Reinaldo Astudillo, *Delft University of Technology, Department of Numerical Analysis*; Fred van Keulen, *Delft University of Technology, Department of Precision and Microsystems Engineering*; Martin van Gijzen, *Delft University of Technology, Department of Numerical Analysis*; Matthijs Langelaar, *Delft University of Technology, Department of Precision and Microsystems Engineering*;

The dynamical structural performance of devices and components in terms of linear frequency-dependent input-output behavior, is expressed by frequency response functions (FRFs). Topology optimization for a FRF usually requires many linear solves of a finite element model per design iteration (e.g. minimizing the dynamic compliance in a range of frequencies requires two linear solves per frequency in every design iteration). To keep the computation time low, a reduced model can be constructed in every design iteration which is used to approximate the FRF at many different frequencies. The eigenmodes are often used as reduction basis inside the topology optimization process [1]. However, eigenmodes are relatively expensive to calculate compared to linear solves and poor accuracy can be expected when insufficient higher modes are included for frequency response type of problems. Additionally, the reduced model should not only maintain accuracy for the response function, but also for the design sensitivities which require an additional adjoint solve [2]. Up to now, only Galerkin projections have been used in topology optimization, which do not provide accurate sensitivity information. In this contribution, we propose the use of moment matching for topology optimization of FRFs. Moment matching is an existing method, which is able to create a comparatively cheap rational interpolation of the FRF by using Krylov methods as described in [3]. It works by applying a Petrov-Galerkin projection using basis vectors which are calculated using the two-sided Arnoldi algorithm, also described in [3]. The basis contains information to solve both the response and adjoint problems for the sensitivities with high accuracy, since the Krylov vectors are based on both the input (response) and output (adjoint) of the system. Using test cases, we compare computational effort and convergence between the full model, model reduction with eigenvectors, and model reduction with moment matching, while varying the number of basis vectors. These tests demonstrate the effectiveness of the reduced model based on moment matching in topology optimization of FRFs. References [1] H. Liu, W. Zhang, and T. Gao. A comparative study of dynamic analysis methods for structural topology optimization under harmonic force excitations. Structural and Multidisciplinary Optimization, 51(6):1321{1333, jun 2015. [2] G. H. Yoon. Structural topology optimization for frequency response problem using model reduction schemes. Computer Methods in Applied Mechanics and Engineering, 199(25-28):1744{1763, may 2010. [3] A. C. Antoulas. Approximation of Large-Scale Dynamical Systems. SIAM Advances in Design and Control, 2005.

15th U.S. National Congress on Computational Mechanics
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Title: The Double Adaptivity Paradigm or How to Circumvent Discrete inf-sup Conditions of Babuska and Brezzi

Author(s): *Leszek Demkowicz, *Oden Institute*; Thomas Fuehrer, *Pontificia Universidad Catolica de Chile*; Norbert Heuer, *Pontificia Universidad Catolica de Chile*; Xiaochuan Tan, *UT-Austin*;

In the mixed formulation of the ideal Petrov-Galerkin method with optimal test functions, one solves for an approximate solution coming from a discrete trial space, along with the Riesz representation of the corresponding residual coming from the exact test space. The residual provides an ideal a-posteriori error estimate providing a basis for adaptive refinements of trial space. This is the outer adaptivity loop. To arrive at a practical method, we need to approximate somehow the residual. In the standard DPG method this is done by employing a sufficiently large discrete (enriched) test subspace of the test space. For (benign) single scale problems, this can be done by implementing elements of higher (enriched) order and constructing appropriate Fortin operators to assess the lost of stability due to the approximation of the exact residual. The situation is quite different for singular perturbation problems where one strives for the robustness, i.e. uniform stability with respect to the perturbation parameter. Alternatively, with the given approximate trial space, one can solve for the approximate residual ADAPTIVELY. This is the inner adaptivity loop. For singular perturbation problems the challenge comes from the need for a ROBUST a-posteriori error estimation technique. We propose an inner adaptivity loop built upon the classical duality theory and a-posteriori error estimation based on duality gap estimate (the classical hypercircle methodology). The methodology will be illustrated with a convection-dominated diffusion (``confusion'') problem. The double adaptivity algorithm delivers solutions for the diffusion constant epsilon = 10^-7 in a fully automatic mode. The adapted trial meshes with the corresponding adaptively obtained test meshes do NOT satisfy the robust inf-sup condition.

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Title: Topology Optimization for Nonlinear Metamaterials Design with Bezier-based Density Representation Algorithm

Author(s): *Hao Deng, *University of Pittsburgh*; Albert To, *University of Pittsburgh*;

Motivated by key advances in manufacturing techniques, the tailoring of materials to achieve novel properties such as stretchability or dissipation properties has been the focus of active research in engineering and materials science over the past decade. The goal of metamaterial design is to determine the optimal spatial layout to achieve a desired macroscopic constitutive response. However, the manufacturing abilities are the key factors to constrain the feasible design space, e.g. minimum length and geometry complexity. From the mathematical view, resolving above problems is equivalent to find an appropriate density field representation methodology to take the place of traditional density-based method. Traditional density-based method, where each element works as a variable, always results in complicated geometry with large number of small intricate features, while these small features are unfavorable for manufacture and lose its geometric accuracy after post-processing. To address above challenges, a new density field representation technique, named as Bezier-based explicit geometric representation scheme is proposed at the first time, where density field is described by Bezier-based Heaviside function. Bezier curves are widely used in computer graphics to produce curves which appear reasonably smooth at all scales. Compared to NURBS or B-spline, Bezier curves have less control parameters and easier to handle for sensitivities derivation, especially for distance sensitivities. Due to the powerful curve fitting ability, using Bezier curve to represent density field can explore design space effectively, and generate graceful structures without any intricate small features at borders. Furthermore, this density representation method is mesh independent and design variables are reduced significantly so that optimization problem can be solved efficiently using small-scale optimization algorithm, e.g. sequential quadratic programming. To demonstrate the powerful ability in design metamaterial of proposed density representation algorithm, two different metamaterial designs is presented, one design is to tailor material to present super stretchability under large deformation with fully recoverable properties. The other design is to optimize buckling-induced energy dissipation metamaterials to achieve desired energy dissipation capacity.

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Title: High-order Generalized-α Method

Author(s): *Quanling Deng, *Curtin University*; Pouria Behnoudfar, *Curtin University*; Victor Calo, *Curtin University and CSIRO*;

The generalized-α method generalizes a wide range of time integrators including the Newmark method, the HHT-α method by Hilber, Hughes, and Taylor, the WBZ-α method by Wood, Bossak, and Zienkiewicz. The method possesses high-frequency dissipation while minimizing unwanted low-frequency dissipation and the numerical dissipation can be controlled by the user. The method is unconditionally stable and is of second-order accuracy in time. We generalize the second-order generalized-α method to third-order accuracy in time while the numerical dissipation can be controlled in a similar fashion. We establish that the third-order method is unconditionally stable. Generalization to higher order scheme is presented. The high-order schemes can be easily implemented into programs that contain the generalized-α method.

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Title: Quantifying Fibrinogen-induced Aggregation of Red Blood Cells in Type 2 Diabetes Mellitus

Author(s): *Yixiang Deng, *School of Engineering and Division of Applied Mathematics, Brown University*; Xuejin Li, *Department of Engineering Mechanics & Center for Soft Matter Science, Zhejiang University*; Ming Dao, *Department of Materials Science and Engineering, Massachusetts Institute of Technology*; Dimitrios Papageorgiou, *Department of Materials Science and Engineering, Massachusetts Institute of Technology*; Nikolaos Perakakis, *Beth Israel Deaconess Medical Center*; George Karniadakis, *Division of Applied Mathematics, Brown University*;

Plasma proteins such as fibrinogen induce the aggregation of red blood cells (RBCs) into rouleaux, which is a normally occurring phenomenon and has a major impact on blood rheology and hemodynamics, especially in pathological conditions including type 2 diabetes mellitus (T2DM). Using a multiscale RBC model with parameters derived from patient-specific data, we present a mesoscopic computational study of the aggregation characteristics of T2DM RBCs under flow conditions mimicking those in post-capillary venules. We first calibrate our model at the level of RBC doublets for patients with metabolic syndrome, treated as healthy group, through matching the disaggregation force required to rupture RBC doublets with selected experimental measurements using atomic force microscopy and optical tweezers. Informed by microfluidic experiments that provide in vitro quantitative information on cell-cell aggregation dynamics, we then quantify the aggregation strength of T2DM RBCs at both the doublet and multiplet levels, through the investigation of the effect of cell alignments in triggering the breakup events. These findings may aid in the understanding of the complex dynamics of multicellular aggregation and disaggregation in arterioles and capillaries.

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Title: An AI-guided Design Space Exploration Technique to Determine Lithology-optimized Drill Bit Geometry for Oil and Gas Recovery

Author(s): *Prathamesh Desai, *Rice University*; Nicholas Wolf, *Rice University*; Joshua Wagner, *Rice University*; C. Fred Higgs III, *Rice University*;

In oil and gas extraction, the rock drilling step consumes approximately half of the entire process time. There is a constant thrust to improve the efficiency of this step. Traditionally, rock drilling has been studied using vertical turret lathe testing or single cutter on rock tribometry. However, there is a need to better predict the lithology-optimized penetrating action of the entire drill bit which is a function of the operating parameters, e.g., weight on bit (WoB) and rotations per minute (rpm). The present work introduces a new process to perform exploratory design search for a drill bit geometry optimized for a particular rock lithology. To experimentally study this, a benchtop rig with a miniaturized PDC drill bit is used to drill into sandstone rock cores in dry and aqueous conditions. Then a modeling framework [1-3] based on bonded particle discrete element method (DEM) and computational fluid dynamics (CFD) is employed to simulate the benchtop drilling. The DEM module has been parallelized using the massive parallelism offered by GPUs. The CFD module numerically solves the entire 3D Navier Stokes equations for incompressible fluids using the projection method for velocity and pressure coupling [2,3]. Adaptive mesh refinement and immersed boundary method are employed to treat the solid geometries. The multiphysics model is used to predict loss of weight on bit (WoB) due to lubrication and rate of penetration (RoP) of the bit. The model is computationally expensive thus a lower-order surrogate model [4] is developed using artificial intelligence (AI). This AI-guided model is ultimately used to provide a design chart which can be used to determine the drill bit shape optimized for a particular rock lithology. Keywords: PDC drill bit, benchtop drilling, sandstone, Discrete Element Method (DEM), Computational Fluid Dynamics (CFD), Artificial Intelligence (AI) References: [1] Terrell, E. J., & Higgs III, C. F. (2009). A particle-augmented mixed lubrication modeling approach to predicting chemical mechanical polishing. Journal of tribology, 131(1), 012201. [2] Mpagazehe, J. N. (2013). A physics-based, Eulerian-Lagrangian computational modeling framework to predict particle flow and tribological phenomena. PhD thesis, CMU (Advisor: C. Fred Higgs III) [3] Desai, P. (2017). Tribosurface Interactions involving Particulate Media with DEM-calibrated Properties: Experiments and Modeling. PhD thesis, CMU (Advisor: C. Fred Higgs III) [4] Zhang, W., Mehta, A., Desai, P.S., Higgs III, C.F. Machine Learning enabled Powder Spreading Process Map for Metal Additive Manufacturing (AM). SFF Symposium., Austin, Aug, 2017

15th U.S. National Congress on Computational Mechanics
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Title: Consistent High-order Approximations Spaces for Mixed Finite Elements on Hybrid 3D Meshes Including Pyramids

Author(s): *Philippe R. B. Devloo, *Unicamp*; Sônia M. Gomes, *Unicamp*; Omar Duran, *Cepetro*; Mark Ainsworth, *Brown University*;

The combination of tetrahedral and hexahedral elements in a single conformal mesh requires pyramids or prims to make the transition between triangular and quadrangular faces. For the pyramids, the approach is to consider composite polynomial approximations based on local partitions of them into two or four internal tetrahedra. The traces associated with triangular faces of the internal tetrahedral elements are constrained to quadrilateral shape functions of the neighboring element. Two classes of composite approximation spaces with exact sequences are constructed, one using classic Ne?de?lec spaces of the first kind, and a second one formed by enriching them with properly selected higher order functions with vanishing traces. Projection-based interpolants commuting the de Rham diagram are presented in a general form, for all element geometry, and the hybrid space configurations. Furthermore, we study applications to the mixed formulation of Poisson problems based on compatible pairs of approximations in {H(div, ?), L2(?)} for such hybrid meshes. An error analysis is outlined, showing optimal orders of approximation in terms of the mesh size as one would obtain using homogenous hexahedral or tetrahedral partitions. Enhanced accuracy for potential and flux divergence variables are obtained when enriched space configurations are applied. These predicted convergence orders are verified by the simulations of some Poisson test problems.

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Title: A New Numerical Approach for the Solution of PDE with Optimal Accuracy on Regular and Irregular Domains and Cartesian Meshes. Comparison with FEM.

Author(s): *Bikash Dey, *Texas Tech University*; Alexander Idesman, *Texas Tech University*;

A new numerical approach to solve the time dependent wave and heat equations as well as the time independent Poisson and Helmholtz equations is developed for the regular[1, 2] and irregular domains in the general multi-dimensional case. Trivial matched and non-matched Cartesian meshes with 3 points, 9 points and 27 points stencils are used in the 1-D, 2-D and 3-D cases, respectively. The idea of the local truncation error in space of the stencil equation is used and the order of this error is minimized to obtain the optimal accuracy of the numerical solution. The application of the new approach to the test problems on irregular domains shows the order of accuracy is close to four for the wave, heat and Helmholtz equations and is close to five for the Poisson equation. This is in agreement with the theoretical results. The comparison of the numerical results obtained by the new approach and by FEM shows that at similar 9 points stencils in the 2-D case and 27 points stencils in the 3-D case, the accuracy of the new approach is at least two orders higher than that for the linear finite elements. Moreover, the new approach yields even much more accurate results than the higher order finite elements with much wider stencils. [1] Idesman, A., and B. Dey. "Optimal reduction of numerical dispersion for wave propagation problems. Part 2: Application to 2-D isogeometric elements." Computer Methods in Applied Mechanics and Engineering 321 (2017): 235-268. [2] Idesman, A., and B. Dey. "The use of the local truncation error for the increase in accuracy of the linear finite elements for heat transfer problems." Computer Methods in Applied Mechanics and Engineering 319 (2017): 52-82.

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Title: On Geometry-based High-order Unstructured Methods for Structural-acoustics

Author(s): *Saikat Dey, *US Naval Research Laboratory*; Romain Aubry, *KeW Corporation*; Michael Williamschen, *KeyW Corporation*; Eric Mestreau, *KeyW Corporation*; Dylan Williams, *KeyW Corporation*;

We discuss recent developments in high-order finite and infinite element based approaches for accurate solution of problems in structural acoustics. We present several applications related to vibratory and scattering response of elastic structures excited by mechanical and/or acoustic sources. We identify and highlight the importance of high-order discretizations and the role of geometry for accurate solution of such wave-dominated problems.

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Title: A Lagrangian Approach to Interacting Particles Moving on Elastic Membranes

Author(s): *Sanjay Dharmavaram, *Bucknell University*; Luigi Perotti, *University of Central Florida*;

A system of interacting point particles free to move on an elastic medium while remaining embedded in the latter serves to model many interesting problems of softmatter and membrane biophysics such as the equilibrium configurations of protein clusters on cell membranes and protein capsomers on viral capsids (e.g., the immature HIV capsids and the maturation of Archaeal viruses [1].) Modeling the coupled interaction between particles and an elastic medium, while maintaining the particles freely moving on the underlying elastic surface is computationally challenging. Standard methods used in the literature include adding explicit constraints to anchor particles to the medium, use multi-step minimization to update particles and medium configurations sequentially, or identify particles to the nodes of the FEM mesh of the elastic medium. These methods are either expensive or introduce spurious restrictions on particle configurations. In this talk, we present an improved variational method that circumvents the existing challenges. Our method differs from existing approaches in that we use a Lagrangian description to represent the particle positions, where instead of using particle positions on the current surface as the degrees-of-freedom, particle positions on the reference configuration (the ``pull-back'' with the deformation map of the elastic medium) are defined as the degrees-of-freedom. Thus, the particles are automatically constrained to lie on the surface and no multi-step minimizations or additional constraints are necessary. Furthermore, as the particles are not artificially restricted to lie at the nodes of the mesh, they are free to explore all possible equilibrium configurations. We demonstrate the efficacy of this method by applying it to three benchmark problems in different dimensions and show that the theoretical convergence rates in energy and displacement norms are realized. We also discuss applications of the method to problems of membrane biophysics.
[1] Useful scars: Physics of the capsids of archaeal viruses, L.E. Perotti et. al, Phys Rev E 94 (2016).

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Title: Coupled Experimental-Computational Investigations of Grain Scale Mechanics in Complex Metallic Microstructures

Author(s): *Martin Diehl, *Max-Planck-Institut für Eisenforschung*; Franz Roters, *Max-Planck-Institut für Eisenforschung*; Dierk Raabe, *Max-Planck-Institut für Eisenforschung*;

Modern metallic materials for structural applications have a complex microstructure. For instance, alpha-beta-titanium alloys and dual phase steels consist of two phases with different properties and martensitic steels possess a multi-level internal structure. Such microstructures are often a result of mechanism-based alloy design, i.e. the complexity was introduced with the purpose of improving certain mechanical properties. When simulating the mechanical behavior of engineering alloys it is therefore necessary to incorporate the relevant microstructural details. In the context of crystal plasticity modelling [1], incorporation of microstructural details can be done directly in the constitutive law (e.g. by modelling mechanical twins or phase transformation) and/or by taking measured microstructures as input. Here, different crystal plasticity models implemented in DAMASK [2] are presented together with application examples based on measured microstructures. If applicable, the deformation behavior observed in the simulation is directly compared to the corresponding experimental investigation. As mechanical loads are accompanied by thermal and chemical loads during production and in service, it is beneficial to incorporate the materials response to these loads into crystal plasticity models [3]. Some aspects of enhancing crystal plasticity models into multiphysics models for Integrated Computational Materials Engineering (ICME) are also presented. [1] Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications, Acta Materialia, 58(4), 2010. doi:10.1016/j.actamat.2009.10.058 [2] DAMASK – The Düsseldorf Advanced Material Simulation Kit for Modelling Multi-Physics Crystal Plasticity, Damage, and Thermal Phenomena from the Single Crystal up to the Component Scale. Computational Materials Science, 157, 2019. doi:10.1016/j.commatsci.2018.04.030 [3] Review and outlook: mechanical, thermodynamic, and kinetic continuum modeling of metallic materials at the grain scale. MRS Communications, 7(4), 2017. doi:10.1557/mrc.2017.98

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Title: Computational Analysis of Coupling Methods for Classical Continuum Mechanics and Peridynamics Models

Author(s): *Patrick Diehl, *Louisianna State University*; Serge Prudhomme, *Polytechnique Montreal*;

Local-nonlocal coupling approaches provide a means to combine the computational efficiency of local models and the accuracy of non-local models. This talk will focus on the coupling of models from peridynamics (PD) and classical continuum mechanics. All approaches currently available in the literature introduce a coupling scheme at the discrete level using the finite element method for the discretization of the classical continuum model and the so-called EMU nodal discretization for PD. We will consider a one-dimensional benchmark problem to review and compare the different approaches and analyze how the matching of forces/displacements between PD nodes and finite element degrees of freedom and the choice of interpolation schemes may affect the accuracy in the solutions of the coupled models. The main objective of the talk will be to provide a general overview of the state-of-the-art and to emphasize the differences and similarities between the existing coupling approaches using the numerical results obtained on the one-dimensional benchmark problem.

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Title: A Development of a SPH Model for Simulation of Abrasive Waterjet Machining Process

Author(s): *Xiangwei Dong, *University of Petroleum (East China)*; Zengliang Li, *University of Petroleum (East China)*;

A fully Lagrangian model for simulating abrasive waterjet (AWJ) impacting on metallic surfaces is established based on smoothed particle hydrodynamics (SPH) method. In the model, both the fluid and the solid are described by SPH, where the waterjet is modeled as the viscous fluid and the metallic target is modeled as the elastic–plastic material. The main novelty of the model is that abrasives are explicitly included in the waterjet flow and modeled as arbitrarily-shaped rigid bodies. The interactions among the fluid, solid, and single abrasives are modeled through suitable techniques that are commonly used in SPH. The simulation of machining process of continuous waterjet flows containing abrasives is conducted as a challenging example to verify the applicability of the model. Results show that it is capable of capturing the physics of micro-machining caused by particle impacts and enclosing all critical factors related to AWJ including mass flow rate of abrasives, waterjet processing parameters, abrasive properties, etc. This new model is attractive for relevant applications, such as solid particle erosion. The advantages of the model lie in its conceptual simplicity, straightforward and the relative ease of incorporating new physics.

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Title: Improving Stability of Numerical Methods for Recovering Governing Equations from Noisy Data

Author(s): Paul Diaz, *University of Colorado, Boulder*; Alexandre Cortiella, *University of Colorado, Boulder*; *Alireza Doostan, *University of Colorado, Boulder*;

In modern science and engineering, coupled systems of non-linear ordinary differential equations are frequently employed to represent a dynamical system of interest. However, in many applications the underlying governing equations of a dynamical system are either unknown or not fully understood and must be informed by experimental data. Our work focuses on the discovery of governing equations for such systems when the amount of data is limited and the data is corrupted with noise. We explore improvements to the Sparse Identification of Non-linear Dynamics (SINDy) method. Approximating solutions via SINDy often involves solving a large over-determined linear system via sparse regression, where the data is evaluated using a candidate dictionary of potential basis functions and gradients are either measured or approximated from data. Problems may arise when the condition number of the dictionary grows due to a poor choice of basis functions or a large number of data points. Ill-conditioning limits the accuracy of approximations considerably given the presence of noise in the data. We explore methods from statistical regression to address this problem.

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Title: Formation Process and Time Evolution of Creases in Elastomers and Gels

Author(s): *Berkin Dortdivanlioglu, *Stanford University*; Christian Linder, *Stanford University*;

Hydrogels are polymeric networks swollen with water and they can undergo large nonlinear deformations. As a result, various unique phenomena, such as pattern formation, can be observed as combined effects of transient and inhomogeneous swelling and nonlinear elastic deformations. In general, swelling follows the diffusion of water inside the hydrogel. In the transient state, maximum amount of isotropic swelling is observed on the surface neighboring the water solvent. This differential swelling initially results in very fine transient surface instabilities forming localized self-contacting cusps referred to as creases. With further swelling, they coalesce and form similar, but successively coarser patterns. Stimuli-responsive polymeric gels that display transient patterns with controlled critical conditions such as onset, geometry, and evolution are useful in applications ranging from sensors and responsive coatings, to bioadhesives and cell substrates. Numerical modeling of hydrogels requires strong coupling between the deformation of the solid matrix and the diffusion of the water. Here, we adopt the mixed variational formulation for finite elasticity coupled with diffusion to model hydrogels. Due to the incompressibility constraint, numerical results suffer from (spurious) numerical oscillations in the nodal chemical potential solution; the formulation fails to satisfy the Ladyzhenskaya-Babuska-Brezzi (LBB) condition. Hence, a numerically stable subdivision-based mixed isogeometric analysis is adopted to obtain oscillation-free solution fields. The coalescing creases form self-contacting surface regions, which further complicates the simulations. A fictitious contact medium method is adopted to enable self-contact and help study a complete and transient description of the evolution of crease patterns in gels. The objective of this presentation is to understand and identify mechanisms leading to coalescence of creases upon diffusion-driven swellings. Furthermore, this study systematically investigates the pattern formation dynamics for the characteristic size of these patterns such as the wavelength, amplitude, and contact length of growing and disappearing creases. We show that the geometrical parameters (finite thickness of the hydrogel slab), material parameters (initial water content, solvent quality, and shear modulus), and diffusion kinetics play a critical role on the interaction among creases and the final characteristic size of patterns. Our proposed framework and numerical results allow a better understanding of pattern formation in hydrogels as well as structurally similar biological tissues, and consequently promote novel engineering and biomedical applications.

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Title: The Surrogate Matrix Methodology: Applications in Isogeometric Analysis

Author(s): *Daniel Drzisga, *Technical University of Munich*; Brendan Keith, *Technical University of Munich*; Barbara Wohlmuth, *Technical University of Munich*;

It has been well-established that isogeometric methods face a great computational challenge at the point of matrix assembly. This is due, in part, to the large support of the basis functions involved in the IGA discretization procedure. Although many computational challenges are naturally alleviated by the IGA paradigm, this particular challenge is clearly evidenced by the expansive and growing literature on new quadrature rules and accelerated assembly algorithms for IGA; see e.g., [1,2]. We present a simple strategy to avoid over-assembling the matrices appearing in IGA discretizations which already has been successfully applied to low-order finite element discretizations [3]. Roughly speaking, our approach involves only assembling a small fraction of the rows in the relevant matrices and then interpolating the remaining entries. Our strategy, which may be viewed as constructing a surrogate for each matrix, works because the IGA framework naturally allows a correspondence between matrix entries and a large class of smooth functions. The procedures we derive for IGA applications are independent of the quadrature rule used at the individual element or basis function level. This allows it to interface with many of most cutting edge quadrature rules for IGA. In order to underscore this fact, we implemented the new surrogate IGA methods by making some minor modifications to the existing assembly routines in the open-source GeoPDEs library. We provide a priori error estimates which certify the convergence of the surrogate method for Poisson's equation. In numerical experiments, the flexibility of the methodology is demonstrated for membrane vibrations, plate bending, and Stokes' flow problems. At only around one million degrees of freedom, we demonstrate assembly speed-ups of up to twenty times for a simple second-order NURBS basis. [1] Calabro, F., Sangalli, G. and Tani, M., 2017. Fast formation of isogeometric Galerkin matrices by weighted quadrature. Computer Methods in Applied Mechanics and Engineering, 316, pp.606-622. [2] Sangalli, G. and Tani, M., 2018. Matrix-free weighted quadrature for a computationally efficient isogeometric k-method. Computer Methods in Applied Mechanics and Engineering, 338, pp.117-133. [3] Bauer, S., Huber, M., Mohr, M., Rüde, U. and Wohlmuth, B., 2018, June. A New Matrix-Free Approach for Large-Scale Geodynamic Simulations and its Performance. In International Conference on Computational Science (pp. 17-30). Springer, Cham.

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Title: A Two-phase Computational Model for Arterial Thrombosis

Author(s): *Jian Du, *Florida Institute of Technology*; Aaron Fogelson, *University of Utah*;

Blood clots which form in the major arteries supplying the heart and brain with blood are the cause of most heart attacks and many strokes. These clots are made up largely of platelet aggregates that are adherent to the vessel wall. We present a two-phase continuum model of platelet aggregation in coronary-artery-sized blood vessels. The model tracks the number densities of different platelet populations characterized by their activation and binding status, as well as the concentration of platelet activating chemicals. Protein-mediated platelet cohesion is modeled through the distribution of elastic bonds between platelets, which generate stresses that can strongly influence the fluid motion. The most important feature of the model is that it treats individual unactivated and activated platelets as part of the viscous bulk fluid and treats the bound platelets as another viscoelastic material with its own velocity field. Movement of the bound platelet material and that of the background fluid are coupled through an interphase drag and an incompressibility constraint. The mechanical properties of an evolving thrombus (elasticity, plasticity, permeability) and the dynamical platelet-fluid interactions are directly related to the model parameters such as the packing densities of bound platelets, the rates of formation/breaking for different interplatelet bonds, and the various flow conditions. Therefore, the model is well suitable for the study of occlusive thrombosis in large arteries, where a fundamental question is how platelets can quickly adhere to the vessel wall and hold together in the face of fast flows and large hydrodynamic forces. Computational results indicate that the two-phase model can overcome the significant limitations of the single-phase model. This sets the stage for use of more realistic parameter values in order to have clot development on physiological time scales, and to add more comprehensive treatment of platelet-surface and platelet-platelet binding by two important proteins vWF and fibrinogen and their platelet receptors. Reference: A Two-phase Mixture Model of Platelet Aggregation. Jian Du, Aaron Fogelson, Mathematical Medicine and Biology, 35 (2018), pp. 225-256.

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Title: Machine Learning Based Vehicle Crashworthiness Design

Author(s): *Xianping Du, *Embry-Riddle Aeronautical University*; Feng Zhu, *Embry-Riddle Aeronautical University*;

A new data-driven methodology has been proposed and used in the vehicle crashworthiness design. The method allows exploring the big dataset of crash simulations to discover the implicit complicated relationships between performance and design variables, and derive design rules based on the structural response to make decisions towards the component design. An S-shaped beam is used as an example to demonstrate the performance of this method. A large number of crash simulations are conducted and a surrogate model is constructed with an Artificial Neural Network (ANN), which is further used to build a decision tree. Based on the decision tree, the interrelationship among the geometric design variables are revealed, and then the design rules are derived to implement the structural design. The accuracy of this method is verified by comparing the data mining model prediction and simulation data.

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Title: Effect of Plasticity and Fracture on the Hot-spot Formation in Energetic Materials

Author(s): *Camilo Duarte Cordon, *Purdue University*; Marisol Koslowski, *Purdue University*; Nicolo Grilli, *University of Oxford*;

?-HMX is an energetic crystal used in polymer-bonded explosive's (PBX) formulations. Ignition in PBXs occurs due to the formation of regions of localized high temperature termed as hot-spots. Preferential nucleation sites of hot spots are usually defects in the energetic crystal such as micro-cracks and voids. Several mechanisms of hot spot formation at the meso-scale have been proposed such as void collapse, shear banding, crack propagation and crack surface/interfacial friction. It has been observed experimentally that when ?-HMX is impacted at low strain rates the crystal behaves as brittle. However, when the crystal is impacted at high strain rates, e.g. during gas gun experiments, plastic deformation is observed. Similar transition from brittle-to-ductile has been observed in molecular dynamics (MD) simulations of energetic crystals subjected to shock load. In this work, we study the effect of plasticity in the fracture evolution and hot-spot formation of shock-loaded ?-HMX single crystals. A thermodynamically consistent finite strain model is used with a crystal plasticity model for the energetic crystal. The volumetric part of the deformation is described by a Birch-Murnaghan equation of state. Fracture evolution is simulated using a continuum phase field model of damage. Simulations are carried out in the finite element solver MOOSE, developed by the Idaho National Laboratory.

15th U.S. National Congress on Computational Mechanics
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Title: Computational Generation and Stochastic Upscaling of Concrete Microstructure

Author(s): *Vasav Dubey, *Texas A&M University, College Station, USA*; Christa E. Torrence, *Texas A&M University, College Station, USA*; Yang Lu, *Boise State University, USA*; Edward Garboczi, *National Institute of Standards and Technology, USA*; Zachary Grasley, *Texas A&M University, College Station, USA*; Arash Noshadravan, *Texas A&M University, College Station, USA*;

The mechanical behavior of concrete is strongly influenced by the characteristics of its highly heterogeneous microstructure. The mesoscale structure of concrete can be described as a composite with aggregates (inclusions) embedded in mortar (matrix). There is inherent randomness in composition and mechanical properties of these constituents, which in turn causes spatial heterogeneity in the local material behavior. The randomness in the morphological features includes size, shape, local volume fraction, spatial distribution of aggregates, and mechanical properties of different phases. In order to improve the microstructural representation, a spherical harmonic expansion is used to recreate the irregular geometry of real aggregates [1]. A custom meshing framework is also utilized to produce periodic finite element model of these microstructures. The existing homogenization schemes are often based on idealized descriptions of micro-heterogeneities and as such they do not take into account the randomness in the morphological features. In this research, we use a nonparametric stochastic model describing the mesoscale mechanical behavior of concrete microstructure, which relies on the theory of micromechanics, random matrix theory and maximum entropy principle [2]. We calibrated the model using a calibration process based on the numerical homogenization of digitally generated random microstructures. The proposed model provides a stochastic mesoscale material description exhibiting random fluctuations that are connected to the subscale microstructural randomness. Furthermore, a global sensitivity analysis is conducted to characterize the link between the uncertainty of model output and model input parameters related to the composition and mechanical behavior of subscale constituents. This upscaling model provides a computationally efficient material description that can be used for macroscale simulation taking into account local fluctuations in material properties that can influence the mechanical behavior of structures. [1] Z. Qian, E. Garboczi, G. Ye, E. Schlangen, Anm: a geometrical model for the composite structure of mortar and concrete using real-shape particles, Materials and Structures 49(1-2) (2016) 149-158. [2] J. Guilleminot, A. Noshadravan, C. Soize, R. Ghanem, A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures, Computer Methods in Applied Mechanics and Engineering 200(17-20) (2011) 1637-1648.

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Title: A Stabilized Finite Element Method for Enforcing Stiff Anisotropic Cohesive Laws Using Interface Elements

Author(s): *Ravindra Duddu, *Vanderbilt University*; Gourab Ghosh, *Vanderbilt University*; Chandrasekhar Annavarapu, *Lawrence Livermore National Laboratory*;

Numerical simulation of fracture propagation in multi-dimensions is a challenging problem, in part due to mixed-mode interactions and stiff anisotropic cohesive response at arbitrarily shaped crack interfaces, particularly under compression. Cohesive zone models (CZMs) have been widely used to analyze and predict mixed-mode fracture or delamination propagation at anisotropic and/or dissimilar material interfaces, despite their limitations. There are broadly two types of CZMs: intrinsic with initially elastic cohesive laws and extrinsic with initially rigid cohesive laws. Cohesive laws with large initial stiffness may be required for accurate fracture analysis and contact enforcement in intrinsic CZMs; however, stiff cohesive laws may also need to be enforced during cycle-by-cycle fatigue analysis even in extrinsic CZMs. It is well-known that the standard (penalty-like) method for enforcing stiff anisotropic cohesive laws using interface elements suffers from a distinct numerical instability that is often manifested by spurious oscillations in crack-face tractions, which may cause inaccuracies in peak-load prediction and convergence issues. To overcome these numerical issues, we develop a stabilized finite element method that generalizes Nitsche's method for enforcing stiff anisotropic cohesive laws with different normal and tangential stiffness. For smaller values of cohesive stiffness, the stabilized method resembles the standard method, wherein the traction on the crack surface is enforced as a Neumann boundary condition. Conversely, for larger values of cohesive stiffness, the stabilized method resembles Nitsche's method, wherein the cohesive law is enforced as a kinematic constraint. We present several numerical examples, in two-dimensions, to compare the performance of the stabilized and standard methods. Our results illustrate that the stabilized method enables accurate recovery of crack-face tractions for stiff isotropic and anisotropic cohesive laws; whereas, the standard method is less accurate due to spurious traction oscillations. Interestingly, the stabilized method could improve computational efficiency by allowing the use of larger displacement increment in mixed-mode fracture simulation owing to its stability and accuracy.

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Title: Topology Optimization of Lattice Structure Unit Cell for Thermal Fluid Applications

Author(s): *Florian Dugast, *University of Pittsburgh*; Albert To, *University of Pittsburgh*;

The determination of optimal structures is a relevant issue in many engineering problems. The corresponding geometry to satisfy a given objective can be obtained via topology optimization. This method has been applied first in structural mechanics and then to a large range of physics as heat transfer and fluid flow for example. The strength of topology optimization relies in the important number of degrees of freedom involved in the search of an optimal design, which allows the creation of complex geometries. Nowadays, additive manufacturing is useful to realize such geometries but the utilization of too many supports can be cumbersome (waste of material, difficult removal). The use of repetitive lattice structures can be used to deal with such issues. At the macroscale, the material distribution is then modified via the volume ratio of each lattice unit cell. At the microscale, the geometry of the unit cell can also be subject to optimization. Simple geometry such as simple cubic cell can be used but this choice is arbitrary and not necessarily justified from an optimization point of view. Therefore, this communication aims to propose an optimized lattice structure unit cell for convective heat transfer applications. A gradient-based method is used to find the optimal geometry. The calculation of the cost function gradient, with respect to design variables, involves the solution of the forward problem at each iteration of the optimization. This latter can be solved via classical methods with Navier-Stokes and energy equations, but the Lattice Boltzmann method (LBM) is an interesting alternative to solve this problem. LBM has an explicit formulation and its algorithm is well suited for high-performance parallel computing. Added to that, LBM can treat in a simple way the boundary conditions, which is another interesting feature for topology optimization where the geometry can be complex. The numerical application is based on a 3D laminar flow with heat transfer. The computational domain is composed of 100*100*100 elements. The objective of the topology optimization problem is to increase the heat transfer efficiency of the unit cell. As the minimal surfaces are good candidate for heat transfer intensification due to their high surface area, a comparison between the optimal geometry and classical minimal surfaces (gyroid for example) is also presented.

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Title: A Multiscale Hybrid Method for Darcy's Problems Using Mixed Finite Element Local Solvers

Author(s): *Omar Duran, *Cepetro*; Philippe R. B. Devloo, *Unicamp*; Sônia M. Gomes, *Unicamp*;

Multiscale Hybrid Mixed (MHM) method refers to a numerical technique targeted to approximate systems of differential equations with strongly varying solutions. For fluid in porous media, normal fluxes (multiplier) over macro element boundaries, and coarse piecewise constant potential approximations in each macro element are computed (upscaling). Then, small details are resolved by local problems, using fine representations inside the macro elements, setting the multiplier as Neumann boundary conditions (downscaling). In this research, a variant of the method is developed, denoted by MHM-H(div), adopting mixed finite elements at the downscaling stage, instead of continuous finite elements used in all previous publications of the method. Thus, this alternative MHM method inherits improvements typical of mixed methods, as better flux accuracy, and local mass conservation at the microscale level inside the macro elements, which are important properties for multi-phase flows in rough heterogeneous media. Different two-scale stable space settings are considered. Vector face functions are supposed to have normal components restricted to a given finite-dimensional trace space defined over the macro element boundaries. In each macro element, the internal flux components, with vanishing normal traces, and the potential approximations, may be enriched in different extents: with respect to internal mesh size, internal polynomial degree, or both, the choice being determined by the problem at hands. Both MHM versions are compared for 2D test problems, with smooth solutions, for convergence rates verification, and for Darcy's flow in heterogeneous media. MHM-H(div) 3D simulations are presented for a known singular Darcy's solution, using adaptive macro partitions, and for an oscillatory permeability scenario.

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Title: Deriving Pade Finite-Difference Summation-by-parts Operators for Spectral Resolvability on Coarse Grids

Author(s): *Ayaboe Edoh, *ERC, Inc. (AFRL Edwards)*; David Del Rey Fernandez, *NASA Langley and National Institute of Aerospace*;

Summation-by-parts (SBP) operators provide a tractable way of constructing schemes that are provably conservative and stable at the discrete level on bounded domains. The development of such schemes has largely been tied to achieving high-order convergence, which yields more efficient methods relative to grid refinement efforts. Besides asymptotic order, however, another important aspect that can be considered is the spectral accuracy of the discretization. This latter perspective takes into account numerical performance as a function of scale and more explicitly reframes the concept of accuracy to include coarse grid scenarios. For example, considering the behavior of a scheme for under-resolved dynamics is imperative in practical engineering calculations such as LES. The subject of spectrally-resolving stencils for SBP methods has been addressed with respect to explicit Dispersion-Relation-Preserving (DRP) stencils [1]. In addition to such optimization-based efforts, however, one can seek to achieve DRP characteristics by adopting Pade (i.e., implicit) formulations. These latter methods can be shown to yield improved spectral and asymptotic properties compared to explicit schemes for a given order or stencil DOF. Carpenter et al. [2] provide the only Pade finite difference SBP (FD-SBP) operator in the literature, constructed relative to the classic fourth-order tri-diagonal interior stencil. Their FD-SBP operator employs a full norm and is constructed such as to preserve global fourth order accuracy. The current work seeks to further explore the potential benefits associated with Pade schemes in the context of FD-SBP. Emphasis is placed on a new derivation procedure based on “cascaded-norms” [3] which enables simple derivation of SBP operators for arbitrary implicit interior stencils. While the current methods are limited to second-order global accuracy, they are seen to benefit from the Pade formulation, which maintains spectral accuracy towards high wavenumbers (i.e., small grid scales). Performances relative to classic diagonal- and block-norm FD-SBP methods, as well as the original Pade scheme of Carpenter et al., are to be assessed in order to further evaluate potential benefits of full-norm FD-SBP operators. 1. Linders, V., Kupiainen, M., and Nordstrom, J., “Summation-by-parts Operators with Minimal Dispersion Error for Coarse Grid Flow Calculations,” Journal of Computational Physics, 2017. 2. Carpenter, M. H., Gottlieb, D., and Abarbanel, S., “Time-stable Boundary Conditions for Finite-difference Schemes Solving Hyperbolic Systems: Methodology and Application to High-order Compact Schemes,” Journal of Computational Physics, 1994. 3. Edoh, A. K. and Sankaran, V., “Boundary Prescriptions for Spectrally-tunable Discrete Filters,” AIAA Aerospace Sciences Meeting, AIAA Paper 2019-2170, 2019.

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Title: Modeling Strain Rate Effects in High Performance Concrete with the Lattice Discrete Particle Method (LDPM)

Author(s): *Micael Edwards, *U.S. Army Engineer Research and Development Center*; Mei Chandler, *U.S. Army Engineer Research and Development Center*; Robert Moser, *U.S. Army Engineer Research and Development Center*; Gianluca Cusatis, *Department of Civil and Environmental Engineering, Northwestern University*;

In this work, we present the results of several simulations of dynamically loaded high performance concrete (HPC) using the rate effects parameters and the explicit porosity inputs in the Lattice Discrete Particle Method (LDPM). HPC possesses much higher unconfined compressive strength (> 100 MPa) compared to normal strength concrete (?40 MPa) and is increasingly used for military applications such as protective structures. Modeling and simulation of this type of material at high strain rates are becoming more and more important. The LDPM method combines the discrete particle method with a lattice model. The model takes into account the mesoscale pore and fine aggregate distributions from experimental characterization. The modeling results are compared to experimental results of HPC specimens subjected to the Kolsky bar compression technique under unconfined uniaxial compression and triaxial compression at different strain rates. The objective of this modeling is to investigate the effects of different mesoscale structure properties, such as size and distribution of meso-porosity and fine aggregate, on the damage and failure of HPC under different dynamic loading conditions. Permission to publish was granted by the Director, ERDC Geotechnical and Structures laboratory.

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Title: Metric-aligned Quad-dominant Mesh Adaptation Using a Dual-Weighted Residual Error Estimator

Author(s): *Dirk Ekelschot, *NASA Ames Research Center*; Scott Murman, *NASA Ames Research Center*;

We present a metric-aligned quad-dominant mesh adaptation strategy that uses a Dual-Weighted Residual (DWR) error estimator. Typically, we are interested in determining a target functional like lift or drag as accurately as possible. In order to do that we use a Dual-Weighted Residual (DWR) error estimator which determines where the discretization error in the computational domain affects the error in target functional the most. Typically, compressible flow problems exhibit anisotropic features like shear layer and shock waves for which we want to adapt for. To incorporate the anisotropy in the adaptive cycle, we incorporate Mesh Optimization by Error Estimation and Synthesis (MOESS) which determines the effect of anisotropic refinement through a local sampling operation [1]. The local anisotropic error estimate that is determined using MOESS is then weighted with the adjoint solution so that a metric-aligned goal-oriented error estimate is determined. This discrete error estimate then serves as a metric field which is used to drive a variational meshing algorithm that relies on Lp-Centroidal Voronoi Tessellation [2] in order to compute a corresponding metric-aligned quad-dominant mesh. The adaptive procedure is demonstrated within the framework of the high-order Discontinuous Galerkin solver, eddy, on stated test cases from the literature. [1] M Yano and DL Darmofal, An optimization framework for anisotropic simplex mesh adaptation, Journal of Computational Physics, 231:7626-7649, 2012. [2] D Ekelschot and M Ceze and A Garai and S. Murman, Parallel high-order anisotropic meshing using discrete metric tensors, AIAA Scitech 2019 Forum San Diego, California

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Title: An Adaptive Quasi-continuum Approach for Modeling Fracture in Polymer Networks

Author(s): *Ahmed Elbanna, *University of Illinois Urbana Champaign*; Ahmed Ghareeb, *University of Illinois Urbana Champaign*;

Polymer network is the backbone for many natural and man-made porous and fluid-infused materials such as gets, biological tissues, and rubbers. The load bearing structure of polymer networks may be abstracted as a complex network of non-linearly interacting polymer chains while inter-connected by cross-linkers. Understanding the multiscale behavior of polymer networks holds key for uncovering origins of fragility in many complex systems. However, these processes are intrinsically multiscale, and it is computationally prohibitive to adopt a full discrete approach for large scale structures. To overcome these difficulties, we introduce a new adaptive numerical algorithm for solving polymer networks using an extended version of the Quasi-Continuum method. In regions of high interest, for example near cracks, explicit representation of the local topology is retained where each polymer chain is idealized using the worm like chain model. Away from these imperfections, the network structure is computationally homogenized, to yield an anisotropic material tensor consistent with the underlying network structure and only a fraction of the network nodes is solved. Dynamic adaptivity allows transition between the two resolutions. The method enables accurate modeling of crack propagation without apriori constraint on the fracture energy and without invoking any assumptions of a material characteristic length scale -which is usually needed for other nonlocal approaches such as phase field methods, while maintaining the influence of large-scale elastic loading in the bulk. We demonstrate the accuracy and efficiency of the method by applying it to study the fracture of large-scale problems and study the effects of network topology on the fracture proprieties. We discuss the implications of the method for the analysis of general networked material systems.

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Title: Exploring Greedy Multilevel/Multifidelity/Multi-Index Surrogate Approaches for Forward Uncertainty Quantification

Author(s): *Michael Eldred, *Sandia National Laboratories*; John Jakeman, *Sandia National Laboratories*; Gianluca Geraci, *Sandia National Laboratories*; Alex Gorodetsky, *University off Michigan*;

In the simulation of complex physics, multiple model forms of varying fidelity and resolution are commonly available. In computational fluid dynamics, for example, common model fidelities include potential flow, inviscid Euler, Reynolds-averaged Navier Stokes, and large eddy simulation, each potentially supporting a variety of spatio-temporal resolution/discretization settings. While we seek results that are consistent with the highest fidelity and finest resolution, the computational cost of directly performing UQ in high random dimensions quickly becomes prohibitive. To address these challenges, we have focused on the development and deployment of multilevel/multifidelity/multi-index algorithms that adaptively fuse information from multiple model fidelities and resolutions in order to reduce the overall computational burden. In this presentation, we focus on forward uncertainty quantification using surrogate approaches that utilize projection (e.g., sparse grid polynomial chaos), interpolation (e.g., hierarchical collocation), or regression (e.g., compressed sensing) to form multiple model approximations from adaptively allocated sample sets. Of particular interest are generalizations for multiple model refinement dimensions and we will explore the relationships between generalized greedy approaches, which admit flexibility in supporting different candidate generators and relaxing hierarchical refinement constraints, and fully-integrated multi-index sparse grid approaches, that span both random variable and model resolution domains within an integrated indexing structure. These greedy surrogate approaches will be demonstrated for standard model problems and deployed to engineered systems.

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Title: Deformation of Computational Domains in Primary Manufacturing Methods

Author(s): *Stefanie Elgeti, *RWTH Aachen University*; Florian Zwicke, *RWTH Aachen University*; Fabian Key, *RWTH Aachen University*;

Deforming computational domains in fluid flow can be categorized as follows: (1) The domain deformation is given from an external source (e.g. a fixed deformation or given via another code as in fluid-structure-interaction) or (2) the domain deformation needs to be computed in the frame of a free-boundary problem. Numerically, both domain deformation categories are subject to either interface capturing or interface tracking methods. Interface capturing methods use a separate marker function to track the interface and subsume methods like level-set or volume of fluid. Interface tracking instead uses boundary conforming grids, which adapt to the domain deformation. This presentation will focus on the case of interface tracking, where, in particular, the Deforming-Spatial-Domain/Stabilized-Space-Time (DSD/SST) formulation will be considered. This methods allows to detach the mesh deformation from the flow pattern, which gives additional flexibility when developing mesh deformation procedures. Recent developments in domain deformation methods will be presented. These include rotational, translational, and arbitrary deformations [1,2]. The application area are primary manufacturing methods. The category of primary shaping manufacturing processes have in common that — using a mold or die — they form material from an initially unshaped state (usually melt) into a desired shape. A general challenge in primary manufacturing is that the exact design of the mold cannot be determined directly and intuitively from the product shape. This is due to the nonlinear behavior of the material regarding the flow and solidification processes. This field of application gives rise to a number of challenges in the area of domain deformation, ranging from fixed deformations, via free-surface flows to shape optimization. [1] F. Key, L. Pauli, S. Elgeti, The Virtual Ring Shear-Slip Mesh Update Method, Computers and Fluids, 172:352-361, 2018. [2] F. Zwicke, S. Eusterholz, S. Elgeti, Boundary-Conforming Free-Surface Flow Computations: Interface Tracking for Linear, Higher-Order and Isogeometric Finite Elements, Computer Methods in Applied Mechanics and Engineering, 326C:175-192, 2017.

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Title: An Embedded Isogeometric Kirchhoff-Love Shell Formulation for the Shape Optimization of Non-conforming Multi-patch Structures

Author(s): Thibaut Hirschler, *Univ Lyon, INSA-Lyon, CNRS, LaMCoS UMR5259*; Robin Bouclier, *Univ Toulouse, UPS, UT1, UT2, INSA, CNRS, IMT UMR5219*; Arnaud Duval, *Univ Lyon, INSA-Lyon, CNRS, LaMCoS UMR5259*; *Thomas Elguedj, *Univ Lyon, INSA-Lyon, CNRS, LaMCoS UMR5259*; Joseph Morlier, *Univ Toulouse, UPS, INSA, ISAE-SUPAERO, MINES-ALBI, CNRS, ICA UMR5312*;

Isogeometric shape optimization uses a unique model for the geometric description and for the analysis. The benefits are multiple: in particular, it avoids tedious procedures related to mesh updates. However, isogeometric shape optimization has so far been mainly applied to simple structures modelled by single patch geometries. It is known that for real-world structures, multipatch models are required. Furthermore, non-conforming junctions and trimmed configu- rations are often inevitable. This issue is not only challenging for the analysis, but it also raises geometric difficulties during the shape updates. Thus, we develop a new approach by employing the Free-Form Deformation principle. Surfaces are embedded into volumes in order to tackle the geometric constraint of connecting interfaces between given patches during the shape modifications. For the analysis, we introduce the embedded Kirchhoff-Love shell formulation where the mid-surface is represented by a NURBS composition while the displacement field is approximated using the spline functions as for the embedded surface. Finally, a new mortar method is formulated to couple the non-conforming Kirchhoff-Love shells. It provides the pos- sibility to use domain decomposition methods which allows to distribute the patches amongst several processors running in parallel, at a very competitive cost. We apply the developed method to optimize stiffened structures widely used in aeronautics.

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Title: Calibration of Imperfect Subsurface Flow Models Using Noise as Regularizer

Author(s): *Ahmed H. Elsheikh, *Heriot-Watt University*; Muzammil H. Rammay, *Heriot-Watt University*;

Efficient calibration of subsurface flow models has a direct impact on the forecast skill of the calibrated model. A high-quality forecast is important for optimal decision making and robust management of operational risks. The model calibration process is often challenging and relies on many factors including the quality of the calibration data, the diversity and information content of these datasets and the quality of the computational model in-terms of validity of modelling assumption and the parameterization of the key uncertain model parameters. As a general rule, a good match to the historical data is not sufficient to assume a high-quality forecast due to modelling errors which often exists in every model. In the current presentation, I will discuss different approaches for calibration of subsurface flow model while assuming an unknown modelling errors within a general Bayesian inversion framework [1, 2]. We build on recent techniques developed in the machine learning literature where noise is used for regularization to avoid overfitting. We also rely on annealing ensemble techniques [3] for sequential estimation of the amount of noise-based regularization terms corresponding to the modelling error. The presented ideas are evaluated on subsurface flow models with various sources of errors including aggressive up-scaling, imperfect geological parameterization and simplified physical modelling assumptions. Our numerical investigation shows that accounting for modelling errors while calibrating imperfect models manages to eliminate the bias in the estimated model parameters which is tightly linked to the data overfitting problem. The developed techniques provide a powerful tool that could be used to guide the model refinement/assessment process within a general framework for data integration of subsurface flow models. References: [1] C Köpke, J Irving, AH Elsheikh, Accounting for model error in Bayesian solutions to hydrogeophysical inverse problems using a local basis approach, Advances in Water Resources 116, 195-207, 2018/ [2] MH Rammay and AH Elsheikh, Y Chen, Identifiability of model discrepancy parameters in history Matching, SPE-193838-MS, Reservoir Simulation Conference, Galveston, Texas, USA, 10 – 11 April 2019. [3] AS Stordal, AH Elsheikh, Iterative ensemble smoothers in the annealed importance sampling framework, Advances in Water Resources 86, 231-239, 2018.

15th U.S. National Congress on Computational Mechanics
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Title: Improved Structural Performance Models for Qualification of Metal AM Components

Author(s): *John Emery, *Sandia National Laboratories*; Kyle Johnson, *Sandia National Laboratories*; Mircea Grigoriu, *Cornell University*; Jay Carroll, *Sandia National Laboratories*; Joseph Bishop, *Sandia National Laboratories*;

Metal additive manufacturing (AM) provides manufacturing benefits that include automation and flexibility, enabling fabrication of geometries that otherwise require jointed connections. Presently, AM pars can exhibit a host of material defects that can compromise structural reliability. Sandia has been developing models and modeling methodology to predict residual stresses and performance, considering uncertainties, with intent to prove/qualify AM components. Experimentally, we have been advancing the state of knowledge with novel measurements and experiments, including micro-computed tomography (uCT), electron backscatter diffraction (EBSD) imaging, and novel mechanical properties characterization techniques. We outline a proposed hierarchical approach that first uses engineering-scale, lower-fidelity models to identify hotspots where later concurrently coupled models containing explicitly-represented materials defects are employed to refine performance predictions. The talk will share preliminary results from efforts to implement this approach, which may include the following types of results. The engineering-scale models use uCT data characterizing materials defects to locally-seeded void-volume fractions in a damage mechanics plasticity model. Substantive residual stresses exist in AM, sometimes above the base material yield strength, and are likely to play an important role in structural reliability. Our approach considers their effects in the engineering-scale models. The fine-scale models develop subvolumes of AM materials, explicitly meshing the geometry of statistically informed porosity, and couple them to the engineering scale with multi-point constraints. Preliminary predictions of reliability are compared, and computational efficiency is discussed. Two additive systems are considered, SS316 and AlSi10Mg, and their similarities and differences are discussed. Acknowledgment: Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

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Title: Design of Compliant Mechanism Actuated by Pneumatic Chambers Using Level Set Topology Optimization with Stress Constraints

Author(s): *Helio Emmendoerfer Junior, *University of Sao Paulo*; Eduardo Alberto Fancello, *Federal University of Santa Catarina*; Emilio Carlos Nelli Silva, *University of Sao Paulo*;

This work presents a level set topology optimization problem to design compliant mechanisms under local stress constraints. Different from the classical flexible structure designs, here the mechanism is actuated by means a pneumatic chamber. Our objective is to obtain a compliant mechanism which both the structure and the shape of the pressurized chamber are optimized. The resulting forces due to the pressure acting on the chamber boundaries are classified as design-dependent loads since their direction and location may change with the structural design. A standard approach of maximizing the output displacement with a (distributed) spring at the output port, representing the stiffness of the external medium, is proposed. Three technical issues are related to solving this problem. The first one is to include local stress constraints using an augmented Lagrangian scheme. The second refers to the unwanted flexible joints (hinges) usually obtained for flexible structure designs. This difficulty is overcome by controlling the von Mises stresses level. Finally, the third issue deals with design-dependent load problems in which is established an appropriate association between the moving load boundary and the pressure acting on it. This difficulty is easily overcome by the level set method that allows for a clear tracking of the boundary along the optimization process. In the present approach, a level set evolution via reaction-diffusion is used. This evolution equation allows for the generation of new holes inside the domain and no need for reinitialization steps. Numerical examples to design a (hinge-free) compliant mechanism with stress level under control and actuated by an optimized pressurized cavity are presented.

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Title: Boomerang Cracks and Toughness Enhancement through Detailed Designs of Composite Architecture

Author(s): *Randall Erb, *Northeastern University*; Robert Zando, *Northeastern University*; Chunzhou Pan, *Northeastern University*;

Ceramic reinforced polymer matrix composites (PMCs) offer routes toward increased specific strength and toughness. However, reinforced PMCs are highly anisotropic. Apply a stress perpendicular to the reinforcement, and easy failure can occur. In this work, we use complex reinforcement architectures to combat this weakness of anisotropy. To achieve control of the fiber architecture, we make use of 3D Magnetic Printing in which we can control the orientation of ceramic reinforcement within every voxel of printed material. Specific to this presentation we have investigated a family of new 2d fiber architectures that are linked to creating what we call "boomerang cracks". In these samples, advancing cracks get turned in the opposite direction through interaction with an underlying fiber architecture. With such an approach, we are able to significantly increase the toughness of the reinforced composites. In this talk, we will offer some early results on next generation samples.

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Title: Accuracy of Energy Stable SBP-SAT Finite Difference Operators Approximating the Second Derivative

Author(s): *Sofia Eriksson, *Linnaeus University*; Anna Nissen, *KTH Royal Institute of Technology*;

In this talk we study the accuracy of spatial discretizations of the Poisson equation and the heat equation with Dirichlet boundary conditions. We use a special family of finite difference schemes, that lead to dual consistency. Dual consistency is a concept which is valuable when one is interested in functionals of the solution, because the accuracy order of the functionals can for such a scheme be substantially higher compared to the accuracy order of the scheme itself. We consider finite difference operators fulfilling the summation by parts (SBP) property, combined with a penalty technique denoted simultaneous approximation term (SAT) for imposing the boundary conditions. The SBP-SAT finite difference operators usually have different design order in the interior and at the boundary, which gives rise to the question how accurate the resulting numerical solution will be. A common measure for accuracy is convergence rate, often in the L2-norm. A rule of thumb says k orders are gained in the convergence rate for a partial differential equation (PDE) with kth order spatial derivative. However, determining the precise convergence rate of a numerical scheme for a specific PDE has been a long-standing research topic. For the time-independent case, a singular spatial discretization operator makes it impossible to find a numerical solution. Besides, when the discrete operator is close to being singular the order of accuracy is reduced. The reduction of accuracy also occurs for the time-dependent problem. At worst, when the operator is sufficiently close to being singular, the time-dependent discretization error has the same order as the truncation error, and the k orders are thus not gained. In this talk we derive expressions of exact inverses of the discrete operators for the time-independent problem (i.e. for the Poisson equation) and find out precisely which choices of SAT penalty parameters in the imposition of the boundary conditions that make the discretization operator singular. For the corresponding time-dependent problem (the heat equation) we use the energy method to determine the penalty parameters, which guarantees a stable numerical solution. It turns out that within the particular family of penalty parameters leading to dual consistency, the stability limit from the energy method coincides with the condition for singularity.

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Title: Constitutive Modeling of Extra- and Intra-Parenchymal Bronchi Experiments Using Inverse Finite Element Analysis and Digital Image Correlation

Author(s): Mehrzad Tartibi, *Delbeat, LLC*; *Mona Eskandari, *University of California Riverside*;

Pulmonary biomechanics research is at the epicenter of understanding chronic lung disease and the millions of lives claimed by it each year. The combined fluid-structure system of the lung complicates analysis, and the lack of fundamental experiments and models characterizing bronchial material response impractically compels the mechanics of fluid flow and tissue expansion to be disconnected [3]. To address this need, here we present a constitutive model of extra- and intra-parenchymal bronchi using material characterization, inverse finite element analysis, and digital image correlation. Experiments are conducted on axially and circumferentially oriented porcine airway specimens, collected from the trachea, large bronchi, and small bronchi regions [1]. Non-linear, incompressible, fiber-reinforced, hyperelastic models with material convexity represent direction- and region-dependent measured stress-strain responses parameterized from uniaxial tensile tests [2]. Incremental elongation to 35% strain is displacement-controlled, with planar deformation directly informed by correlated surface speckles. Tracking of lateral material contraction informs the constitutive model. Accuracy is verified through the predictive response of uncalibrated samples, and is well simulated by the finite element model. Establishing the anisotropic and heterogeneous behavior of the airway network primes the development of realistic physiological models, facilitating whole lung-level simulations through the coalition of fluid and structure mechanics, setting the stage for future pulmonary computational methods capable of optimizing surgery and diagnosing disease. [1] Eskandari, M. et al. (2018). Mechanical Properties of the Airway Tree: Heterogeneous and Anisotropic Pseudoelastic and Viscoelastic Tissue Responses. J App. Physiol. [2] Eskandari et al. (2019) Mechanics of Pulmonary Airways: Linking Structure to Function Through Constitutive Models, Biochemical Analysis, and Histology, submitted. [3] Wall, W. A., Rabczuk, T. (2008). Fluid–structure interaction in lower airways of CT-based lung geometries. Int. J Num. Meth. Fluids.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Shape and Topology Optimization of Architectured Materials Either Linear and Non Linear Elastic: from the Design to Real Structures

Author(s): *Rafael Estevez, *Université Grenoble Alpes*; Alexis Faure, *Université Grenoble Alpes*; Georgios Michailidis, *Université Grenoble Alpes*; Charles Dapogny, *Université Grenoble Alpes*;

Shape optimization methods are promising methods and are gradually becoming industrialized. They provide the ability to automatically design structures with optimal behavior. They are outstanding tools for exploration and design of new materials and in particular architectured materials which are expected to “fill the holes” in the materials space [Ashby & Bréchet, 2003, Acta Mater.]. We first focus on the plausible manufacturing solution to process architectured materials. Additive manufacturing is a relevant option. We introduce several strategies to circumvent some limitations and side effects of these processings during optimization stage. We focus on Fiber Deposition Molding [Dapogny et al., 2019, CMAME], which induces an important mechanical anisotropy. In particular, we present a contribution to the modelling of the effective properties of the constituve partof structures fabricated by additive manufacturing technologies, and how they influence the design optimization process. On the one hand, emphasizing on the case where the particular material extrusion techniques are used, we propose a model for the anisotropic material properties of shapes depending on the (user-defined) trajectory followed by the machine tool during the assembly of each of their 2D layers. On the other hand, we take advantage of the potential of additive manufacturing technologies for constructing very small features, and we consider the optimization of the infill region of shapes with the goal to improve at the same time their lightness and robustness. The optimized and constraint functionals of the domain involved in the shape optimization problems in these two contexts are detailed, by relying on the notion of signed distance function. Eventually, some numerical experiments are conducted in two dimensions to illustrate the main points of the study. In a second part, we investigate the influence of non linear effects, either geometrical with account of the Green-Lagarnge strain measure or non linear elastic response of the constitutive phases. This is relevant for the design of actuators and outcomes are provided from the cases investigated. First, as reported in the literature, account for the full deformation does not drastically change the fnal design but captures the critical load that trigger the onset to some buckling in the structure. How this is prevented in an optimization process is pointed out. The influence of a non linear elastic response is then explored and it is shown that depending on the materials’ parameters and the load level, distinct optimum designs are derived and discussed.

15th U.S. National Congress on Computational Mechanics
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Title: A Pressure-Robust Residual-Based Stabilized Method for the Incompressible Navier-Stokes Equations

Author(s): *John Evans, *University of Colorado Boulder*; David Kamensky, *Brown University*;

Mixed methods for the incompressible Navier-Stokes equations whose velocity error is independent of the pressure field are said to be pressure-robust. While most mixed methods do not have this property, methods which return a divergence-free velocity field are indeed pressure-robust. However, the application of residual-based stabilization, including Streamline-Upwind Petrov-Galerkin (SUPG) stabilization, typically results in a loss of pressure-robustness as such stabilization induces additional coupling between the velocity and pressure fields. This is unfortunate as stabilization is required in the case of dominant convection. In this talk, we introduce a new residual-based stabilized method for the incompressible Navier-Stokes equations which, when coupled with a divergence-conforming velocity/pressure pair, is provably pressure-robust. As opposed to classical residual-based stabilized methods such as the SUPG method, our method involves the curl of the residual rather than the residual itself. For the setting of linearized Oseen flow, we prove error estimates for the velocity field that are independent of both the pressure field as well as the Reynolds number by appealing to a strong SUPG-like norm. We numerically confirm these error estimates for two divergence-conforming mixed methods, divergence-conforming B-splines and Scott-Vogelius finite elements, using a suite of benchmark problems. Finally, we demonstrate the potential of our new residual-based method in the large eddy simulation of turbulent flow.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Existence of Solutions in Topology Optimization: the Nonlocal Perspective

Author(s): *Anton Evgrafov, *Technical University of Denmark*; Jose C. Bellido, *University of Castilla-La Mancha*;

One of the most popular methods for optimal design in continuum mechanics is topology optimization. Within this framework, which has been made particularly relevant owing to the recent advances in additive manufacturing, at each point in the design domain one takes a decision about which material should be placed there. Computationally one solves a relaxed version of this problem, which reduces to optimal control in the coefficients of partial differential equations. In most interesting and relevant cases the problem is non-convex and lacks optimal solutions. There are essentially two strategies for dealing with this issue. One is to restrict the set of allowable controls by applying external regularization tools to the problem, thereby only allowing designs satisfying certain explicit or implicit regularity criteria. The alternative is to extend the set of allowable controls by also considering limits of highly oscillatory designs, interpreting them as composite materials in the sense defined by the homogenization process. We present a completely different approach to this optimal design problem. Namely we replace the governing partial differential equations of the continuum mechanical model with a non-local, integral, peridynamic model. The control variables still enter the problem as coefficients of the governing non-local equation. On the one hand, we verify that in the limit of small interaction horizons we recover the governing PDE with coefficients we control. On the other hand the resulting control problem, in spite of its non-convexity, attains its infimum and therefore admits globally optimal solutions without the need for any external regularization techniques. We will illustrate our results with numerical examples related to steady state heat conduction.

15th U.S. National Congress on Computational Mechanics
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Title: Robust and High-Fidelity Reduced-Order Model for Structural Vibration Analysis of Multiscale Spent Nuclear Fuel Containers

Author(s): *Olivier Ezvan, *University of Southern California*; Xiaoshu Zeng, *University of Southern California*; Roger Ghanem, *University of Southern California*; Bora Gencturk, *University of Southern California*;

We propose an efficient reduced-order model (ROM) for a robust and high-fidelity prediction of the structural vibrations of a spent nuclear fuel (SNF) container. The ROM is intended for inverse identification of the structural integrity of the sealed container internal components. The internals consist of 68 identical fuel assemblies placed in a honeycomb shaped basket. Each fuel assembly holds a hundred of long and slender nuclear fuel rods, maintained in position by 8 spacer grids. The several structural scales and the repetition of components (pseudo-periodicity) lead to a large-scale finite element (FE) model with hundreds of millions of degrees of freedom (DOFs). Due to the isolated (local) vibrations of the numerous components, the FE model also exhibits a very large number of vibration eigenmodes. For these reasons, a vibration analysis is nearly intractable with standard methods. To tackle this difficulty and leverage the particular structure of the nuclear package (pseudo-periodicity and localized structural connections between sub-components), Craig-Bampton (CB) substructuring technique is used and further adapted to the SNF package specificities (large number of component modes and small number of boundary DOFs). Two nested CB reductions are carried out. The inner CB deals with the eigenvalue analysis of the fuel assembly, whereas the outer CB deals with the whole SNF package, using the inner CB modes as component modes. Each CB eigenvalue problem consists of a sparse generalized eigenvalue problem for which a large percentage of the eigenpairs are sought and for which the dimension precludes the use of the usual direct solvers. Spectrum slicing with shift-invert Lanczos (SIL) is thus used for an efficient and parallel solution, further enhanced through block factorization by Schur complement. The system eigenmodes obtained are partially validated against a reduced set of so-called dominant modes (according to a mode filtering process) that are exactly computed. The rank and eigenfrequency of the dominant modes are obtained from the CB approximation, and the corresponding eigenmodes are exactly computed with SIL, by targeting thin frequency slices and using Schur complement method. This yields a reference model against which further truncations and mode filtering are performed for an enhanced speed-up with controlled accuracy. The computational cost for constructing the validated ROM is of several orders of magnitude less than standard modal analysis. Furthermore, the multilevel CB enables the efficient integration of the parametric and nonparametric approaches to uncertainty quantification, which allows to account for both model and model-parameter uncertainties.

15th U.S. National Congress on Computational Mechanics
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Title: A Coupled Phase-Field and Deformation Theory of Multi-constituent Tumor Growth

Author(s): *Danial Faghihi, *The University of Texas at Austin*; Ernesto Lima, *The University of Texas at Austin*; Xinzeng Feng, *The University of Texas at Austin*; Thomas Yankeelov, *The University of Texas at Austin*;

Mechanical stresses of the solid phase of a tumor play a vital role in the expansion, invasion, and metastasis of tumors. These stresses mainly arise due to heterogeneous tumor growth and the effect of surrounding tissue confinement, and moderate the development of solid tumors by lowering the proliferation rate and inducing apoptosis of the tumor cells. This contribution focuses on developing a continuum model to simulate the effect of mechanical stress in an avascular model of tumor growth at the tissue scale, while accounting for a range of important cell and sub-cellular interactions. The model is developed based on continuum mixture theory coupling diffusion (phase-field) with deformation (hyperelastic) responses of multiple interacting constituents. The mixture theory also accounts for balance laws at the microscale (subcellular and cellular scale interactions) in addition to the macroscale balance laws (tissue level). Special attention is given to model the effects of mechanical deformation in tumor progression. In this regard, growth effects and their interaction with the deformation are included in the model through a physically and mathematically consistent construction. The numerical approximation of the proposed model using mixed finite elements are also presented. The numerical experiments indicate the ability of the model to capture key features of an avascular tumor growth in various microenvironments of living tissue. Ongoing studies are designed to calibrate and validate the model using in vivo magnetic resonance imaging measurements of the spatio-temporal evolution of the tumor cell in pre-clinical models of glioma.

15th U.S. National Congress on Computational Mechanics
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Title: A Hierarchical Multilevel Markov Chain Monte Carlo Approach for Large-Scale Bayesian Inference

Author(s): *Hillary Fairbanks, *Lawrence Livermore National Laboratory*; Panayot Vassilevski, *Lawrence Livermore National Laboratory*;

Markov chain Monte Carlo (MCMC), while a standard approach for nonlinear Bayesian inference of high-dimensional problems, is not feasible for large-scale applications. With the increase in problem size and thus simulation cost, MCMC becomes intractable, and acceleration approaches become necessary. Of particular interest within the scope of acceleration methods is the recently developed hierarchical multilevel MCMC approach in Dodwell et al. 2015 based on the Karhunen-Loeve expansion (KLE) that performs MCMC on the coarse grid problem and adds MCMC estimates of multilevel correction terms to account for the error between solutions on adjacent grids. While it has been shown to reduce the cost in comparison to standard MCMC for model 2D problems, a drawback is that the KLE-based hierarchy is not well-suited (and not even feasible) for 3D problems, as the KLE-based hierarchical sampling approach does not scale with the size of the problem. In this work, we explore a new PDE-based hierarchical sampling formulation based on algebraic multigrid and apply it to this existing multilevel MCMC framework. In particular, we form a scalable hierarchical sampling method for a 3D subsurface flow example, and investigate the cost reduction and scaling of this approach in comparison to standard MCMC. T.J. Dodwell, C. Ketelsen, R. Scheichl, and A.L. Teckentrup. A hierarchical multilevel Markov chain Monte Carlo algorithm with applications to uncertainty quantification in subsurface flow. SIAM/ASA Journal on Uncertainty Quantification, 3(1):1075–1108, 2015. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

15th U.S. National Congress on Computational Mechanics
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Title: On the Stability of the Nonlinear Reduction of Scale-Resolving Turbulent Flow Models

Author(s): *Charbel Farhat, *Stanford University*; Sebastian Grimberg, *Stanford University*;

The construction of nonlinear Projection-based Reduced-Order Models (PROMs) for scale-resolving, CFD-based, turbulent flow computational models using Large Eddy Simulation (LES), or when possible, Direct Numerical Simulation (DNS), is a topic of interest to the model reduction community. Such models exhibit multiscale features over large spatial and temporal ranges, which can pose problems for model reduction. Indeed, convection-dominated phenomena generally lead to the slow decay of the singular values of the snapshots computed to construct a Reduced-Order Basis (ROB). This means that in this case, PROMs typically require many modes to maintain solution accuracy, or may suffer a severe loss of information it the computed modes are truncated. Of specific concern however is the often reported numerical instability exhibited by nonlinear PROMs constructed for the fast solution of turbulent flow problems. It is often claimed that this instability originates in the removal of low-energy modes during the construction of the ROB, which eliminates the ability of the PROM to dissipate energy. Various approaches for remedying this instability have been proposed, including adding dissipation at the PROM level via some eddy-viscosity model. Unfortunately, this destroys consistency between the PROM and its underlying High-Dimensional computational Model (HDM). In this work, it is first pointed out that the aforementioned numerical instability has always been reported for Galerkin PROMs. Then, it is argued that this instability originates primarily in the Galerkin projection process. It is also shown that for numerous LES simulations, Petrov-Galerkin PROMs [1] exhibit a stable behavior. Hence, it is argued — with some theoretical support — that the multiscale nature of the flow problem may necessitate a large ROB in order to maintain accuracy, but the truncation of the ROB does not impact numerical stability. It is also shown that the error of the flow solution computed using a Petrov-Galerkin PROM monotonically decreases when the size of the ROB is increased. This is however generally false in the case of nonlinear Galerkin PROMs. Hence, it is concluded that it is better to construct a nonlinear PROM for an LES model using a Petrov-Galerkin than a Galerkin projection. References [1] K. Carlberg, C. Bou-Mosleh, C. Farhat, Efficient Non-linear Model Reduction via a Least-Squares Petrov-Galerkin Projection and Compressive Tensor Approximations, International Journal for Numerical Methods in Engineering, vol. 86, no. 2, pp. 155-181, 2011.

15th U.S. National Congress on Computational Mechanics
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Title: Performance Evaluation of a Two-Bar Bridge Rail Using Finite Element Analysis

Author(s): *Joshua Fatoki, *University of North Carolina at Charlotte*; Howie Fang, *University of North Carolina at Charlotte*; Emre Palta, *University of North Carolina at Charlotte*; Zheng Li, *University of North Carolina at Charlotte*;

Roadside barriers are important safety devices installed on highways to mitigate the severity of serious crashes by errant vehicles. Safety features such as longitudinal barriers are commonly used to contain and redirect errant vehicles. The two-bar metal bridge rail is a frequently used longitudinal barrier in North Carolina and is recognized for its performance and aesthetics. Currently, all safety devices used on U.S. highways must be tested to meet the safety criteria specified by the Manual for Assessing Safety Hardware (MASH) issued by the American Association of State Highway and Transportation Officials (AASHTO). While full-scale crash testing is a valid means to evaluate the safety performance of bridge rails, physical crash testing is very expensive, time-consuming, and difficult to perform. With the rapid development of computing hardware and commercial software for high performance computing, computer simulations have been increasingly used to assess the performance of roadside safety systems. In this study, the FE model of a two-bar bridge rail was developed and used in the evaluation of its compliance with MASH Test Level 3 (TL-3) requirements. The test vehicles used for MASH TL-3 tests include a small passenger car (a 2016 Toyota Yaris) and a pickup truck (a 2016 Chevy Silverado). The bridge rail was evaluated at an impact speed of 62 mph and at an angle of 25 degree [1]. Post-impact performance and structural adequacy of the Two-bar bridge rail were accessed and evaluated. Reference [1] AASHTO (2016). Manual for Assessing Safety Hardware (MASH-2), 2nd Edition. American Association of State Highway and Transportation Officials (AASHTO), Washington, D.C.

15th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification in Inelastic Problems via Stochastic Finite Element Methods

Author(s): *Nan Feng, *University of Notre Dame*; Guodong Zhang, *University of Notre Dame*; Kapil Khandelwal, *University of Notre Dame*;

Due to the inherent randomness in various systems, e.g. randomness in material properties, loading and boundary conditions, etc., deterministic approaches may not be able to satisfactorily characterize the system response. In such cases, stochastic approaches that can simulate various uncertainties have to be employed. In the past, a number of stochastic methods have been developed for uncertainty quantification (UQ), among which the perturbation methods, intrusive and non-intrusive polynomial chaos expansion (PCE) methods and stochastic collocation methods have received considerable attention. In the past, due to computational restrictions, most of the applications of these methods are confined to relatively simple problems, and the applicability and performance of these methods to complex nonlinear solid mechanics problems are not clear. This study carried out a detailed investigation on exploring the use of perturbation methods and non-intrusive PCE to inelastic solid mechanics problems. In particular, the use of these methods is considered in conjunction with elastoplastic and nonlocal coupled elastoplastic-damage models. Numerical studies are carried out to compare the performance of the considered UQ methods. The uncertainties in the inelastic system responses are quantified, and the importance of incorporating randomness for capturing the inherent variability in the system's response is demonstrated by comparing the results with deterministic models. Keywords: Stochastic Finite Elements; Perturbation Methods; Polynomial Chaos Expansion; Plasticity; Nonlocal Elastoplastic Damage.

15th U.S. National Congress on Computational Mechanics
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Title: Development of a Constitutive Model Incorporating a Deformation Dependent Stiffness for Soft Porous Media

Author(s): *Eanna Fennell, *University of Limerick*; Szymon Leszczynski, *Procter & Gamble Service GmbH*; Jacques Huyghe, *University of Limerick*;

Soft porous media have a wide range of applications from medical devices to tissue engineering to industrial health products. The numerical modeling of these porous structures can provide insight into their in-situ performance. However, an accurate constitutive model to replicate the stress-strain behavior of the process is essential in ensuring the efficacy of the simulation. A particular subset of soft porous media, known as super absorbents, are a form of hydrogel with the capability of swelling up to 100 times their original volume. As a result of this finite deformation, the stiffness of the structure changes dramatically throughout the course of swelling. Therefore, this study presents a constitutive equation incorporating a deformation dependent stiffness to model finite swelling in soft porous media. Experimental data of the response of stiffness to volumetric deformation for polyacrylate super absorbents of various cross-link densities is also presented. A Neo-Hookean strain energy density function is derived with respect to the right Cauchy Green strain tensor to define the effective Cauchy stress acting on the solid matrix of the gel. This constitutive equation is implemented into a mixed hybrid finite element model to replicate the large deformation of polyacrylate gels under osmotic loading. Through numerical simulations on spherical geometries using the experimental data as input, the effect of both cross-link density and dynamic stiffness is investigated against a control model. For each of the cross-link densities tested, the equilibrium swelling ratio differed significantly from the control model. The higher the cross-link density, the stiffer the gel and therefore a reduced equilibrium swelling ratio. The results align well with previous experimental studies on the effect of cross-link density on swelling gels. A stiffness gradient across the radius of the gel is also demonstrated as a result of the dynamic modulus. Subsequently, extremely large surface azimuthal stresses form. The higher cross-link density models experience higher stresses which correspond to a larger radial stiffness gradient. These large surface stresses are seen as the source of surface instabilities in many materials. In summary, a constitutive model accounting for dynamic stiffness and cross-link density is presented and numerically tested with experimental data. This model can be tailored to all applications of deforming soft porous media.

15th U.S. National Congress on Computational Mechanics
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Title: Computational Experience with Part-scale Modeling of Powder Bed Fusion Additive Manufacturing

Author(s): *Robert Ferencz, *Lawerence Livermore National Laboratory*; Rishi Ganeriwala, *Lawerence Livermore National Laboratory*; Ryan Vignes, *Lawerence Livermore National Laboratory*; Neil Hodge, *Lawerence Livermore National Laboratory*;

Many researchers are exploring thermomechanical modeling of the laser powder bed fusion (PBF) process to gain insights into residual stresses and distortions arising during this metal additive manufacturing process. This challenging problem encompasses a range of scales: temporally from miliseconds for local material transformation to hours and days for overall part fabrication; spatially from 100 microns for the local melt pool versus overall part dimensions [1]. Various approaches are being pursued to identify and implement abstractions rendering the problem computationally tractable while still yielding results providing meaningful insights. We are adapting a general purpose, nonlinear thermal-mechanical finite element code to model the PBF process [2]. First touching upon some of our earlier successes modeling PBF for a stainless steel [3], we survey more recent successes and challenges we have encountered as we attempt to model more general configurations and material systems. These efforts have motivated reexamination of our assumptions and approaches, pointing the way toward more general and robust modeling. References [1] W.E. King, A.T. Anderson, R.M. Ferencz, N.E. Hodge, C. Kamath, S.A. Khairallah, A.M. Rubenchik, “Laser powder bed fusion additive manufacturing of metals; physics, computational, and materials challenges”, Applied Physics Reviews, 2 (4) 041304 (2015). [2] N.E. Hodge, R.M. Ferencz, J.M, Solberg, “Implementation of a thermomechanical model for the simulation of selective laser melting”, Computational Mechanics 54 (1), 33-51 (2014). [3] N.E. Hodge, R.M. Ferencz and R.M. Vignes, “Experimental comparison of residual stresses for a thermomechanical model for the simulation of selective laser melting”, Additive Manufacturing, 12, 169-168 (2016).

_____ This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

15th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Multiple Deformable Bodies in Contact

Author(s): *Felipe Fernandez, *University of Illinois at Urbana-Champaign*; Mike Puso, *Lawrence Livermore National Laboratory*; Jerome Solberg, *Lawrence Livermore National Laboratory*; Daniel A. Tortorelli, *Lawrence Livermore National Laboratory*;

Works in topology optimization of structures with contact boundary conditions are primarily restricted to the two-dimensional rigid obstacle problem. This is because the contact analysis of multiple three-dimensional deformable bodies with meshes which are non-matching across the contact interface requires state-of-the-art contact algorithms which are computationally complex and as such have been beyond the scope of previous investigations. Our research is devoted to addressing topology design problems with multiple deformable three-dimensional components in contact using state-of-the-art contact algorithms. We formulate and resolve the design simulation problem using large deformation continuum mechanics and the finite element method. The contact conditions are discretized via the mortar segment-to-segment approach which provides smooth force variations over the contact surface. Since the contact problem is computationally expensive to solve, we solve the optimization problem using efficient nonlinear programming algorithms which require the sensitivities of the cost and constraint functions. To this end, we formulate analytical adjoint sensitivity expressions to compute the gradients of general functionals. Additionally, we use a B-spline design parameterization to reduce the number of design variables compared to usual element-wise parameterizations and regularize the topology optimization problem. Numerical examples are presented to validate our study.

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Title: Continuum and Multiscale Modeling of Rubber Toughened Glassy Polymers at Finite Strains

Author(s): *Bernardo Ferreira, *Department of Mechanical Engineering, Faculty of Engineering, University of Porto*; Mohsen Mirkhalaf, *Chalmers University of Technology, University of Gothenburg*; Francisco Pires, *Department of Mechanical Engineering, Faculty of Engineering, University of Porto*;

Over recent years, the modeling of heterogenous multi-phase materials has been a topic of extensive research by the scientific community. Among other approaches, computational homogenization-based multiscale modeling has emerged as an effective way to relate the macroscopic behaviour of materials with their underlying heterogeneous microstructure by continuous interchange of information between scales. Under the key assumption of the principle of separation of scales, the hierarchically coupled multi-scale finite element method is based on the nested solution of two coupled boundary value problems: (i) at the macroscale, where the material's macroscopic response is sought, and (ii) at the microscale, where computations are conducted over representative volume elements in order to account for microstructural phenomena in the macroscopic response, through an homogenization procedure. A considerable effort has been made by the scientific community to develop constitutive models that are able to accurately describe the deformation behaviour of polymeric based materials. Concerning their fracture thoughness, it is well known that glassy polymers show brittle behaviour, particulary under specific conditions such as low temperatures and high strain rates. One important and well-known technique to improve their fracture toughness is termed rubber toughnening, which consists in dispersing rubbery particles in the polymeric matrix in order to hinder the propagation of microfractures. Associated with these rubbery particles is the phenomenon of internal cavitation, meaning that they will behave as voids during the deformation of the rubber toughened polymer. In the present contribution, a continuum constitutive model is developed in order to predict the behaviour of porous polymeric materials. This model fully couples the finite strain elasto-viscoplastic constitutive model proposed by Mirkhalaf et al. [1] with the yield surface of the well-known micromechanical void growth model proposed by Gurson [2]. A first order homogenization-based multiscale model [3] is then employed to critically assess the predictive ability of the developed continuum model, through several numerical comparisons between the continuum approach and the homogenized response of a voided representative volume element. [1] Mirkhalaf, S. M., Pires, F. M. A., and Simoes, R. (2016). An elasto-viscoplastic constitutive model for polymers at finite strains: Formulation and computational aspects. Computers and Structures, 166:60–74. [2] Gurson, A. L. (1977). Continuum theory of ductile rupture by void nucleation and growth: Part I – yield criteria and flow rules for porous ductile media. Journal of Engineering Materials and Technology, 99. [3] Reis, F.J.P. & Andrade Pires, F.M. (2013). An Adaptative Sub-incremental Strategy for the Solution of Homogenization-based Multi-scale Problems, Computer Methods in Applied Mechanics and Engineering, Vol. 257, pp. 164– 182.

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Title: Error Estimation and Goal-Oriented Adaptation for High-Order Hybridized Discontinuous Galerkin Methods

Author(s): *Krzysztof Fidkowski, *University of Michigan*;

This talk presents techniques for estimating numerical errors and optimizing computational meshes for high-order hybridized discontinuous Galerkin (HDG) methods. We consider both the standard HDG method and the embedded discontinuous Galerkin (EDG) method. EDG offers memory and computational time advantages compared to both the discontinuous Galerkin (DG) method and to DG through its decoupling of elemental degrees of freedom and the introduction of continuous face degrees of freedom that become the only globally-coupled unknowns. In hybridized DG methods, additional equations of weak flux continuity on each interior face introduce new residuals that augment output error estimates and complicate existing element-centric mesh optimization methods. This work presents a technique for converting face-based error estimates to elements and sampling their reduction with refinement in order to determine element-specific anisotropic convergence rate tensors. The sampling uses fine-space adjoint projections and does not require any additional solves on subelements. Together with a degree-of-freedom cost model, this error model for hybridized discretizations drives metric-based unstructured mesh optimization. Adaptive results for two-dimensional flow problems demonstrate the improvement of mesh optimality when using the new error model compared to one that does not incorporate face errors, and performance benefits of hybridization relative to the traditional discontinuous Galerkin method.

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Title: CRIMSON, an Open-source Computational Hemodynamics Platform: Present and Future

Author(s): *C. Alberto Figueroa, *University of Michigan*; Christopher J. Arthurs, *King's College London*;

In this lecture we will provide an overview of CRIMSON, a computational hemodynamics platform based on state-of-the art open-source standards for medical image data visualization and segmentation, mesh generation, boundary condition specification, multi-scale formulations for boundary condition specification, fluid-structure interaction methods, and more (www.crimson.software). In addition to discussing the capabilities of the platform, we will describe ongoing work in the fields of simulation of coupled scalar transport problems, methods for machine learning, and cloud computing. We will finish the presentation summarizing aspects of the open-sourcing process, and the infrastructure set in place to aid with global participation of the community of users.

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Title: Patient-specific Multiscale Computational Modeling of Pulmonary Arterial Hypertension

Author(s): *Vasilina Filonova, *University of Michigan*; Christopher Tossas, *University of Michigan*; Hamidreza Gharahi, *Michigan State University*; Seungik Baek, *Michigan State University*; C. Alberto Figueroa, *University of Michigan*;

We present the patient-specific computational modeling of blood flow in compliant pulmonary vasculature to study the progression of Pulmonary Arterial Hypertension (PAH). Progressive thickening and stiffening of distal pulmonary vessels yield to an increase in pulmonary arterial pressure which can lead to fatal right heart failure. Thus, from a modeling perspective there is a need to couple the hemodynamics in distal and proximal vasculature beds with vessel wall growth and remodeling formulations. This leads to a multi-scale fluid-structure interaction problem in space and time. First, we must estimate the homeostatic baseline state for the distal pulmonary arterial tree [1] by means of homeostatic optimization based on energetic considerations and a previously developed fluid-solid growth formulation. The distal vasculature is represented by a fractal tree. Pulsatile blood flow in the distal tree is calculated from analytical solutions using Womersley's theory of pulsatile flow in deformable vessels [2]. This approach includes pulse wave propagation and provides an input impedance function for outflow boundary conditions on the proximal vasculature. Second, the blood flow simulations in the proximal pulmonary vessels are conducted in the fluid-solid interaction solver (CRIMSON) using patient-specific anatomical and physiological data of pediatric patients with PAH (acquired in collaboration with Michigan Medicine clinicians). This solver is based on the Coupled-Momentum Method, recently verified against Womersley's theory deformable wall analytical solution [3]. Lastly, we will discuss the needs and challenges of building representative models of the distal pulmonary arterial tree using mice lung data. References [1] V. Filonova, H. Gharahi, N. Nama, S. Baek, and C. A. Figueroa, "A Multiscale Framework for Defining Homeostasis in Vascular Trees: Applications to the Pulmonary Circulation," Submitted. [2] J. R. Womersley, "Oscillatory Flow in Arteries?: the Constrained Elastic Tube as a Model of Arterial Flow and Pulse Transmission," Phys. Med. Biol., vol. 2, no. 2, pp. 178–187, 1957. [3] V. Filonova, C. J. Arthurs, I. E. Vignon-Clementel, and C. A. Figueroa, "Verification of the Coupled-Momentum Method with Womersley's Deformable Wall Analytical Solution," Submitted.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: State Reconstruction of Highly Flexible Structures

Author(s): *Timothy Fitzgerald, *Gonzaga University*;

The combination of high speed photogrammetry, geometrically exact finite element models, and extended Kalman filters provides a very general tool capable of reconstructing the motion of complicated structures. This work presents the formulation, implementation, and demonstration of this tool on test structures. High-speed photogrammetry of complicated systems presents a useful method to measure the dynamics of a system without contacting it. This can be advantageous when it would be difficult or too time-consuming to alter or modify a system my mounting sensors. Additionally if the structure is very light, such as in biological systems like flying insects, mounting sensors is not an option. Issues arise since the use of correlated image data is incomplete and noisy. The entire surface of a body's motion may not be visible throughout a dynamic event, thus introducing more uncertainty. To mitigate this, as well as provide an estimate of the error, an extended Kalman filter is used to approximate the states of a geometrically exact finite element model. Though computationally expensive, this filter is well-studied and robust. The finite elements are discretized in time using the Generalized alpha method, which is a member of the well-known Newmark family of time stepping methods. Previous efforts include the use of shadow castings to build the maximal volume in which the deformed body must be inside. The minimization of an energy function then provided a solution for the state of the body for a specific instance in time. This method does not provide an estimate of the uncertainty, and that motivates the use of the extended Kalman Filter. This filter also permits the generalization to uncertainty in the parameters of the structure as well. This work presents tests on several mechanically excited structures. It is the first step towards building the apparatus to study free-flying insects. Using multiple, synchronized cameras to capture free flying insects permits natural untethered flight and behaviors to be captured, reconstructed, and analyzed. The ability to accurately reconstruct the motion of free flying insects presents a treasure trove of data. Using this information as inputs to numerical fluid-structure simulations would permit modeling and load estimation.

15th U.S. National Congress on Computational Mechanics
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Title: Coupled Multibody and Finite Element Modeling of Rail Substructure

Author(s): *Craig Foster, *University of Illinois at Chicago*; Ahmed El-Ghandour, *Ozen Engineering*; Mohammad Hosein Motamedi, *Rowan University*; Sarvesh Masurekar, *University of Illinois at Chicago*;

Railway substructure, including ties, ballast, subballast, and subgrade, plays an important role in the support of the train as well as drainage, damping of vibrations, and other functions. While sophisticated models of train and rail-wheel interaction have been developed in the rail industry, the effects of the substructure are often neglected or treated with very simple models such as discrete springs. In this research, we employ a co-simulation approach, coupling a high-fidelity multibody code developed to simulate a locomotive and rail-wheel interaction, with a finite element model for the track and substructure. The finite element model is developed and, for the linear case, modal information is exported into the multibody software SAMS/rail. For efficiency, the mode shapes are truncated to only include the nodes in contact with the other bodies, those on the rail in this case. In this way a relatively complicated substructure can be represented without adding greatly to the computational cost. Using the stiffness of the substructure model, the multibody runs the dynamic train-track simulation in the time domain, calculating the rail contact force and modal deformation. Using modal displacements, the deformation, and stress in the entire substructure over time can be reconstructed. The model shows that simplified representations of the substructure are not always accurate [1], and that the new model can better predict some deformation characteristics of the soil. The model is applied to the bridge approach problem, where well documented changes in the stiffness at the approach slab can result in high contact forces and track quality degradation. Variable-thickness approach slabs are modeled as a potential solution. The model is also applied to examining vibrations in nearby structures from passing trains. Finally, soil nonlinearity is modeled through an iterative procedure. A viscoplastic model is used to simulate permanent displacement under loads. The contact forces from the train are determined from the linear case and run in the finite element model to determine permanent settlement, tangent stiffness, and geometric forces. Preliminary results of the settlement at a stiffness transition are shown. [1] A.I. El-Ghandour, M.B. Hamper, and C.D. Foster. “Coupled Finite Element and Multibody Dynamics Systems Modeling of a 3D railroad system”. Journal of Rail and Rapid Transit, Vol. 230 No. 1, 2016, 283-294. DOI: 10.1177/0954409714539942

15th U.S. National Congress on Computational Mechanics
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Title: Coupling FEM and Meshfree Peridynamics for the Simulation of Hydraulic Fracturing

Author(s): *John Foster, *The University of Texas at Austin*; Jason York, *The University of Texas at Austin*;

Over the last several years we have developed a nonlocal multiphysics model based on peridynamic theory for the simulation of hydraulic fracture processes.As we've added complexity including fully implicit poromechanics and plasticity to the model, we have struggled with expensive computational run times even while utilizing a massively parallel implementation of the full peridynamics model. In this talk, we present a coupling method for simulating hydraulic fracture growth with peridynamics in regions near the fractures and using a standard Galerkin finite element formulation with adaptive mesh refinement in regions far from the growing fractures. This includes a method of converting the finite element nodes to meshfree peridynamics nodes “on the fly”. The model, implementation, and efficacy of the technique are discussed.

15th U.S. National Congress on Computational Mechanics
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Title: Multiscale Modeling of Soil Loaded by the Detonation of Buried Explosives

Author(s): *David Fox, *US Army Research Laboratory*; Justin McKee, *US Army Research Laboratory*; Robert Spink, *US Army Research Laboratory*;

Continuum and grain scale methods for the treatment of soil are combined to yield grain scale dynamic outputs suitable for application to problems involving the response of flesh and fabric subjected to erosion by high velocity soil particles. In the present work buried explosives are used to accelerate the soil. The explosive is modeled at the continuum scale using a general particle algorithm, programmed burn detonation kinetics, and a Jones Wilkins Lee equation of state to model the expansion of the explosive's detonation product gases. Next, the soil is modeled at a continuum scale, also using the general particle method, along with a hybrid elastic plastic approach to the treatment of the constitutive and yield behavior. Finally, the mass and momentum flux of the continuum scale particles passing through a relevant control surface are measured and used as boundary conditions for the much smaller elements used to model the high velocity dynamics of the soil at the grain scale.

15th U.S. National Congress on Computational Mechanics
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Title: Predicting the Mechanical Response of Oligocrystals with Deep Convolutional Neural Networks

Author(s): *Ari Frankel, *Sandia National Laboratories*; Reese Jones, *Sandia National Laboratories*; Coleman Alleman, *Sandia National Laboratories*; Jeremy Templeton, *Sandia National Laboratories*;

Additive manufacturing is an attractive approach for developing highly customizable parts, but the resulting parts can demonstrate a high variability in their mechanical properties. This variability is often due to differences in the parts at a microstructural level, including grain structure, pores, and defects. Predicting the effects of these microstructural properties can be challenging and often relies on inaccurate semi-empirical treatments of homogenized properties. Rather than relying on such normative approaches, data-driven models have been increasingly gaining attention for their high capacity and flexibility in application to different problems. In this study we consider the use of advanced deep neural network architectures to learn the mechanical properties of microstructures directly from computational realizations of the oligocrystal aggregates. We will first discuss the dataset, in which randomly textured oligocrystals were subjected to uniaxial tension through elastic and plastic flow. The question of representing the individual grain orientations under crystal symmetry for machine learning purposes will also be discussed. We apply deep neural networks to predict the elastic and plastic response of these microstructures and compare the predictions to bounds from classical homogenization theory. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

15th U.S. National Congress on Computational Mechanics
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Title: Phase Field Modeling of Microstructure Evolution during Solidification at Varying Cooling Rates

Author(s): *Yao Fu, *University of Cincinnati*; Balachander Gnanasekaran, *University of Cincinnati*;

Designing novel structural materials with complex shape and geometry is enabled with the advancement of additive manufacturing processes, to meet specific performance requirements that are not imaginable with traditional subtractive manufacturing techniques. The microstructure evolution during the repeated heating/cooling process determines the various properties of manufactured products. Modeling and simulation can advance our fundamental understanding of the underlying physical processes. In this study, we demonstrate the microstructure evolution involving the nucleation and grain growth of a binary alloy during the continuous cooling process via a combined multiphase field model and stochastic nucleation computational model. The nuclei are initiated by adding into the total free energy a term of the nucleation energy related to the variables that represents grains of different orientation. It was found that the temperature dependent nucleation rate and interface mobility are the main materials properties controlling the features of the resultant microstructures. More even-sized and fine grains can be formed under a high cooling rate given the specified temperature dependent nucleation rate. Solute trapping is the most prominent and solute segregation is the slightest at the highest cooling rate. Equipped with a grain-tracking method, this computational framework provides a viable and computationally efficiently pathway to investigate the large-scale microstructure evolution under various temperature histories that could occur in manufacturing processes.

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Title: Using High-order DPG Finite Element Methods to Study Form-wound Medium-voltage Coils

Author(s): *Federico Fuentes, *Cornell University*; Leszek Demkowicz, *ICES, The University of Texas at Austin*; Aleta Wilder, *CEER, The University of Texas at Austin*;

A geometry relevant to form-wound medium-voltage coils sitting inside large electric machinery was analyzed in detail. This included studying its behavior under an array of physical scenarios involving different forcing and boundary conditions ranging from low-frequency thermoviscoelastic effects to high-frequency Lorentz forces. High-order discontinuous Petrov-Galerkin (DPG) finite element methods were used to simulate these scenarios. Their inherent stability along with their natural a posteriori error indicators were fundamental in being able to resolve the fine details of the solutions produced by the computations.

15th U.S. National Congress on Computational Mechanics
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Title: Representative Volume Element and Irreducible Brillouin Zone Path Choice for Complete Band Gap Search in 3D Acoustic and Phononic Crystals

Author(s): *Pavel I. Galich, *Rice University*; Edwin L. Thomas, *Rice University*;

Recent advances in computational facilities and commercial finite element software such as COMSOL Multiphysics enabled exploration of many new designs of 3D acoustic and phononic crystals. Recall that acoustic crystals are utilized for managing pressure wave propagation in air or liquid, while phononic crystals are used for control of elastic pressure and shear waves propagating in solids. A main goal of the majority of current publications is finding and reporting the biggest complete band gap – the frequency region where waves of all polarizations are forbidden to propagate in all directions. However, frequently the choice of the representative volume element (RVE) and the first irreducible Brillouin zone (IBZ) are not consistent. Usually the particular choice of the IBZ path for declaring complete (omnidirectional) band gaps is not justified, and, moreover, it is inadequate for claiming a complete band gap. In this talk, we will propose a methodology for correctly defining RVE and IBZ path for band gap analysis in periodic structures. We demonstrate using both 3D acoustic and phononic crystals with face- and body-centered cubic Bravais lattices how an incorrect choice of RVE and IBZ path can lead to erroneous conclusions regarding omnidirectional or especially directional band gaps.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Global Equilibrium in Computational Methods Coupling Peridynamics with Classical Mechanics

Author(s): *Ugo Galvanetto, *Dept. Industrial Engineering, University of Padua, Italy*; Tao Ni, *College of Civil and Transportation Engineering, Hohai University, Nanjing, China*; Greta Ongaro, *Dept. Industrial Engineering, University of Padua, Italy*; Pablo Seleson, *Computer Science and Mathematics, Oak Ridge National Laboratory, USA*; Mirco Zaccariotto, *Dept. Industrial Engineering, University of Padua, Italy*;

Coupling of PD-based software with computational tools using classical mechanics to solve problems of structural engineering is the topic of a growing research effort [1-3]. The aim of that is to generate a computational method exhibiting the efficiency of those based on classical mechanics and the capability to simulate crack propagation problems typical of peridynamics. An often-overlooked issue in the use of coupled computational methods is the verification of overall structural equilibrium: coupling different models of solid mechanics, to describe the mechanical behavior of a body, can affect the satisfaction of the equilibrium equations for the overall body. Simple examples of statically determinate structures, partially discretized with a PD method and partially with a classical mechanics FEM approach, will illustrate the problem. In our examples, using the coupling method presented in [2], the magnitude of the out of balance forces is small, compared to that of the acting forces, but it cannot be assumed to be a numerical error. We observe that this is the case even if the method described in [2] satisfies the usual numerical tests: rigid body motion, uniform strain cases, patch test ... Our work will examine how the variation of various features of the coupled model, such as position and size of the PD region, length of the coupling boundary, rate of change of the strains …, can affect the magnitude of the out of balance forces. Moreover, we will propose new criteria for coupling methods in order to reduce the magnitude of the out of balance forces. 1) SA Silling, M Epton, O Weckner, J Xu, E Askari, ‘Peridynamic states and constitutive modeling’, Journal of Elasticity 88 (2), 2007, 151-184. 2) Mirco Zaccariotto, Teo Mudric, Davide Tomasi, Arman Shojaei, Ugo Galvanetto, ‘Coupling of FEM meshes with Peridynamic grids’, Computer Methods in Applied Mechanics and Engineering, Volume 330, 1 March 2018, Pages 471-497. 3) P. Seleson, Y.D. Ha, S. Beneddine, Concurrent Coupling of bond-based Peridynamics and the Navier equations of classical elasticity by blending, Int. J. Multiscale Comput. Eng. 13 (2), 2015, 91–113. The authors U. Galvanetto and M. Zaccariotto would like to acknowledge the support they received from University of Padua under the research project BIRD2017 NR.175705/17.

15th U.S. National Congress on Computational Mechanics
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Title: Generation of Extensive Virtual Topology Layers to Enable Automatic CAD Topology Suppression During Meshing

Author(s): *Mark Gammon, *ITI Ltd*; Sam Whyman, *ITI Ltd*; Chris Fellows, *ITI Ltd*;

Summary: CAD clean-up and simplification is an expensive bottleneck that is often quoted [1] as the source of meshing failures and delays. The clean-up process often involves manual modifications to the CAD geometry, introducing deviations from the intended design. We present an alternative approach that is based on the generation of extensive virtual topology (VT) layers that suppress geometrically irrelevant topology, e.g. short edges and sliver faces. Each VT layer is embedded in a robustly parametrised C1 continuous surface formed of Clough Tocher patches [2]. The VT layers act as an accurate replacement for the CAD geometry enabling rapid but accurate mesh generation without the constraint of respecting irrelevant CAD details. Details: VT layers are typically generated from collections of tangential CAD faces. One of the key strengths of the approach we will present is that the VT layers can be very extensive and highly non-planar. The VT layers can also contain regions of non-tangential faces, e.g. a small step that is below the desired mesh resolution and should not feature in the final mesh. For a VT layer to be used for mesh generation a suitable global parametrisation needs to be generated across the collection of CAD faces in the VT layer. To achieve this a curved triangular mesh using Clough Tocher patches is generated from the original CAD surfaces with adaptive refinement that guarantees sufficient capture of the CAD details. The curved mesh is the parametrized using a novel combination of the ARAP [3] parametrisation technique combined with a robust untangling strategy. We will demonstrate the robustness of the VT layer generation on examples of complex real-world CAD geometry. Finally the parametrized VT layers will be meshed using a Delaunay-based meshing algorithm coupled with a robust adaptive curvature refinement stage capable of working across large VT layers that contain significant areas of localised high curvature. [1] NASA, "CFD Vision 2030 Study: A Path to Revolutionary Computational Aerosciences," NASA CR-2014-218178, 2014. [2] R. Clough and J. Tocher, "Finite element stiffness matrices for analysis of plates in bending," in Conference on Matrix Methods in Structural Mechanics, Wright Patterson Air Force Base, Ohio, 1965. [3] L. Liu, L. Zhang, Y. Xu, C. Gotsman and S. Gortler, "A Local/Global Approach to Mesh Parameterization," in Eurographics Symposium on Geometry Processing, 2008.

15th U.S. National Congress on Computational Mechanics
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Title: Solutal-thermocapillary Phenomena in Additive Manufacturing

Author(s): *Zhengtao Gan, *Northwestern University*; Wing Liu, *Northwestern University*;

To introduce chemical inhomogeneities within the liquid metal pool and attempt to manipulate the melt pool dynamics and solidification, we postulate that melt pool dynamics and resulting crystal microstructure can be predictably manipulated by surface-active agents. This prediction requires a predictive theory and in-/ex-situ validation experiments and we believe it could improve final product reliability and printability of material systems in additive manufacturing. Here, dynamics within the melt pool is described as solutal-thermocapillary flow: a surface-tension-driven flow with chemical inhomogeneities in the form of solutes.

15th U.S. National Congress on Computational Mechanics
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Title: Effect of Part Geometry on Process Control and Modeling during Laser Powder Bed Fusion

Author(s): *Rishi Ganeriwala, *Lawrence Livermore National Laboratory*; Neil Hodge, *Lawrence Livermore National Laboratory*; Robert Ferencz, *Lawrence Livermore National Laboratory*; Nachiket Patil, *Lawrence Livermore National Laboratory*; Wayne King, *Lawrence Livermore National Laboratory*;

The production of metal parts via laser powder bed fusion (L-PBF) additive manufacturing is rapidly growing. However, parts built via L-PBF may exhibit critical defects, such as porosity and/or high residual stresses and distortion. These issues can often be mitigated through appropriate selection of process parameters. These optimal process parameters will vary as a function of material and part geometry. Frequently, it is also necessary to vary the process parameters throughout an individual build as thermal conditions within a part evolve. For example, certain geometries will heat up during a build, especially if they contain large overhangs or increasing cross-sectional areas. Being able to predict the temperature evolution of such parts is a critical component of feed forward process parameter control to avoid overheating, which can lead to increased defects. This temperature evolution additionally needs to be captured properly for any model to produce accurate residual stress predictions at the part scale. In this work the multiphysics finite element code Diablo, developed at Lawrence Livermore National Laboratory, is used to simulate the interlayer part temperature throughout an entire build for various geometries. Adaptive mesh refinement is employed to run these simulations at nearly the physical layer scale. Experimental validation of the actual interlayer part temperature is provided from data taken using a calibrated forward-looking infrared (FLIR) camera. These experimental measurements help inform the necessary amount of physics required in a model to accurately predict these temperatures. The effects of various modeling simplifications on accuracy will be explored. Finally, the ramifications of the predicted interlayer temperature on feed forward process control and residual stress modeling will be discussed. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

15th U.S. National Congress on Computational Mechanics
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Title: Data-driven Multiscale Modeling for Unidirectional Carbon Fiber Reinforced Polymer

Author(s): *Jiaying Gao, *Northwestern University*; Gino Domel, *University of Notre Dame*; Wing Kam Liu, *Northwestern University*;

In this work, a data-driven multiscale modeling framework for Unidirectional (UD) Carbon Fiber Reinforced Polymer (CFRP) is presented. A UD CFRP microstructure database is established through the two-stage Self-consistent Clustering Analysis (SCA) [1-3], a Reduced Order Modeling (ROM) approach including an offline data compression by unsupervised learning, and online stage of UD CFRP responses prediction with decent efficiency and accuracy. The UD CFRP database can be integrated directly into any composite structures to provide physical UD material responses under arbitrary loading conditions. The macroscale structure and the microscale constituents stress, strain, and stage variables evolution are captured simultaneously. This work will link microstructure and macroscopic structure responses for general Polymer Matrix Composites (PMC), allowing one to investigate the effect of basic constituents on the final structure performance. To illustrate the potential of the framework, a sample case study of a composite bolted joint is analyzed. Reference: 1. Liu, Zeliang, M. A. Bessa, and Wing Kam Liu. "Self-consistent clustering analysis: an efficient multi-scale scheme for inelastic heterogeneous materials." Computer Methods in Applied Mechanics and Engineering 306 (2016): 319-341. 2. Liu, Zeliang, Mark Fleming, and Wing Kam Liu. "Microstructural material database for self-consistent clustering analysis of elastoplastic strain softening materials." Computer Methods in Applied Mechanics and Engineering 330 (2018): 547-577. 3. Bessa, M. A., et al. "A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality." Computer Methods in Applied Mechanics and Engineering 320 (2017): 633-667.

15th U.S. National Congress on Computational Mechanics
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Title: Stress Modulated Phase Transition in 2D Materials

Author(s): *Wei Gao, *University of Texas at San Antonio*;

The polymorphism of 2D transition metal dichalcogenides (TMDs) has shown great potential for applications in electrical and optoelectronic devices. Single-layered TMDs appears in two distinct symmetries: the 2H and 1T phases. The two phases exhibit completely different electronic structures, with the 2H phase being semiconducting and the 1T phase metallic. In addition, the transition between these two phases can be modulated by external stress. In this talk, using MoTe2 as a model material, I will present our recent computational study on the mechanism of stress dependent phase transition. Our results will shed light on the application of MoTe2 by strain engineering.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Dynamic Behavior Modeling of Core-Shell Si Nano-particles Cycling under Impact Loading

Author(s): *Xiang Gao, *UNCC*; Jun Xu, *UNCC*;

Silicon is one kind of promising electrode materials for Lithium-ion batteries in the near future because of its high capacity. But the large volume expansion/contraction of Si during lithiation/delithiation cycling have been the main barrier of its broad application. In order to reduce the impact of this volume change, many managements have been proposed in the Si electrode. Core-shell structure is a typical configuration in stress management of Si and some experimental and numerical studies have been carried out on this structure. Nonetheless, few works were done about the dynamic behaviors of core-shell structured (CSS) Si nanoparticles under impact loadings. Dynamic behaviors of the CSS Si nanoparticle during electrochemical cycling were modeled in a finite element software. A core-shell-structured model that contained a Si nanoparticle wrapped with amorphous carbon was established. The system containing two touching CSS Si nanoparticles were charged and discharged under different voltages with an impact loading applied on the surface of one particle. The volume change and associated stress simulated by the model without external loading were compared with the experiment data and matched well. The effects of the amorphous carbon with different thicknesses on the volume change and stress evolution in the particles were calculated. Besides, the effects of loading rate were introduced into this model to see the dynamic effects on the stress evolution and failure behavior of the Si particles. The present study showed a best combination of charge/discharge strategy and the thickness of wrapping layer and illustrate the dynamic behavior under impact loading, which would give guidance for the Si based battery design and help to understand the coupling effects of dynamic loading and electrochemical cycling on Si.

15th U.S. National Congress on Computational Mechanics
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Title: A General Approach to Efficiently Compute Derivatives with Hypercomplex Finite Element Methods Using a Block Solution Scheme

Author(s): *Manuel Garcia, *Angelo State University*; Andres Aguirre, *University of Texas at San Antonio*; Harry Millwater, *University of Texas at San Antonio*; Daniel Ramirez, *University of Texas at San Antonio*; Mauricio Aristizabal, *Universidad EAFIT*;

Hypercomplex finite element analysis is a numerical technique that allows the computation of arbitrary order derivatives by redefining the problem in terms of hypercomplex variables. A perturbation is applied to the imaginary axis of the independent variables. Then the problem is operated using hypercomplex-algebra, usually by overloading operators, and derivative information is recovered from the imaginary values of the solution. The method has been successfully used in a variety of problems as: crack propagation [1], fluid mechanics, bioheat transfer [2], nonlinear materials, plasticity, and shape sensitivity, among others. While the method is accurate and easy to use, its main drawback is the high memory requirements and long computing times. This work presents advances in a general approach for hypercomplex differentiation called block solver. By using the Cauchy-Riemann matrix representation of a hypercomplex variable the finite element sensitivities can be calculated as a particular load case of the original system. The highlight of this method is that it unifies and automates other well-known methodologies such as direct differentiation and the semi analytical method. The method has been integrated to the commercial finite element software Abaqus through user element subroutines. A numerical implementation for a linear elastic case of study shows that a new sensitivity can be calculated in less than 30% of the standard real-variable solution time. [1] A. Montoya, D. Ramirez Tamayo, H.R. Millwater, and M. Kirby, “A Complex-Variable Virtual Crack Extension Finite Element Method for Elastic-Plastic Fracture Mechanics, Engineering Fracture Mechanics”, 202 (2018) 242-258 [2] J. Monsalvo, M. García, H Millwatter, Y. Feng. Sensitivity analysis for radiofrequency induced thermal therapies using the complex finite element method. Finite Elements in Analysis and Design. 2017, Vol 135,C, p 11-21.

15th U.S. National Congress on Computational Mechanics
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Title: A Graph Theoretic Framework for Representation, Exploration and Analysis on Computed States of Physical Systems

Author(s): *Krishna Garikipati, *University of Michigan*; Rik Banerjee, *University of Michigan*; Koki Sagiyama, *Imperial College, Lonton*; Gregory Teichert, *University of Michigan*;

A graph theoretic perspective is taken for a range of phenomena in continuum physics in order to develop representations for analysis of large scale, high-fidelity solutions to these problems. Of interest are phenomena described by partial differential equations, with solutions being obtained by computation. The motivation is to gain insight that may otherwise be difficult to attain because of the high dimensionality of computed solutions. We consider graph theoretic representations that are made possible by low-dimensional states defined on the systems. These states are typically functionals of the high-dimensional solutions, and therefore retain important aspects of the high-fidelity information present in the original, computed solutions. Our approach is rooted in regarding each state as a vertex on a graph and identifying edges via processes that are induced either by numerical solution strategies, or by the physics. Correspondences are drawn between the sampling of stationary states, or the time evolution of dynamic phenomena, and the analytic machinery of graph theory. A collection of computations is examined in this framework and new insights to them are presented through analysis of the corresponding graphs.

15th U.S. National Congress on Computational Mechanics
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Title: Explicit and Implicit Approaches for Characterization and Fracture Analysis of Anisotropic Rock

Author(s): *Justin Garrard, *University of Tennessee*; Reza Abedi, *University of Tennesee*; Robert Haber, *University of Illinois at Urbana-Champaign*;

Fracture in rock as a heterogeneous brittle material, having significant inherent randomness, requires including probabilistic considerations at different scales. Crack growth in rocks is generally associated with complex features such as crack-path oscillations as well as microcrack and crack branching events. Two methods will be presented to address rock inhomogeneity and anisotropy. In the first method, microcracks are explicitly realized in a domain based on specific statistics of crack length and location. In the second, a statistical model implicitly represents an inhomogeneous field for fracture strength. We use statistical volume elements to derive an angle-dependent fracture strength for a given population of in-situ microcracks and construct a mesoscopic fracture-strength field, In contrast to the explicit approach, no macroscopic cracks exist at the initial time of a failure analysis. Cracks are only nucleated at weak points of the domain (based on the mesoscopic fracture-strength field) and / or at stress concentration points. Both approaches can be applied to rock in which the natural fractures are biased to specific orientations. as in, for example, bedding planes in sedimentary rocks. At the macroscale, crack growth is modeled by an interfacial damage / contact model. We will present an effective stress (a scalar stress value to derive the damage evolution) that is consistent with the Mohr-Coulomb model. The Mohr-Coulomb model and the interaction between friction angle and rock bedding planes produce interesting physics. Under a uniaxial stress loading and an isotropic rock strength, the Mohr-Coulomb model predicts cracks at angles +/-(45 - ??????where ??is the friction angle. Introduction of anisotropic rock strength not only alters the angles, it also favors one angle over the other. We will present numerical results that demonstrate the effect of anisotropy on compressive rock fracture with explicit and implicit approaches. In addition, we demonstrate how the statistics of an in-situ population of microcracks, e.g., the mean and standard variation of microcrack length, affects the macroscopic response. For a given problem set-up we show that a more uniform population of in-situ microcracks results in higher fracture strength and toughness at the macroscale. However, these advantages are offset by more brittle rock response.

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Title: A Fictitious Domain Approach for Fluid-Structure Interaction

Author(s): *Lucia Gastaldi, *University of Brescia*;

The approach of the fluid-structure interaction problem with the fictitious method is originated from the finite element version of the Immersed Boundary Method (FE-IBM) developed by Peskin in the finite difference framework. Actually, the introduction of a Lagrange multiplier allows to consider the FE-IBM as a Fictitious Domain formulation for FSI for which existence and uniqueness results have been proved. We are going to present some results on the analysis of the scheme including error estimates both in time and space and the stability of a time splitting approach. At the end, we shall show how our technique can handle the case of compressible solids as well.

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Title: Efficient Preconditioning of hp-FEM Matrices by Hierarchical Low-Rank Approximations

Author(s): *Paolo Gatto, *RWTH Aachen University*; Jan Hesthaven, *Ecole Polytechnique Federale de Lausanne (EPFL)*;

In this talk, I will introduce a preconditioner based on low-rank compression of Schur complements. The construction is inspired by the well-known nested dissection strategy, and relies on the assumption that the Schur complements that arise in the elimination process can be approximated, to high precision, by compressible matrices. The preconditioner is built as an approximate LDM^t factorization of a given matrix A, and no knowledge of A in assembled form is required by the construction. The LDM^t factorization is amenable to fast inversion, and the inverse can be applied fast as well. I will present numerical experiments that investigate the behavior of the preconditioner in the context of Discontinuous Galerkin finite element approximations of positive-definite problems, as well as indefinite wave propagation problems.

15th U.S. National Congress on Computational Mechanics
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Title: Multi-phase Topology Optimization for Additive Manufacturing: Elimination of Enclosed Pores in Self-supporting Structures

Author(s): *Andrew Gaynor, *U.S. Army Research Laboratory*; Raymond Wildman, *U.S. Army Research Laboratory*;

In order to properly harness the potential of additive manufacturing (AM), one must design to the capabilities of the machine. Beyond the typical self-supporting design requirement for additive manufacturing to eliminate sacrificial support material [1,2] (an extremely popular topic in topology optimization (TO) for AM), it is also critical to design-away the occurrence of topological features that trap unprocessed material. For example, laser powderbed fusion (LPBF) AM has the opportunity to trap powder, while stereolithography (SLA) AM may trap resin. To address these needs, a multi-phase, projection-based method is presented to concurrently design for the guarantee of self-supporting structures and for the elimination of enclosed pores. The presented TO algorithm, which has been generalized to work with typical unstructured meshes, ultimately employs the same underlying “path-dependent” algorithmic logic to tackle both design considerations. Here, the solid projection phase designs for the self-supporting condition, where the solid must “grow” from a specified direction – the build plate – at allowable prescribed angles (machine dependent). Likewise, the void projection phase designs for enclosed void elimination, stipulating that voids must “grow” from defined surfaces, guaranteeing an exit path for all void regions. The two phases are combined in a typical, weighted multi-phase TO approach. The combined algorithm is first demonstrated in 2D, allowing for the voids to “exit” in specified directions. As more void design freedom is allowed through an embedded multi-projection scheme, the optimization problem’s nonlinearity relaxes. Since the algorithm severely constrains the design space in 2D, it is extensively demonstrated in 3D for various combinations of self-supporting overhang angle and void drainage diameters. Beyond exhibiting the novel multiphase approach, there will be discussion of implementation details and observed behavior and trends. Notably, the additional phase adds computational cost, but, contrary to initial expectations, the added complexity allows for an easier exploration of the design space. This often results in superior performing solutions when compared to the aforementioned single-phase self-supporting TO algorithm [1]. There will be additional discussion on extensions to design for sacrificial support structures and other pertinent additive manufacturing considerations. [1] Johnson, T., Gaynor, A. “Three-dimensional projection-based topology optimization for prescribed-angle self-supporting additively manufactured structures,” Additive Manufacturing Journal, vol 24, pp 667-686, 2018. [2] Langelaar, M. “An additive manufacturing filter for topology optimization of print-ready designs,” Structural and Multidisciplinary Optimization, vol 55(3), 871–883, 2016.

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Title: An Extended Phase-field Finite Element Method for Fracture Using Numerically Constructed Enrichment Functions

Author(s): *Rudy Geelen, *Duke University*; John Dolbow, *Duke University*;

Phenomena spanning multiple spatial scales and encompassing multiple physics disciplines are prevalent in many modern engineering applications. For example, structural failure is often caused by microstructural crack growth and coalescence. Over recent years, much attention has focused on gradient-based damage and phase-field models of fracture, see e.g. Miehe et al. (IJNME, 2010) and Lorentz and Godard (CMAME, 2011). However, a persistent limitation in these approaches is that resolving the regularization length scale with high fidelity can be extraordinarily expensive under traditional analysis techniques. The use of highly refined finite element meshes is imperative to accurately capture the physics of localized interacting cracks. While the computational expense of phase-field models has recently gained more importance, we know of no universally effective remedy. In this talk we outline a computational framework for regularized crack propagation based on the two-scale approach using coarse-generalized FEM meshes from Duarte and Kim (CMAME, 2008). Such a procedure combines classical global-local finite element method concepts with the partition of unity approach. It involves the solution of local boundary value problems using boundary conditions from a global problem defined on a coarse discretization. These local solutions are, in turn, employed to enrich the global space using the partition of unity framework. The method can handle approximation spaces which evolve in time by updating enrichment functions generated from local boundary value problems throughout the analysis while maintaining a fixed global mesh. In this work we describe an implementation for two-way coupled phase-field descriptions of multi-crack propagation. For problems exhibiting strong localization, as is common in quasi-brittle fracture, the fine-scale domain is updated on the fly to minimize the computational effort.

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Title: A Framework for Hex-dominant Meshing

Author(s): *Christos Georgiadis, *Universite catholique de Louvain*; Jean-François Remacle, *Universite catholique de Louvain*;

In this presentation, we will present a complete framework that aims at generating hex-dominant meshes in a robust fashion. Starting from a triangulation (STL), a 3D frame field is computed and surfaces are remeshed accordingly. A volulme mesh is subsequently generated using the same frame field. A hex-dominant mesh is finally produced, possibly including boundary layers. This research has been developed in the framework of the HEXTREME ERC Advanced Grant project.

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Title: Recent Advancements for Multifidelity UQ and OUU in Dakota: Capability Overview and Perspectives

Author(s): *Gianluca Geraci, *Sandia National Laboratories*; Michael Eldred, *Sandia National Laboratories*; Alex Gorodetsky, *University of Michigan*; John Jakeman, *Sandia National Laboratories*;

The Dakota software (http://dakota.sandia.gov [1]) is the premier vehicle at Sandia National Laboratories for delivering both state-of-the-art research and robust, usable software for optimization, uncertainty quantification (UQ) and optimization under uncertainty (OUU). Its architecture and algorithmic advancements are motivated by the need to handle complex applications spanning defense programs for DOE and DOD, climate modeling, computational materials, nuclear power, renewable energy, and many others. Often, these complex physical/engineering systems require high-fidelity, computationally-intensive simulations to accurately represent the range of physics of interest. In addition, this increasing level of complexity is often accompanied by an increasing number of sources of uncertainty that affect the physical/numerical modeling. The combined effect of the large number of uncertain parameters and the high numerical cost of each realization makes both UQ and OUU extremely challenging. In order to alleviate this prohibitive numerical cost, we have invested in the development and implementation of multilevel/multifidelity strategies. The main idea is to aggregate a small number of high-fidelity evaluations with a large number of realizations from less expensive, lower accuracy models to decrease the aggregate computational cost without sacrificing the accuracy of these methods. In this talk, we will present an overview of Dakota's multilevel/multifidelity capabilities, spanning sampling and surrogates-based approaches for UQ and derivative-free and gradient-based methods for OUU. We will show several examples of their deployment for realistic applications and also provide a preview of generalized multilevel/multifidelity capabilities that we are currently developing for future Dakota releases. [1] Adams, B.M., Bauman, L.E., Bohnhoff, W.J., Dalbey, K.R., Ebeida, M.S., Eddy, J.P., Eldred, M.S., Hough, P.D., Hu, K.T., Jakeman, J.D., Stephens, J.A., Swiler, L.P., Vigil, D.M., and Wildey, T.M., "Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.0 User’s Manual," Sandia Technical Report SAND2014-4633, July 2014. Updated November 2018 (Version 6.9).

15th U.S. National Congress on Computational Mechanics
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Title: A Numerical Verification of the inf-sup Conditions of a Class of Mixed Finite Element Methods for Nonlinear Elasticity

Author(s): *Ali Gerami Matin, *Ph.D. Candidate at George Washington University*; Arzhang Angoshtari, *Assistant Professor at George Washington University*;

We study the stability of a class of three-field mixed finite element methods for nonlinear elasticity called CSFEMs near regular solutions. To this end, we write suitable material-independent and material-dependent inf-sup conditions. The material-independent condition is only a necessary condition for the stability while the material-depend one is sufficient as well. By considering several combinations of first-order and second-order elements, we study the validity of these inf-sup conditions by using singular values associated to the matrix form of the inf-sup conditions.

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Title: On Penalization Of Irreversibility In Variational Phase-Field Modeling Of Brittle Fracture

Author(s): *Tymofiy Gerasimov, *Technische Universität Braunschweig, Germany*; Laura De Lorenzis, *Technische Universität Braunschweig, Germany*;

Irreversible evolution is one of the central concepts as well as implementation challenges of both the variational approach to fracture by Francfort and Marigo (1998) and its regularized counterpart by Bourdin, Francfort and Marigo (2000, 2007 and 2008) commonly referred to as a phase-field model of (brittle) fracture. Irreversibility of the crack phase-field imposed to prevent fracture healing leads to a constrained minimization problem, whose optimality condition is given by a variational inequality. In our study, the irreversibility is handled via simple penalization. Provided the penalty constant is well-tuned, the penalized formulation is a good approximation to the original one, with the advantage that the induced equality-based weak problem enables a much simpler algorithmic treatment. We propose an analytical procedure for deriving the optimal penalty constant, more precisely, its lower bound, which guarantees a sufficiently accurate enforcement of the crack phase-field irreversibility. Our main tool is the notion of the optimal phase-field profile, as well as the so-called gamma-convergence result. It is shown that the explicit lower bound is a function of two formulation parameters (the fracture toughness and the regularization length scale) but is independent on the problem setup (geometry, boundary conditions etc.) and the formulation ingredients (degradation function, tension-compression split etc.). The optimally-penalized formulation is tested for two benchmark problems, including one with available analytical solution. We also compare our results with those obtained by using the alternative irreversibility technique based on the notion of the history field by Miehe et al. (2010).

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Title: A New Time-splitting Scheme for Unfitted Mesh Approximations of FSI with Immersed Solids

Author(s): *Fannie Gerosa, *Inria Paris, J.-L. Lions Laboratory (UPMC)*; Miguel Ángel Fernández, *Inria Paris, J.-L. Lions Laboratory (UPMC)*;

The mechanical interaction of an incompressible viscous fluid with an immersed structure appears in a wide variety of engineering fields (from micro-encapsulation to aeroelasticity) and is particularly ubiquitous in nature (from heart valves to the wings of a bird). For this type of multi-physics systems, Nitsche based unfitted mesh approximations are very appealing from a mathematical and computational point of view (see [1]). Indeed, they allow for weak and strong discontinuities, respectively in the discrete velocity and the pressure (which guarantees accuracy), and are Lagrange multiplier free (no additional unknowns are introduced). These advantages come however at a price: the weak treatment (à la Nitsche) of the kinematic coupling complicates the design of efficient time splitting schemes (i.e., which avoid strong coupling). For instance, standard loosely coupled schemes do not necessarily retain their time splitting features when formulated in an unfitted mesh framework (see [2]). In this work we generalize the projection based semi-implicit coupling paradigm introduced in [3] to the case of unfitted mesh approximations with cut-elements. The fundamental idea consists in combining a fractional-step time-marching of the unfitted mesh fluid approximation with an explicit-implicit treatment of the interface conditions (which avoids added-mass stability issues). The proposed method retains the time-splitting features and the energy stability properties of the original splitting scheme with fitted meshes. Numerical results in 2D, motivated by biomedical applications and involving dynamic interfaces, illustrate the capabilities of the proposed approach. References: [1] E. Burman, M.A. Fernández. An unfitted Nitsche method for incompressible fluid–structure interaction using overlapping meshes. Comput. Methods Appl. Mech. Engrg., vol. 279, pp. 497-514, 2014. [2] M.Landajuela, M.A.Fernández. Unfitted mesh formulations and splitting schemes for incompressible fluid/thin-walled structure interaction. IMA J. Numer. Anal., DOI: 10.1093/imanum/dry098, 2018. [3] M.A. Fernández, J.-F. Gerbeau and C. Grandmont. A projection semi-implicit scheme for the coupling of an elastic structure with an incompressible fluid. Int. J. Num. Meth. Engrg., vol. 69, num. 4, pp. 794–821, 2007.

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Title: Modeling Fracture in 3D Printed Polymer Materials Considering Layer Interfaces and Surface Patterns

Author(s): *Rojin Ghandriz, *PhD student, Mechanical Engineering Department, University of Massachusetts Dartmouth, North Dartmouth, M.A*; Jun Li, *Assistant Professor, Mechanical Engineering Department,University of Massachusetts Dartmouth, North Dartmouth, M.A*;

Additive manufacturing (or 3D printing) is coming of age as a viable advanced manufacturing technology that is already serving a substantial impact on a wide variety of subdivisions, from biomedical, electronics, automotive to aerospace industries. However, the reduced fracture resistance often observed in 3D printed materials limits its application to functional components. The fracture of 3D printed polymer materials with various layer orientations and surface patterns is studied using the extended finite element method (XFEM) and phase filed fracture method (PFFM) implemented in finite element software ABAQUS [1,2]. The XFEM with cohesive segment approach is employed to model the inter-laminar fracture (fracture between layers), cross-laminar fracture (fracture through layers), as well as mixed inter-/cross- laminar fracture of 3D printed specimens made of acrylonitrile-butadiene-styrene (ABS) materials. Both elastic and elastic-plastic fracture models are developed for the inter-laminar and cross-laminar fracture, respectively. For mixed inter-/cross- laminar fracture, an anisotropic damage model is developed to predict the kinked crack propagations. The model was implemented through user-defined damage initiation subroutines with ABAQUS/XFEM to capture fracture behaviors under various layer orientations. Furthermore, various 3D printed surface patterns are studied to enhance the fracture resistance. A robust PFFM is developed to predict the complicated crack deflections in 3D printed samples with patterned surfaces. 1. J. Li, S. Yang, D. Li, V. Chalivendra. Numerical and experimental studies of additively manufactured polymers for enhanced fracture properties. Engineering Fracture Mechanics, 204 (2018) 557–569. 2. M.A. Msekh, J.M. Sargado, M. Jamshidian, P.M. Areias, T. Rabczuk. Abaqus implementation of phase-field model for brittle fracture. Computational Materials Science 96(2015) 472484.

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Title: Multi-fidelity Diffusion Map Projections

Author(s): *Roger Ghanem, *University of Southern California*;

Diffusion maps synthesized from physics model of varying fidelity provide ROMs that are adapted both to the underlying physics and the particular training set. Each of these ROMs is defined by an RKHS. In this presentation we investigate the relationships between these RKHS and discuss the accuracy and pitfalls of multi-fidelity pooling using DMAPS. Examples will be drawn using problems from across science and engineering.

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Title: Hemodynamics and Homeostatic Conditions in a Multiscale Model of the Coronary Arterial Tree

Author(s): *Hamidreza Gharahi, *Michigan State University*; Seungik Baek, *Michigan State University*; Vasilina Filonova, *University of Michigan*; C. Alberto Figueroa, *University of Michigan*; Ravi Namani, *Michigan State University*; Lik Chuan Lee, *Michigan State University*;

Coronary arteries are responsible for supplying oxygenated blood to myocytes in the cardiac wall. In addition, the coronary microcirculation plays a major role in maintaining homeostasis of the heart and responding to the changes in the workload of the heart via autoregulatory responses. The coronary circulation, however, is unique among the regional vascular beds in that its microvascular network of vessels is embedded inside the myocardium and is constantly under compressive forces from the myocytes. Since the intramyocardial pressure varies across the ventricular walls, the homeostatic (e.g. equilibrium) baseline state of the arteries and their autoregulatory response depends heavily on their transmural location in the heart wall. Therefore, there is a crucial need to identify the structural and functional differences in arteries located at different layers of the myocardium. The objective of the present study is, therefore, to estimate the homeostatic states of the distal coronary arterial tree and model their hemodynamics. We construct a multi-scale model of the coronary arterial tree whereby each vessel is composed of collagen fibers, elastin, and smooth muscle cells. Using an extension of Murray's law [1], each vessel radius and wall compositions are determined as a target state via a minimization problem involving the metabolic cost of maintaining the blood volume, the power needed to overcome viscous drag by the blood flow, and the metabolic cost of the vessel wall constituents. The problem is optimized under the constraint of mechanical equilibrium imposed through steady state hemodynamics and interaction of vessel wall with the surrounding myocardium [2]. Once the composition and the geometry of the arteries are estimated, the stiffness of each individual blood vessel can be calculated using the small on large theory [3]. Then, the baseline characteristics of the arterial tree will be used to study the pulsatile hemodynamics of the coronary vessels and their autoregulatory response. References [1] S. B. Lindström et al. Biomech. Model. Mechanobiol., 14 (2015), 83-91. [2] D. Algranati et al. Am. J. Physiol. Heart Circ. Physiol., 298 (2010), H861–H873 [3] S. Baek et al., Comput. Methods Appl. Mech. Engrg. 196 (2007), 3070-3078.

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Title: A Robust Approach for Patient-specific Parameter Estimation of Lumped Coronary Boundary Conditions in a Case of Intermediate Coronary Stenosis

Author(s): *Arash Ghorbanniahassankiadeh, *Marquette University and the Medical College of Wisconsin*; John F. LaDisa, Jr., *Marquette University and the Medical College of Wisconsin*;

Autoregulation and vasodilation are two important control mechanisms of the coronary vasculature. These mechanisms are influenced by the flow-dependent significance of intermediate epicardial stenosis, which makes parameter estimation of boundary conditions an iterative and time-consuming process. Therefore, a robust parameter estimation approach is required to replicate these physiological mechanisms under rest and pharmacological stress at a reasonable computational cost. An Idealized aortic model with intermediate stenoses in the left coronary artery having fractional flow reserve (FFR) values of 0.7-0.9 was used to study the local hemodynamics of the epicardial coronary system. Computational fluid dynamics was performed using an open source software package (Simvascular; simtk.org) to solve the time-dependent Navier-Stokes equations. Inflow boundary conditions consisting of a time-varying blood flow waveform were imposed at the aortic inlet. A five-element coronary boundary condition was used to model the out-of-phase behavior of the coronary vasculature [2]. An open-loop iterative approach was used for parameter estimation under rest and pharmacological stress conditions (i.e. 140 µg/kg/min Adenosine). The parameter estimation process was based on whether the downstream vasculature was in autoregulatory or maximum vasodilation states, differentiated by a threshold of 40 mmHg. A modified Bernoulli approach was used to estimate the epicardial pressure drop across the stenosis due to viscous and separation loss [1]. Results show FFR of 0.8 in the case with minimum lumen area (MLA) 4.5 mm2, which is in close agreement with standard threshold criteria for percutaneous coronary intervention of a left main stenosis [3] and points to the accuracy of simulations. It was observed that using pressure-flow relationship specific to the hemodynamic state of coronary vasculature (i.e. constant and linear in autoregulatory and maximum vasodilation, respectively) can result in less computational cost compared to traditional tuning algorithms. [1] Duncker DJ, Koller A, Merkus D, Canty JM Jr. (2015) Regulation of coronary blood flow in health and ischemic heart disease. Prog Cardiovasc Dis 57: 409–422. [2] Kim HJ, et al. Patient-specific modeling of blood flow and pressure in human coronary arteries. Ann Biomed Eng. 2010; 38:3195–3209. [3] Park SJ, Ahn JM, Kang SJ et al. Intravascular ultrasound-derived minimal lumen area criteria for functionally significant left main coronary artery stenosis. JACC Cardiovasc Interv. 2014; 7:868–74.

15th U.S. National Congress on Computational Mechanics
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Title: A Semi-Implicit Algorithm for the Simulation of High-Z Plasma Interpenetration

Author(s): *Debojyoti Ghosh, *Lawrence Livermore National Laboratory*; Thomas Chapman, *Lawrence Livermore National Laboratory*; Richard Berger, *Lawrence Livermore National Laboratory*; Jeffrey Banks, *Rensselaer Polytechnic Institute*; Dylan Copeland, *Lawrence Livermore National Laboratory*;

High-energy density physics (HEDP) experiments often involve laser-induced counterstreaming plasmas that interpenetrate each other and interact through electrostatic and collisional forces. The simulation of such flows requires a multifluid model that allows distinct velocity fields for the plasma streams. Recently, we developed EUCLID (Eulerian Code for pLasma Interaction Dynamics) [1] that solves the inviscid Euler equations for each plasma stream and species. This approach allows distinct flows, including cases where the same species need to be partitioned into multiple populations or streams. The fluids interact with each other through electrostatic forces, friction, and thermal equilibration. We further simplify our model by assuming inertia-less electrons and a quasi-neutral plasma, and remove the necessity to solve the Poisson's equation for the electrostatic potential. One of the primary challenges in solving the resulting equations is that the collisional (friction and thermal equilibration) time scales are significantly faster than the acoustic and advective time scales. This difference is exacerbated for higher-Z species such as aluminum and gold. Explicit time integration methods are thus inefficient since the time steps are constrained by the collisional scales. We investigate the use of high-order implicit-explicit (IMEX) Additive Runge-Kutta (ARK) methods, where the friction and thermal equilibration terms are integrated implicitly in time, while the advective flux and the electrostatic terms are integrated explicitly. The equations are discretized in space on a three-dimensional Cartesian grid using a conservative finite-difference formulation and the 5th order MPWENO scheme. The semi-implicit time integration results in a nonlinear system of equations that are solved using the Jacobian-free Newton-Krylov approach. In this talk, we report on our implementation and we present simulations of several one- and two-dimensional plasma interpenetration cases that are representative of the HEDP experiments. In particular, we present results showing the interaction of high-Z species. [1] D. Ghosh et al., "A Multispecies, Multifluid Model for Laser-Induced Counterstreaming Plasma Simulations", Submitted. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 and funded by the LDRD Program at LLNL under project tracking code 17-ERD-081. LLNL-ABS-765541

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Title: A posteriori Error Bounds for Linear and Nonlinear Reduced Order Models: Application to Uncertainty Quantification

Author(s): Nurtaj Hossain Md, *Indian Institute of Science, Bangalore*; *Debraj Ghosh, *Indian Institute of Science, Bangalore*;

Usage of reduced order models (ROM) of dynamical systems has emerged as a very effective way of reducing computational cost. Its efficiency is more pronounced when the solution of higher dimensional model (HDM) is sought at multiple parameter values. However, due to approximation in a lower dimensional subspace, ROMs incur error in the solution. Moreover, since ROMs are trained for a particular set of parametric values, they lack robustness. To address these two issues, first, two a posteriori error bounds are developed for linear and nonlinear dynamical systems, respectively, based on the residual in the governing differential equation. For uncertainty quantification, these error bounds are then used in conjunction with a greedy search algorithm. The greedy search is performed using a multi-frequency particle swarm optimization. To get an accelerated convergence, at each iteration of the greedy search, the ROM is updated for the global as well as for few local maxima. Numerical studies are performed on structural vibration and Burgers' equation to demonstrate the accuracy and efficiency of the proposed error bounds and the algorithm. Proper orthogonal decomposition based ROMs are used for these studies. Failure probability estimated using the adaptive ROM is found to match closely with the estimate using the HDM. A significant speed up is achieved.

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Title: Coupling CPFEM with Phase Field Modeling from Crack Propagation in Polycrystalline Materials

Author(s): *Somnath Ghosh, *Johns Hopkins University*; Jiahao Cheng, *Oak Ridge National Laboratory*; Ahmad Shahba, *Johns Hopkins University*;

Modeling fracture in polycrystalline materials is computationally complicated due the grain morphology, material anisotropy and heterogeneous deformation fields. This talk will discuss a coupled crystal plasticity FE model (CPFEM) of deformation analysis and phase-field model (PFM) for crack propagation, to predict failure in polycrystalline metals and alloys. Tasks in this module will include: A. Image-Based Microstructural CPFEM: Microstructure-based statistically equivalent representative volume elements (M-SERVEs) of polycrystalline and polyphase microstructures are generated from experimentally obtained 2D or 3D data from EBSD and SEM data. These SERVEs form the computational domains for image-based, time-dependent finite strain crystal plasticity FE models (CPFEM). Dislocation density-based rate-dependent crystal plasticity model with evolution of statistically stored dislocations (SSDs) and geometrically necessary dislocations (GND) are implemented for modeling deformation. B. Coupled Phase-Field CPFEM for Crack Propagation in Polycrystalline Microstructures: The phase field modeling (PFM) manifests a regularized discontinuous crack surface by introducing an auxiliary scalar field variable to represent the crack topology. A hallmark of PFM is defining a Helmholtz free energy density, which is a function of both the displacement field, internal state variables representing the defect state and crack phase field. It leads to a two-way coupling between the displacement field and crack phase field. A severe limitation of PF models coupled with CPFEM is high computational cost associated with extremely fine mesh resolutions. A wavelet-based hierarchical adaptation method will be developed for projecting evolving variables from the scale of crystal plasticity simulations in CPFEM to that of phase field simulations. This projection will transfer elastic and defect energy densities from the coarse crystal plasticity mesh to the fine phase field mesh for driving the phase field evolution, and also to transfer the phase field variables back to CPFE simulations. The talk will discuss a variety of methods in ICME for coupling image-based crystal plasticity FEM with PFM in the pursuit of propagating cracks in polycrystalline microstructures of Ti and Al alloys.

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Title: Influence of Thermomechanical Loads on the Energetics of Precipitation in Magnesium Aluminum Alloys

Author(s): *Swarnava Ghosh, *California Institute of Technology*; Kaushik Bhattacharya, *California Institute of Technology*;

Magnesium is the lightest among most commonly used structural metals, and has a high strength to weight ratio, and therefore has the potential to be significantly integrated into a wide range of applications. Existing magnesium alloys show low spall strength, which inhibits their applicability in dynamic environments. Magnesium alloys achieve their desirable mechanical properties via age hardening, and controlling the size of precipitates is necessary for spall strength. We use first principles calculations to understand the energetics of precipitation in magnesium-aluminum binary alloys and report the influence of thermomechanical loads on the energetics of the precipitation process.

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Title: Asynchronous and Heterogeneous Coupling for Co-Simulation of Fluid-Structure Interaction

Author(s): *Marie Gibert, *Lamcos, Université de Lyon, Insa Lyon, CNRS UMR 5259, F-69621, France and ANSYS France SA*; Aline Bel-Brunon, *Lamcos, Université de Lyon, Insa Lyon, CNRS UMR 5259, F-69621, France*; Michaël Brun, *GEOMAS, Université de Lyon, Insa Lyon,F-69621, France*; Michel Rochette, *ANSYS France SA*; Anthony Gravouil, *Lamcos, Université de Lyon, Insa Lyon,F-69621, France*;

This abstract presents a coupling method for fluid-structure interaction problems, validated using the piston test case introduced by Piperno. This method is inspired by the GC coupling methods, which involves coupling several structural sub-domains with their own temporal integrations and spatio-temporal scales, without any loss of energy. Concerning FSI, various methods have already been proposed, due to the numerous fields of application. Most of them are partitioned methods, where the problem is treated as uncoupled, which is easy to implement but lacks accuracy due to the time-lag involved by the method. The other methods are monolithic, more efficient in terms of stability and accuracy but also diffcult to implement and generalize. One improvement, among others, was the extension of the GC method to FSI problems. For instance, Meduri has recently proposed a fully Lagrangian finite elements coupling for fluid and structural sub-domains. The aim here is to extend this coupling method to more classical spatio-temporal discretization methods for each sub-domain. The middle-term objective is to build a co-simulation methods using commercial codes, from Ansys products. In this way, the structural sub-domain is discretized in space by the finite elements method and in time by the Newmark implicit scheme. The fluid sub-domain is discretized by the finite volume cell centered method and explicit second order Rung-Kutta scheme. The coupling condition of velocities continuity is driven thanks to the Lagrange multiplier methods. Finally, each sub-domain is driven by its proper time-step. Thus the proposed method takes full advantage of both partitioned and monolithic methods; the monolithic formulation ensuring the energy conservation, and the asynchronous and heterogeneous co-simulation algorithm allowing the generalization. REFERENCES [1] Gravouil, Combescure, Brun. Heterogeneous asynchronous time integrators for computational structural dynamics, Int. J. Numer. eth. Engng, 102(3), 2015. [2] Piperno, Farhat, Larrouturou. Partitioned procedures for the transient solution of coupled aroelastic problems Part I: Model problem, theory and two-dimensional application, Computer Methods in Applied Mechanics and Engineering,124(1), 79-112, 1995. [3] Meduri, Cremonesi, Perego, Bettinotti,Kurkchubasche ,Oancea . Tpartitioned fully explicit Lagrangian Finite Element Method for highly nonlinear Fluid-Structure-Interaction problems, Numerical Methods in Engineering, 113(1), 43-64, 2017.

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Title: Fast Simulations of Coupled Flow and Geomechanics in Ultra-Low Permeability (ULP) Reservoirs Via Reduced-Order Modeling

Author(s): *Eduardo Gildin, *Texas A&M University*; Horacio Florez, *Texas A&M University*;

Global model reduction has been applied extensively in reservoir simulation to mitigate the high computational cost of multiphase flow but, its application to combined multiphysics, as in the case of flow and geomechanics, has been minimal [1]. This work focuses on the development of accurate and fast simulation models for Ultra-Low Permeability (ULP) reservoirs, i.e., tight-sands and shales. We rely on projection-based Model-Order Reduction (MOR) techniques, namely POD-DEIM to reduce the ULP's computational burden. The usage of global basis is not convenient to tackle problems characterized by different regimes, i.e., depletion/build-up. Also having many snapshots to capture all these variations is unfeasible. We thus develop a strategy based on local POD basis to reduce one- and two-way coupled flow and geomechanics computations [2]. Preliminary results focused on linear and nonlinear thermo-poroelasticity, show that our MOR algorithm provides substantial single and double digits speedups, up to 50X if we combine with multi-threading assembling and perform MOR on both physics [3]. [1]. Tan, X., Gildin, E., Florez, H. et al. Comput Geosci (2018). "Trajectory-based DEIM (TDEIM) model reduction applied to reservoir simulation". https://doi.org/10.1007/s10596-018-9782-0 [2]. H Florez, E Gildin. Model-Order Reduction Applied To Coupled Flow and Geomechanics. Published at the European Conference on the Mathematics of Oil Recovery (ECMOR XVI held in Barcelona, Spain. 3 - 6 September 2018. [3]. H Florez, E Gildin. "Fast Simulations of Coupled Flow and Geomechanics in Ultra-Low Permeability (ULP) Reservoirs Via Reduced-Order Modeling and Hyper-reduction". Accepted to be presented at the SPE Reservoir Simulation Conference, Apr 2019., Galveston, Texas, USA

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Finite Element Analysis of Non-reciprocal Wave Propagation in Mechanically-Modulated Continuous Elastic Metamaterials

Author(s): *Benjamin Goldsberry, *The University of Texas at Austin and Applied Research Laboratories*; Samuel Wallen, *Applied Research Laboratories*; Michael Haberman, *The University of Texas at Austin and Applied Research Laboratories*;

Elastic metamaterials with time- and space-dependent effective material properties have received great attention as a means to induce non-reciprocal wave propagation. These materials have promise for applications such as improved acoustic communication devices, vibration isolation components and others. Recent analytical models of spring-mass chains have shown that external application of a nonlinear mechanical deformation, when applied on time scales that are slow compared to the characteristic times of propagating linear elastic waves, may induce non-reciprocity via changes in the apparent elastic modulus for perturbations around that deformation [Wallen et al., Phys. Rev. E., 99, 013001, (2019)]. Unfortunately, it is rarely possible to derive analogous analytical models for continuous elastic metamaterials due to their complex unit cell geometry. In this talk, we present a finite element approach to simulate elastic wave propagation in mechanically-modulated metamaterials. A full transient simulation of the mechanical deformation and elastic wave propagation may not be practical due to computational burdens associated with extracting propagating modes of interest from a broadband signal in complex geometry. Instead, we utilize the small-on-large approximation to separate the nonlinear mechanical deformation (the “large” wave) from the superimposed linear elastic waves (the “small” waves), which are then analyzed via Bloch wave analysis with a Fourier expansion in the harmonics of the modulation frequency. This approach is implemented on a metamaterial supercell to account for the modulation wavelength. Distributed-memory parallel processing is utilized to decrease computation time. Results on non-reciprocal wave propagation in negative stiffness honeycombs, a structure exhibiting large stiffness modulations due to the presence of mechanical instabilities [Correa et al., Rapid Prototyping J., 21(2), 193-200, (2015)], are then shown as a case example. [Work supported by National Science Foundation EFRI award number 1641078.]

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Title: Fluid-Structure Interaction Modeling of Cyclic Aspiration for Acute Ischemic Stroke Patients

Author(s): *Bryan Good, *Pennsylvania State University*; Francesco Costanzo, *Pennsylvania State University*; Scott Simon, *Penn State Health Milton S. Hershey Medical Center, Hershey*; Keefe Manning, *Pennsylvania State University*;

An estimated 700,000 acute ischemic strokes (AIS) occur annually in the United States[1] due to embolic occlusion of a cerebral artery. Despite improved recanalization rates with new stent retriever devices, over 15% of patients cannot be recanalized and another 17% die within 90 days despite successful recanalization[1]. In order to investigate the underlying mechanics of a lodged embolus and determine its optimal surgical removal procedure, we are developing a continuum-based fluid-structure interaction (FSI) model to simulate dislodgement under cyclically applied aspiration. The model will allow for patient-specific geometries, blood and thromboemboli properties, and hemodynamic conditions to be investigated. The current modeling framework combines established viscoelastic blood and embolus models with a cohesive zone model for the interface between the embolus and artery wall. While no computational model has been developed specifically for this interface, cohesive zone concepts have been used for coarsely ligated biofilms and will be used here to apply a traction force as a function of the interface opening displacement and rate[2]. Our primary hypothesis is that a thromboemboli can be removed at lower pressure magnitude under cyclic aspiration compared to static aspiration[3] and avoid fracture and distal embolization. To investigate this hypothesis, all constitutive models were implemented in OpenFOAM in a tightly-coupled finite-volume FSI framework. This framework has been used previously by our group for simulating diaphragmatic motion in Pediatric VADs. To validate the computational solver, an experimental flow loop was developed to track the displacement of an embolus under controlled cyclic aspiration. The flow loop consists of medical aspirator, solenoid valve, Arduino controller, 3D-printed middle cerebral artery chamber, and a rubber embolus analog. Cyclic pressures were applied near the embolus surface via an aspiration catheter at 1 Hz to mimic previous experimental studies[3]. The embolus analog’s motion was then tracked and analyzed with in-house Matlab code to compare with computational predictions. Extreme cases of embolus and cohesive zone properties were investigated (deformable embolus with an infinitely stiff cohesive zone and a rigid embolus with a deformable cohesive zone). Following the solver’s validation in this simplified geometry, patient specific cerebral artery anatomies and their local hemodynamics, currently being collected from AIS patients, will be incorporated into the FSI solver in order to simulate actual surgical aspiration procedures. 1. Grech et al. The Neuroradiology Journal. 2015. 2. Costanzo. International Journal of Engineering Science. 1998. 3. Simon et al. Journal of Neurointerventional Surgery. 2013.

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Title: Unifying Multifidelity Sampling Approaches as Approximate Control Variates

Author(s): *Alex Gorodetsky, *University of Michigan*; Michael Eldred, *Sandia National Laboratories*; Gianluca Geraci, *Sandia National Laboratories*; John Jakeman, *Sandia National Laboratories*;

We consider variance reduction for Monte Carlo sampling algorithms for propagating uncertainty through computational simulation models when additional simulators of varying fidelity are available. Our goal is to estimate, or predict, quantities of interest from a specified high-fidelity model when only a limited number of such simulations is available. To aid in this task, lower fidelity models can be used to reduce the uncertainty in the high-fidelity predictions. We have developed a novel framework that unifies existing variance reduction sampling approaches such as multilevel, multi-index, and multifidelity Monte Carlo through the lens of an approximate control variate. Specifically, we have created a general framework for analyzing the statistical properties, i.e., variance reduction, of approximate control variate estimators. For instance, we demonstrate that existing sampling approaches are in-fact sub-optimal realizations of our framework; they cannot obtain the same variance reduction performance that would be achieved by an optimal (non-approximate) linear control variate scheme. We then describe several estimators arising from this framework that do converge to the optimal linear control variate. Often such estimators can achieve orders of magnitude reduction in estimator variance relative to existing approaches for equivalent computational cost. Examples are demonstrated on both synthetic problems as well as prototypical problems in fluid dynamics.

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Title: Instability-induced Pattern Formations in Soft Magnetoactive Composites

Author(s): *Artemii Goshkoderia, *Department of Aerospace Engineering, Technion - Israeli Institute of Technology*; Vincent Chen, *Air Force Research Laboratory, Wright-Patterson AFB*; Jian Li, *Department of Aerospace Engineering, Technion - Israeli Institute of Technology*; Abigail Juhl, *Air Force Research Laboratory, Wright-Patterson AFB*; Philip Buskohl, *Air Force Research Laboratory, Wright-Patterson AFB*; Stephan Rudykh, *Department of Mechanical Engineering, University of Wisconsin - Madison*;

We study magnetomechanical instabilities in magnetoactive elastomer (MAE) composites undergoing finite strains in the presence of a magnetic field. In particular, we consider MAE composites with chain-like microstructure. We analyze the influence of the applied magnetic field along the chains on the stability of the MAE composites at both microscopic and macroscopic [1] length scales [2]. To this end, we develop a numerical scheme to detect the onset of instabilities at the long wave and finite length-scales. By applying the developed numerical technique, we analyze the influence of the materials microstructure geometrical parameters and applied magnetic field on the onset of instabilities in soft MAEs. We found that under some the identical MAE composites with periodically distributed particles can switch to a variety of new patterns with different periodicity under particular levels of the applied magnetic field. The post buckling analysis is performed to numerically realize the newly formed patterns dictated by the magnitude of the applied magnetic field. References [1] Goshkoderia A. and Rudykh S.: Stability of magnetoactive composites with periodic microstructures undergoing finite strains in the presence of a magnetic field, Composites Part B, 128, 19-29, 2017. [2] A. Goshkoderia, V. Chen, J. Li, A. Juhl, P. Buskohl and S. Rudykh, Instability-induced pattern formations in soft magnetoactive composites. Under review (2018).

15th U.S. National Congress on Computational Mechanics
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Title: Computational Modeling of Pregnant Cervix

Author(s): *Kun Gou, *Texas A&M University-San Antonio*;

Human cervix is an important mechanical organ located immediately below the uterus for keeping the fetus inside the uterus before baby due date. During the whole pregnancy period, the fibers inside the cervix are constantly evolving to suite the mechanical need of the cervix. The water amount inside the cervical tissue also increases to make the cervix become soft enough for smooth baby birth. The cervix is considered as a hyperelastic body surrounded by ligaments to fix the cervix on the pelvic skeleton. The top boundary of the cervix is subjected to both the intrauterine pressure from the uterus contraction and hydrostatic pressure from the fluid and fetus weight inside the uterus. The ligaments around the cervix are employed to provide fixed-displacement boundary conditions. A recent fiber remodeling technique is applied to study fiber modification under a cervical tissue homeostasis status. We study the stress distribution of the loaded and swelling cervix, and how its length and lumen area change during the second trimester period of pregnancy. A finite-element computation approach with an energy penalty method is used to study the modeling. The computational results show stress distribution in the interface area between the cervix and the ligaments. The lumen area is not uniform anymore along the length of the cervix. For a fixed top pressure, the length of the cervix increases when swelling increases, while for a fixed swelling, the length decreases when the top pressure increases. The computational result helps treat a disease called cervical inefficiency, under which the cervix becomes soft and effaced ahead of the time for a normal due date causing miscarriage or immature baby birth. The stress distribution allows us to know where the cervix is under tension and vulnerable. The lumen area also facilitates us to know where the cervix is narrow so that we can use string to tighten the cervix for more secure pregnancy.

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Title: A Computational Framework for Regional Earthquake Loss Estimation

Author(s): Wael Elhaddad, *NHERI SimCenter, University of California, Berkeley*; Frank McKenna, *NHERI SimCenter, University of California, Berkeley*; Michael Gardner, *NHERI SimCenter, University of California, Berkeley*; Adam Zsarnóczay, *NHERI SimCenter, Stanford University*; Chaofeng Wang, *NHERI SimCenter, University of California, Berkeley*; Matthew Schoettler, *NHERI SimCenter, University of California, Berkeley*; *Sanjay Govindjee, *NHERI SimCenter, University of California, Berkeley*; Gregory Deierlein, *NHERI SimCenter, Stanford University*;

A major challenge in natural hazards engineering is the determination of the effects of a given natural event on an entire region. Regional impact estimates of this type are central to effective planning efforts by city and regional planners. For maximum utility, these estimates need to be conducted at as fine a scale as is practically possible. In this presentation we describe a computational framework that was developed at the NSF NHERI SimCenter to study the effects of natural hazards on communities at a regional scale. The modular and extensible framework allows researchers to simulate the response of structures using multiple fidelity models and perform damage and loss estimation for all structures in a region of interest. These large-scale simulations provide aggregated and granular damage and loss estimates for the region taking into account both the uncertainty in the structural material properties and the loading on the structures due to the natural hazard. Two testbed simulations demonstrate the capability of the framework: one for the San Francisco (SF) Bay Area subjected to a synthetic magnitude 7.0 earthquake scenario on the Hayward fault and another for the magnitude 7.0 earthquake in Anchorage, Alaska that occurred on November 30, 2018. These simulations demonstrate the workflow which couples the finite element modeling (FEM) software OpenSees with the uncertainty quantification (UQ) software DAKOTA. The extensibility of the framework is demonstrated by characterizing the earthquake hazards using different models, viz. seismic hazard analysis, stochastic earthquake loading models [1], and physics-based ground motion simulations [2]. Results from both the SF Bay Area and Anchorage regional studies are compared to regional structural damage and loss estimates obtained using HAZUS [3]. References [1] C. Vlachos, K. G. Papakonstantinou and G. Deodatis, "Predictive model for site specific simulation of ground motions based on earthquake scenarios," Earthquake Engineering and Structural Dynamics, vol. 47, no. 1, pp. 195-218, 2018. [2] A. J. Rodgers, A. Pitarka, N. A. Petersson, B. Sjögreen and D. B. McCallen, "Broadband (0–4 Hz) ground motions for a magnitude 7.0 Hayward fault earthquake with three?dimensional structure and topography," Geophysical Research Letters, vol. 45, p. 739–747, 2018. [3] "Hazus®–MH 2.1, Earthquake Model Technical Manual," Federal Emergency Management Agency , Department of Homeland Security, Washington, D.C., 2017.

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Title: Hydraulic Fracturing: Coupling, Multiple Fractures, Dynamics, and XFEM,

Author(s): *Robert Gracie, *University of Waterloo*; Matin Parchei Esfahani, *University of Waterloo*;

In this presentation, we will discuss some recent advances in the simulation of multiple curving fractures, driven hydraulically using XFEM. Specifically we will address issues with iterative coupling, the simulation of multiple fractures, and dynamic HF. First we will discuss two new sequential coupling schemes— the undrained HF split and the fixed-strain HF splits— which allows mechanical equilibrium of the rock mass to be solved separately and in an iteratively fashion from/with the conservation of mass of the fluid flow in the fracture. It will be shown that the new schemes are stable, whereas other more naïve/traditional approaches are unstable. This will be illustrated in the practical situation of HF initiation and propagation multiple fractures from a well from perforations not aligned with the principal in-situ stresses. Next, the topic of the implementation of fluid partitioning algorithms will be discussed for fluid mass/volume injection rate controlled simulations. Lastly, we will discuss recent applications to dynamic HF fracture, in which stimulation is the result of high-rate pressure pulsing, where fracture behavior differs significantly from the quasi-static case

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Title: Computational Assessment of Radiation Dose Enhancement for Gold Nanospheres in a Tumor Using MCNP6.2

Author(s): *Tara Gray, *University of Texas at San Antonio*; Kathryn Mayer, *University of Texas at San Antonio*; Neil Kirby, *University of Texas Health M.D. Anderson Mays Cancer Center*;

The purpose of this study is to computationally quantify dose enhancement effects of using different concentrations and sizes of gold nanospheres in high dose rate (HDR) brachytherapy and external beam radiotherapy. A MicroSelectron HDR Ir-192 brachytherapy source and a Varian 600C gantry head with a 6MV photon energy were modeled using Monte Carlo N-Particle radiation transport software (MCNP 6.2, Los Alamos National Laboratory). The repeating structures capability of MCNP6.2 was utilized to simulate nanospheres of sizes 4.5 nm, 30 nm and 60 nm at varying nanosphere concentrations of 5 nM, 10 nM and 20 nM, inside a tumor, with a diameter of 1 x 1 x 1 cm3. Dose enhancement factors (DEFs) were computed as the ratio of dose to the tumor containing gold nanospheres relative to that without. The highest DEF of 1.7 was observed with the Ir-192 source for a total nanosphere concentration of 20 nM and diameters of 4.5 nm. It was observed that increasing concentration and decreasing the size of the nanospheres produced the greatest dose enhancement for both HDR brachytherapy and external beam radiotherapy cases. This work indicates the potential for significant dose enhancement and more effective tumor cell killing in radiation oncology practice.

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Title: Hyperreduction of Nonlinear Petrov-Galerkin Reduced-Order Models Using ECSW

Author(s): *Sebastian Grimberg, *Stanford University*; Charbel Farhat, *Stanford University*;

To extract the desired computational speed-up from nonlinear Projection-based Reduced-Order Models (PROMs), a second layer of approximations is typically required after the original subspace approximation is performed using a Reduced-Order Basis (ROB). This step, known as hyperreduction, seeks to accelerate specifically the evaluation of the projected nonlinear quantities using an approximate approach whose computational complexity scales only with the dimension of the PROM. All hyperreduction methods that have been applied so far to CFD problems are of the approximate-then-project type — that is, they approximate first the quantity to be projected on the left ROB, then compute its exact projection. They typically rely on an approach that was first developed for the Gappy Proper Orthogonal Decomposition (POD) method. Unfortunately, the implementation of most, if not all, of these hyperreduction methods requires a number of user-specified parameters that are hard to determine. As such, they are less desirable from a practical viewpoint. Alternatives to this first class of hyperreduction methods are of the project-then-approximate type, where the projected nonlinear quantities are directly approximated. The Energy Conserving Sampling and Weighting (ECSW) method [1] is a recent demonstration of the ability of this class of hyperreduction methods to produce stable and accurate hyperreduced Galerkin PROMs for second-order hyperbolic problems. ECSW relies on an approximate, data-driven, generalized quadrature rule determined via the solution offline of an optimization problem for which several distributed solution algorithms have been studied [2]. In this work, a quadrature-based method for hyperreduction of the project-then-approximate type inspired by ECSW is presented for first-order hyperbolic Petrov-Galerkin PROMs, such as those designed for the reduction of nonlinear CFD models. This proposed ECSW-like method represents an improvement of the state of the art of hyperreduction techniques for CFD problems. Its accuracy and computational efficiency will be demonstrated in this lecture for a variety of RANS and LES computations associated with complex geometries. References [1] C. Farhat, T. Chapman, P. Avery, Structure?Preserving, Stability, and Accuracy Properties of the Energy?Conserving Sampling and Weighting Method for the Hyper Reduction of Nonlinear Finite Element Dynamic Models, International Journal for Numerical Methods in Engineering, vol. 102, no. 5, pp. 1077-1110, 2015. [2] T. Chapman, P. Avery, P. Collins, C. Farhat, Accelerated Mesh Sampling for the Hyper-reduction of Nonlinear Computational Methods, International Journal for Numerical Methods in Engineering, vol. 109, no. 12, pp. 1623-1654, 2014.

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Title: Multiscale Uncertainty Propagation for Fasteners

Author(s): *Peter Grimmer, *Sandia National Labs--Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.*; John Emery, *Sandia National Labs--Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.*;

Finite element models of complex structures are used to predict how structures respond to extreme environments. This involves severe loading scenarios that cause material failure, which can greatly affect the structural response. To accurately predict material failure processes detailed models must be used. It is impractical to simulate a model of an entire structure with the level of detail needed to accurately predict failure. This motivates multiscale uncertainty propagation (UP) methods that can include fine details in critical areas, while using a coarser system level model to maintain computational tractability. This work does not seek to develop a new multiscale numerical method, but rather to demonstrate a novel use of one for UP to efficiently gain statistics about system mechanical failure [1]. Here, we demonstrate the developments for a housing with threaded fasteners, representing the fasteners with various levels of geometric fidelity. Here we use a simple joint with four screws as an example of a system that benefits from our multiscale uncertainty propagation approach. In this problem, the failure of the individual bolts in the joint governs the system response. Predicting the fracture in a bolt requires a high level of detail that cannot be included for every bolt in a complex system. The constitutive response (e.g., yield load, ultimate load, elongation-to-failure) of each individual bolt in our example joint varies randomly according to distributions determined from fastener testing. In general, sampling-based methods can be used to understand the effect uncertain inputs have on the system response. Here, the uncertain fastener constitutive parameters were optimally described by a stochastic reduced-order model (SROM) [2], which is a set of parameters that optimally samples the parameter space. This SROM was used to construct a surrogate model of the joint's response using the low fidelity joint model. This surrogate was then sampled 10,000 times to inform which bolt to replace in the low fidelity fastener model with a much higher-fidelity, helical-threaded fastener model using multi-point constraints to couple the models. The results compare the frameworks' estimates of probability of failure against direct numerical simulation for "truth''. [1] J. M. Emery and M. D. Grigoriu, "Efficient uncertainty propagation across continuum length scales for reliability estimates," in Uncertainty Quantification in Multiscale Materials Modeling, Elsevier, 2019. [2] M. Grigoriu, "Reduced order models for random functions. Application to stochastic problems," Appl. Math. Model., vol. 33, no. 1, pp. 161–175, 2009.

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Title: Computing Convergent Stress Intensity Factors Along the Front of a Three-Dimensional Crack on Unstructured Meshes

Author(s): *Benjamin Grossman-Ponemon, *Stanford University*; Leon Keer, *Northwestern University*; Adrian Lew, *Stanford University*;

Robust calculation of the stress intensity factors along the front of a crack is an essential ingredient of computational fracture mechanics. The most popular approach to their calculation is through the use of an extraction integral, namely the J-integral[1] or the interaction integral[2]. In this work, we present a formulation of the interaction integral and a method to compute the mixed-mode stress intensity distribution along the front of a non-planar crack. By our choice of the auxiliary fields, we simplify boundary integrals to require problem data only; the displacement gradient appears solely in volumetric integrals. When our interaction integral is applied to the true solution of the elasticity problem, we recover exactly a weighted integral of the stress intensity factors over the crack front. By introducing a mesh of the crack front and applying the interaction integral to a finite-element approximation of the true solution, we formulate a linear system which we may solve for the stress intensity distributions. Through analysis we are able to define conditions under which our method is guaranteed to converge. We demonstrate the efficacy of our method on several examples. References [1] Nikishkov, G.P., Vershinin, A.V. and Nikishkov, Y.G., 2016. Mesh-independent equivalent domain integral method for J-integral evaluation. Advances in Engineering Software, 100, pp.308-318. [2] Chiaramonte, M.M., Shen, Y., Keer, L.M. and Lew, A.J., 2015. Computing stress intensity factors for curvilinear cracks. International Journal for Numerical Methods in Engineering, 104(4), pp.260-296.

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Title: Thermal Conduction Analysis in Mesoscale Concrete with Refined Bond-Based Peridynamics

Author(s): *Xin Gu, *Hohai University*; Qing Zhang, *Hohai University*; Erdogan Madenci, *University of Arizona*; Yuan Wang, *Hohai University*;

This study reviews the existing bond-based peridynamic (PD) and state-based PD heat conduction models, and further proposes a refined bond-based PD thermal conduction model for homogeneous isotropic materials by using PD differential operator (PDDO). The refined bond-based PD is established by replacing the local spatial derivatives in the classical heat conduction equations with corresponding nonlocal integral expressions from PD differential operator. Considering that the state-based PD constructs the governing equations by substituting for the spatial derivatives in local equations with a certain nonlocal operator as well, this modeling approach is more representative of the state-based PD models while the resulting governing equations appear as bond-based PD models. The refined model can be reduced to the existing bond-based PD heat conduction models by specifying particular influence functions. Also, the refined model does not require any calibration procedure, unlike the bond-based PD. A systematic explicit dynamic solver is introduced to validate 1D-, 2D- and 3D-heat conduction in domains with and without a crack subjected to a combination of Dirichlet, Neumann and convection boundary conditions. All of the PD predictions are in excellent agreement with the classical solutions. Furthermore, we develop a PD modeling approach to analyze heat conduction in heterogeneous mesoscale concretes. It is based on the refined bond-based PD thermal conduction model for homogeneous isotropic materials and the random aggregate model (RAM) for mesoscale concrete specimens. The numerical results concern steady-state heat flow in a 2D mesoscale concrete specimen. The temperature and heat flux distributions are reasonable, and the predicted effective thermal conductivity agrees well with the experimental result. It also presents the effect of insulating cracks on heat flow in a mesoscale concrete. The refined bond-based PD thermal conduction model is shown to be effective for conduction problems involving discontinuities.

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Title: Numerical Modeling of Transport Phenomena in Melt-pool for Laser Direct Deposition Process

Author(s): *Xiaoyi Guan, *McGill University*; Yaoyao Zhao, *McGill University*;

Laser direct deposition process offers an effective way to fabricate fully dense metallic parts through laser irradiation and simultaneous delivery of material such as powder or wire. However, due to the complex physical phenomena involved, especially the short existing time scale of melt-pool at given location, a better understanding of the physical details during the process is still required to built high-quality parts. Numerical simulation provides an efficient approach to virtually build the part, to understand the physical details of the process and to support optimization. In this study, a new comprehensive three-dimensional numerical model is developed and used for the simulation of Laser Direct Deposition processes. Physical phenomena of melt-pool including powder injection, fluid flow, heat transfer, melting and solidification, capillary and thermo-capillary behaviors are all considered in the model. A mesh-free method, i.e. Smoothed Particle Hydrodynamics (SPH), with improved numerical scheme is used in the numerical model to solve the governing equations, which enables the natural tracking of liquid-gas interface and allows for easy handling of droplet or powder injection. The coupled heat transfer between melt-pool and solid heat affected zone is also considered with the emphasis on the shape of melt-pool. Meanwhile, injected mass and heat flux and attenuated laser intensity are collected from the previous simulated results of powder stream simulation to make the model more complete physically. The resulted numerical equations are solved through GPU computing and the simulated thermal profile and history, melt-pool geometry and the geometry of deposited tracks are presented.

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Title: Topology Optimization of 3-D Woven Lattices Considering Topology-Dependent Bonding

Author(s): Hak Yong Lee, *Johns Hopkins University*; *James Guest, *Johns Hopkins University*;

Three-dimensional weaving has recently arisen as viable means for manufacturing metallic, architected, multifunctional micro-lattices. Previous work by the authors and collaborators have shown these lattices inherently offer a suite of unique and useful mechanical and thermal properties, as well as demonstrated the ability to tailor these (and other) properties by designing the architecture, or topology, of these lattices (e.g., [1-2]). As architecture is directly related to the insertion pattern of wires or yarns by the weaving loom, one has the ability to directly realize tailored pore structures within the lattice provided fundamental 3D weaving manufacturing constraints are respected. This work will present topology optimization approaches based on both ground structure (discrete element) and material distribution (continuum) methods for designing the architecture of 3D-woven lattices to achieve desired property sets [2-3]. A key advancement is the development of a novel bonding element that mimics the resulting bond structure when 3D woven materials are bonded by brazing. Past work has shown that this brazing process is remarkably effective and conformal, and necessary to achieve load-bearing in the lattice, but is also topology-dependent. The new bonding element introduces the bonding material with its own set of manufacturing constraints. The approach is demonstrated to design lattices with maximized elastic moduli and structures with tailored dynamic properties. References [1] Zhang Y., Ha S., Sharp K., Guest J.K., Weihs T.P., and Hemker K.J. (2015). Fabrication and mechanical characterization of 3D woven Cu lattice materials. Materials and Design 85: 743-751. [2] Ha S.H., Lee H.Y., Hemker K.J., and Guest J.K. (in press). Topology Optimization of 3D Woven Materials using a Ground Structure Design Variable Representation. ASME Journal of Mechanical Design. [3] Guest J.K. (2015). Optimizing Discrete Object Layouts in Structures and Materials: A Projection-Based Topology Optimization Approach, Computer Methods in Applied Mechanics and Engineering 283: 330-351.

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Title: A Stochastic Framework to Perform Topology Optimization with Topologically Dependent Uncertainties

Author(s): *Johann Guilleminot, *Duke University*; Alireza Asadpoure, *University of Massachusetts Dartmouth*; Mazdak Tootkaboni, *University of Massachusetts Dartmouth*;

Topology optimization under uncertainty requires the definition and sampling of relevant uncertainties on a reference configuration. The latter is generally taken as the initial configuration, which allows for the use of standard representation techniques such as spectral expansions for random fields. In this talk, we present a new framework where the definition of the underlying uncertainties is updated on the fly as the design iterations go on. The overall methodology and theoretical background are first presented. We then discuss numerical aspects, and numerical benchmarks are finally provided to demonstrate the relevance of the approach.

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Title: A Computational Framework for the Morpho-elastic Development of Molluskan Shells by Surface and Volume Growth

Author(s): *Rahul Gulati, *University of Wisconsin-Madison*; Shiva Rudraraju, *University of Wisconsin-Madison*; Derek Moulton, *University of Oxford, U.K.*; Régis Chirat, *Université Lyon1, CNRS France*; Alain Goriely, *University of Oxford, U.K.*; Krishna Garikipati, *University of Michigan, Ann Arbor*;

Molluskan shells are an ideal model system for understanding the morpho-elastic basis of exoskeleton evolution in invertebrates. During the formation of the shell, the mantle tissue secretes proteins and minerals that calcify to form a new incremental layer of the exoskeleton. Most of the existing literature on the morphology of mollusks is descriptive. The mathematical understanding of the underlying coupling between pre-existing shell morphology, de novo surface deposition and morpho-elastic volume growth is at a nascent stage, primarily limited to reduced geometric representations. Here, we propose a general, three-dimensional computational framework coupling pre-existing morphology, incremental surface growth by accretion, and morpho-elastic volume growth. We demonstrate the potential of this formulation by applying it to explain the stepwise morphogenesis of seashells during growth: New material surfaces are laid down by accretive growth on the mantle whose form is determined by its morpho-elastic growth. Calcification of the newest surfaces extends the shell as well as creates a new scaffold that constrains the next generation of the sequence. We study the effects of surface and volumetric growth rates, and of existing shell geometries on the resulting modes of mantle deformation, and therefore of the developing shell's morphology. Connections are made to a range of complex shells ornamentations.

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Title: A Discontinuous Galerkin Method for Elastic-acoustic Coupled Wave Equations in First-order Form

Author(s): *Kaihang Guo, *Rice University*; Jesse Chan, *Rice University*;

Efficient and accurate simulation of wave propagation through coupled elastic-acoustic media has application areas such as geophysics and medical imaging. In this work, we introduce a high order weight-adjusted discontinuous Galerkin (DG) method based on a first-order stress-velocity elastic formulation and velocity-pressure acoustic formulation. The novelty of this method is the derivation of a simple upwind-like penalty numerical flux across the interface between elastic and acoustic media. This method is consistent and provably energy stable for arbitrary heterogeneous media (including anisotropy and sub-cell heterogeneities) and curvilinear meshes consisting of general types of elements. Numerical experiments demonstrate the high order accuracy, stability, and flexibility of the method on triangular and tetrahedral meshes.

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Title: Modelling of Gas Migration through the Gas Hydrate Stability Zone in Marine Geosystems

Author(s): *Shubhangi Gupta, *GEOMAR Helmholtz Center for Ocean Research Kiel*; Barbara Wohlmuth, *Technical University of Munich*; Matthias Haeckel, *GEOMAR Helmholtz Center for Ocean Research Kiel*;

Methane hydrates constitute a dominant organic carbon pool in the earth system and an important intermediate ”capacitor” in the global methane budget. Gas hydrates are predominantly formed from biogenic methane that is generated by methanogenesis in the deep biosphere. This methane migrates upwards as free gas or as methane-rich porewater by advection. This fluid flow is caused by non-steady state sediment compaction (passive margins), compaction of oceanic sediments during subduction (active margins), and dewatering of minerals at elevated temperatures (passive+active margins). Over geological times, the hydrates accumulate close to the bottom simulation reflector (BSR, lower stability limit of gas hydrates) because, the methane flux from below leads to hydrate formation in the gas hydrate stability zone (GHSZ), but the ongoing sedimentation tends to bury the hydrates below the GHSZ where the hydrates dissociate, and the released methane gas migrates back into the GHSZ to re-form the hydrates. Towards the seafloor, the hydrates dissolve due to undersaturation of porewaters as a consequence of anaerobic methane oxidation (AOM). Some methane gas by-passes the GHSZ and AOM zone if the upward flow is larger than the reaction rates. This methane fuels rich cold seep ecosystems. In order to understand the role of gas migration through the GHSZ in the natural carbon cycle, we have developed a multiphysics mathematical model and numerical solution framework for methane hydrate geosystems occurring in marine subsurface. The model considers coupled nonisothermal multiphase multicomponent reactive transport processes on geological time (hundreds of thousand years) and spatial (tens of kilometer) scales. The modelling of gas hydrate geosystems is challenging not only because of its multiphysics nature, but also due to the complex equilibrium and non-equilibrium phase transitions: methane hydrate<->gaseous methane<->dissolved methane, which are strongly coupled through nonlinear source and sink terms and are extremely sensitive to local temperature, pressure, and salinity conditions. To handle these phase transitions robustly, we have developed a semi-smooth Newton scheme where the phase transitions are incorporated within a single Newton iteration loop as variationally consistent nonlinear complementary constraints. In this talk, we will present an application of our model to analyze the sedimentation driven migration of methane gas through the GHSZ in one of the most dynamic natural settings of the Black Sea paleo-Danube gas hydrate system. We will discuss the specific numerical challenges of this problem setting, and show the robustness of our numerical strategy in terms of handling these numerical challenges.

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Title: Artificial Neural Network based Homogenization of Periodic Microstructures

Author(s): *Felix Selim Göküzüm, *University of Stuttgart*; Marc-André Keip, *University of Stuttgart*;

Cutting edge applications at extreme boundary conditions demand materials that can withstand such conditions. Smart design of composite microstructures enables a wide range of general improvements of existing materials as well as their manufacturing with custom-fit effective properties. However, the huge difference in length scales between the actual structural element and the underlying microstructure calls for efficient scaling techniques and simulations with low computational costs. In this contribution, we investigate a solution scheme which is based on an artificial neural network (ANN) discretization with the aim of combining powerful methods of continuum mechanics and innovative concepts of machine learning [1]. The principle ideas follow the work of Lagaris et al. [2], who suggested the construction of ANN-based trial functions that a priori fulfill the given boundary conditions. In our case, the boundary value problem is governed by periodic representative volume elements (RVE), which are representative for the underlying microstructure of the material. We further assume separation of length scales between the macro- and the microscale, which results in a first-order homogenization scheme. The periodic boundary conditions can then be obtained from an energy conservation principle between macro- and microscale, based on the Hill-Mandel condition. We thus can construct trial functions through single- and multilayer ANNs that a priori fulfill the periodic boundary conditions. Finally, a global energy potential is minimized to determine the ANN's parameters and the physical equilibrium state. Due to the construction of the trial function, the minimization can be carried out without any constraints on the ANN's parameters. The numerical framework is tested for linear material laws and two- and three-dimensional microstructures. Comparison to finite element and Fourier-based methods show that accurate results for the local fields can be obtained with a relatively small number of ANN parameters. Furthermore, the selection of features and its impact on the convergence rate of the iterative solver are discussed with a focus on a nested ANN approach using pretrained microstructure recognition. Finally, the implementation in Tensorflow, which can be done in a compact and flexible manner, is discussed. [1] D. R. Rummelhart, J. L. McClelland: Parallel distributed processing: exploration in the microstructure of recognition, IEEE Transactions on Neural Networks, 9, 987, 987-1000, (1998). [2] I. E. Lagaris, A. Lika, D. I. Fotiadis: Artificial neural networks for solving ordinary and partial differential equations, IEEE Transactions on Neural Networks, 9, 987 - 1000 (1998).

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Title: Introduction Of Adaptive W-Refinement Technique: A New Paradigm In Adaptive Isogeometric Analysis

Author(s): *Alireza H. Taheri, *University of Wisconsin Madison*; Krishnan Suresh, *University of Wisconsin Madison*;

It is well-known that smooth tensor product splines, such as NURBS, are inherently weak in capturing rapidly varying fields and sharp local gradients. Hence, when deployed in isogeometric analysis (IGA), they perform poorly in problems with poor regularity containing multiple thin layers or singularities. The prevailing idea for addressing these types of problems, which has recently been extensively explored, is providing the adaptive local refinement property by employing hierarchical splines [1,2]. In this paper, based on a proposed generalization of NURBS (GNURBS), we introduce a novel adaptivity technique in IGA, referred to as adaptive w-refinement technique, as an alternative fundamental approach for dealing with the aforementioned problems. This generalization is obtained by decoupling of the weights associated with the basis functions in geometry and field variable space. Considering the additional unknown control weights in the function space as design variables, we subsequently develop two different adaptivity algorithms to find these unknowns via solving an unconstrained optimization problem. Having access to the full analytical sensitivities, the established optimization problem is solved efficiently using a gradient-based algorithm. This procedure leads to constructing the optimal rational function space associated with the problem under study, while preserving the underlying geometry as well as its parameterization unchanged. These adaptive algorithms which rely on a residual based a posteriori error estimator are the invention of a novel class of adaptive refinement strategies in IGA. To perform the numerical integrations on the arising highly rational knot-elements, an adaptive subdivision integration scheme has been developed. We study the performance of these algorithms on problems with either smoothly or rapidly varying solution. The numerical results demonstrate more than one order higher rate of convergence for smooth problems compared to the results of classic NURBS-based IGA. Further, owing to the high capability of rational functions in capturing rapidly varying fields, the method particularly yields remarkable results in the case of problems containing thin layers and singularities. Overall, the suggested adaptive w-refinement procedures provide a novel powerful adaptivity technique in IGA and a competitive tool with hierarchical splines. [1] A. Vuong, C. Giannelli, B. Jüttler, and B. Simeon, “A hierarchical approach to adaptive local refinement in isogeometric analysis”, Comput. Methods Appl. Mech. Eng., 200, 3554-3567, 2011. [2] E. J. Evans, M. A. Scott, X. Li, and D. C. Thomas, “Hierarchical T-splines: Analysissuitability, Bézier extraction, and application as an adaptive basis for isogeometric analysis”, Comput. Methods Appl. Mech. Eng., 284, 1-20, 2015.

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Title: Distributed Parallel–Adaptive Implementation of Asynchronous Spacetime Discontinuous Galerkin Methods with Application to Seismic Simulation

Author(s): *Robert Haber, *University of Illinois at Urbana-Champaign*; Amit Madhukar, *University of Illinois at Urbana-Champaign*; Xiao Ma, *University of Illinois at Urbana-Champaign*; Ahmed Elbanna, *University of Illinois at Urbana-Champaign*; Reza Abedi, *University of Tennessee Knoxville (UTK) / Space Institute (UTSI)*; Volodymyr Kindratenko, *University of Illinois at Urbana-Champaign*;

The asynchronous Spacetime Discontinuous Galerkin (aSDG) method [1] is a powerful solution scheme for hyperbolic systems. It features unconditional stability, conservation over every spacetime cell, linear computational complexity, and support for arbitrarily high-order elements. However, its most promising advantages are compatibility with an extremely powerful and dynamic form of adaptive spacetime meshing and a highly favorable algorithmic structure for parallel computation. Serial adaptive aSDG solvers typically outperform conventional solvers running in parallel on large clusters, especially for multi-scale problems or problems with rapidly evolving domain geometry; cf. recent work on dynamic fracture [2]. Recent success with parallel–adaptive implementations on shared memory platforms bodes well for a more ambitious implementation intended for large-scale distributed supercomputers. In particular, the asynchronous and latency-tolerant features of our parallel–adaptive software architecture might be particularly well suited for implementation on exascale platforms. This presentation describes the architecture and initial results from our work on a distributed parallel–adaptive aSDG implementation. We begin with a review of the design of our shared-memory implementation, emphasizing our reasons for abandoning the domain decomposition method and introducing a round-robin strategy for parallel task assignment. Then we describe various modifications required to extend our strategy to distributed systems, including nested round-robin schemes for multi-host platforms. We present preliminary performance and scaling efficiency studies and demonstrate an application of the parallel–adaptive aSDG method to a seismic simulation problem in which we model off-fault damage as a random field of explicit small-scale fractures. This approach is expected to deliver physically more realistic behaviour than typical smeared models in which, for example, a continuum plasticity model represents the bulk response of damaged rock. We close with a discussion of directions for continuing development, including integration of our parallel code with new spacetime meshing capabilities for problems defined in 3d×time. References: [1] R. Abedi, R. B. Haber, B. Petracovici. A spacetime discontinuous Galerkin method for elastodynamics with element-level balance of linear momentum, ?Comput. Methods Appl. Mech. Eng. 195 (2006) 3247–3273. [2] R. Abedi, and R. Haber. Spacetime simulation of dynamic fracture with crack closure and frictional sliding, Advanced Modeling and Simulation in Engineering Sciences 5 (2018). doi:10.1186/s40323-018-0116-5

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Title: Solution Adaptation in Embedded Boundary Methods: Adaptive Mesh Refinement vs. Adaptive Remeshing

Author(s): Charbel Farhat, *Stanford University, USA*; Raunak Borker, *Stanford University, USA*; *Elie Hachem, *MINES ParisTech, France*;

Embedded Boundary Methods (EBMs) for the solution of Computational Fluid Dynamics (CFD) and Fluid-Structure Interaction (FSI) problems are typically formulated in the Eulerian setting, which makes them more attractive than Chimera and Arbitrary Lagrangian-Eulerian methods when the structure undergoes large structural motions, large deformations, and/or topological changes. In the presence of viscous flows however, they necessitate the adaptation of the spatial discretization, for example, via Adaptive Mesh Refinement (AMR) or Adaptive Remeshing (AR), because unlike Chimera and ALE methods, they do not track the boundary layers. In general, AMR gives rise to non-conforming mesh configurations and AR necessitates the transport of information from one mesh to another. Hence, both competing approaches for adapting the spatial discretization can complicate the semi-discretization process. A few mesh adaptation approaches that maintain mesh conformity in the context of EBMs have been developed however. The objective of this talk is to describe one such approach [1] based on the bisection method, contrast it with an alternative AR approach based on a mesh metric tensor field [2], highlight the practical benefits of both computational strategies, discuss their intrinsic pros and cons, and contrast their performances for various CFD and FSI problems. [1] R. Borker, S. Grimberg, C. Farhat, P. Avery, J. Rabinovitch, An Adaptive Mesh Refinement Concept for Viscous Fluid-Structure Computations Using Eulerian Vertex-Based Finite Volume Methods, AIAA 2018-1072, AIAA SciTech 2018, Kissimmee, FL, January 8-12 (2018) [2] L. Billon, Y. Mesri, E. Hachem, Anisotropic Boundary Layer Mesh Generation for Immersed Complex Geometries, Engineering with Computers, vol. 33, no. 2, pp. 249-260, 2017.

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Title: Estimation of ARMA-model Parameters to Describe Pathological Conditions in Cardiovascular System Models

Author(s): *Urs Hackstein, *Pforzheim University of Applied Sciences*; Ali Hamie, *Pforzheim University of Applied Sciences*; Stefan Krickl, *Pforzheim University of Applied Sciences / Freie Universität Berlin*; Stefan Bernhard, *Pforzheim University of Applied Sciences / Freie Universität Berlin*;

Cardiovascular diseases cause one of the three major deaths worldwide. Among these diseases especially aortic aneurysms are a highly underestimated problem as they affect 12-14% of the population worldwide on one hand, but are categorical underdiagnosed clinically on the other hand. There are several attempts to model the cardiovascular system known in the literature, mostly based on the Windkessel model and the estimation of its model parameters. The objective is to simulate healthy and diseased conditions of cardiovascular blood flow by means of numerical models. Recall that there is for e.g. a recent report by Casas et al., who created a personalized lumped parameter model and compared it with data from clinical measurements. Note also, that there is a recent review of the variety of models with different levels of complexity from the 90s up to today by Quarteroni et al.. In this work, we used a zero-dimensional lumped model of the cardiovascular system based on the Windkessel model and regard pressure-pressure transfer functions between two systemic measurement locations, modeling them as an AutoRegressive-MovingAverage (ARMA)-model after subtracting its means from input resp. output data and estimating its coefficients. Recall that ARMA-models are a specific class of linear, time-invariant input-output models that is completely characterized by a finite set of adjustable parameters. For the estimation of the ARMA-coefficients (a_k, b_k)_{k=1,...,16} we use a Subspace Gauss-Newton search method with an adaptive cut-off of singular values, implemented as algorithm in the System Identification toolbox of Matlab. The ARMA-coefficients were estimated using signals from the arteria brachialis and femoralis in four cases: Besides the control group, the estimations were performed on signals of two aneurysms located in the thoracic and one in the abdominal aorta. The coincidence obtained for a polynomial model of order 15 was above 95% in comparison to the original output which is equivalent to an average error of less than 5 Pa per sample point. We further quantify the difference between the estimated coefficients in each case, using different distance measures based on the variance, the euclidean distance and its norm. The largest deviation between the pathological conditions and the control group was found in the coefficients (a_3,b_3), (a_8,b_8) and (a_5,b_5). These findings suggest a reasonable situation to distinguish the pathological state of the four underlying modeling from the estimated coefficients.

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Title: A New Approach Towards Estimation of Axonal Damage Location Following Rapid Head Rotation Using Axonal Tract Embedded Finite Element Modeling

Author(s): *Marzieh Hajiaghamemar, *Georgia Institute of Technology & Emory University*; Susan Margulies, *Georgia Institute of Technology & Emory University*;

Finite element (FE) derived injury metrics for predicting traumatic brain injury (TBI) have been limited to predicting absence or presence of TBI rather than estimating the location of injury. We developed an anisotropic FE model with embedded axonal fiber tracts to predict sites of acute traumatic axonal injury (TAI). Piglets experiencing rapid non-impact head rotation (113-203 rad/s) in the axial (n=20) or sagittal (n=24) direction were sacrificed 6-hours post-TBI, brains perfusion-fixed, sectioned and stained for beta-amyloid-precursor-protein, and TAI maps were generated. An idealized pig head FE model [1] was enhanced by adding lateral ventricles and embedding axonal fiber tractography into brain FE model. Brain and axonal fiber were modeled using Holzapfel-Gasser-Ogden hyper-viscoelastic user-defined material in LS-DYNA [2], and validated against in-situ hemisection experiments. We scaled the model to match each subject's brain mass, and simulated each piglet experiment with measured velocities. For each simulation, six maximal brain and axonal fiber deformation values were extracted from each element's history: maximum principal strain (MPS), strain rate (MPSR), and MPSxSR, and maximum axonal strain (MAS), strain rate (MASR), and MASxSR. To determine the best predictor for acute TAI location, TAI maps were co-localized to the FE and the minimum distance d between the location of each brain/axonal element and TAI site was calculated for each simulation. The results of each of the six deformation TAI candidates and d for all elements and all animals were combined. Any element within a distance ds of any TAI was defined as an injured element. All TAI candidates showed higher values at elements closer and lower values at elements farther from TAI sites. For each of the six TAI metric candidates (x), we examined a matrix of different threshold values (thx) and ds to maximize the average of two optimization criteria: correct prediction rate of TAI and TAI detection rate, defined as the percentage of actual TAI sites ?ds from elements ? thx. No optimal ds and thx was found for brain tissue metrics MPS, MPSR, MPSxSR. In contrast, all the three axonal deformation-related TAI candidates showed promise, with a 91-93% TAI detection rate and 72-76% correct prediction rate for TAI. The optimal ds (and thx) for MAS, MASR, and MASxSR were 2.5mm (0.12), 2mm (50/s), and 2mm (3/s). In summary, axonal deformation-related metrics reliably predict the sites of acute TAI acutely ?2.5mm. Acknowledgements: Biocore Co., Ltd., NIH-R01NS097549, and 2R56NS055951-10A1 References: [1] Sullivan S., Biomech Model Mechanobiol, 2015,14(4) p877. [2] Wu T., 18th USNC/TAM Conference, 2018.

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Title: Unstructured Mesh Adaptation for Flow Problems with Evolving Features

Author(s): *Morteza Hakimi, *Rensselaer Polytechnic Institute*; Fan Yang, *Rensselaer Polytechnic Institute*; Alvin Zhang, *Rensselaer Polytechnic Institute*; Rocco Nastasia, *Simmetrix Inc.*; Blair Downie, *Simmetrix Inc.*; Saurabh Tendulkar, *Simmetrix Inc.*; Assad Oberai, *University of Southern California*; Mark Shephard, *Rensselaer Polytechnic Institute*; Onkar Sahni, *Rensselaer Polytechnic Institute*;

Evolving features arise in many flow problems of interest. These features could be related to an evolving solution behavior or geometry/domain. For example, an evolving interface in a multiphase medium or a shock propagating in case of a compressible flow or a moving object in the domain. In such problems mesh resolution around the evolving feature must be controlled to accurately resolve and capture the physics, for example, a boundary layer mesh around a moving object in case of a high Reynolds number flow or a discontinuous field at a multiphase interface such as density. In this talk, we will present adaptation of unstructured meshes (including boundary layer meshes) based on local mesh modification operators for a wide variety of flow problems with evolving features such as level set-based implicit tracking of the interface, a discontinuous interpolation based explicit interface tracking, a moving object with a sliding contact or narrow gap. In cases where the mesh moves or deforms, we apply mesh modification in combination with mesh motion such that the mesh remains consistent with the underlying geometry/domain representation. All steps are done in parallel on distributed meshes. We will demonstrate our approach for few different types of problems (e.g., a projectile moving in a barrel or interfaces undergoing large motions).

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Title: Shell Eigenvalue Problems under Uncertainty

Author(s): *Harri Hakula, *Aalto University*;

Shell eigenproblems are challenging since the smallest eigenmode can have higher multiplicities. Moreover, for shells of revolution the situation becomes even more complex due to symmetries and the spectrum always contains clusters of eigenmodes. If for instance the material parameters are allowed to be random or uncertain, the eigenproblem becomes a multiparametric one. In the multiparametric setting it is possible that the modes within the cluster cross, that is, if the experimental setup is monitoring for instance the smallest mode, it is possible that if the material properties vary from one realization to another, the observed smallest mode changes. Here the focus is on application of recent theoretical results extending our previous work [1]. We present new results on deterministic parameter-dependence (thickness) of the eigenmodes of shells of revolution and demonstrate how the crossing of modes occurs even in the deterministic setting. These concepts are then used in stochastic FEM eigensolution of parabolic and hyperbolic shell model problems leading to computational asymptotic analysis of the expected value of the smallest eigenmode as the thickness tends to zero. One of the fascinating problems inherent in all multiparametric eigenvalue problems is tracking the correct mode within a cluster through the parameter space. To our knowledge there is no agreement on how to do this in a robust manner. We suggest some alternatives and illustrate the underlying issues. [1] Harri Hakula, Mikael Laaksonen, Multiparametric shell eigenvalue problems, Computer Methods in Applied Mechanics and Engineering, Volume 343, 1 January 2019, Pages 721-745

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Title: MD Informed Mesoscale Simulations of Shock to Detonation Transition in Energetic Materials

Author(s): *Ahmed Hamed, *Purdue University*; Marisol Koslowski, *Purdue University*;

The reliable prediction of energetic materials response to different loading conditions and various types of stimuli is of critical importance for efficient performance and safety of their applications. In this regard, developing high fidelity models for the shock to detonation transition is a key challenge. Successful modelling of this problem dictates capturing the heterogeneous nature of hot-spot formation and initiation as well as the interplay between the underpinning mechanisms—spanning different time- and length-scales. In the current study, a novel mesoscale model for the shock to detonation transition in high explosives (RDX and HMX) is presented. The model solves the reactive hydrodynamic system of equations with explicit consideration of the underlying mechanical, chemical, and thermal processes. By coupling with two supplementary models, one for single crystal plasticity while the other is a phase-field damage model, our model accounts for dissipative heating mechanisms by viscoplasticity and fracture, respectively. Moreover, for thermodynamic consistent description, the energy conservation equation incorporates two distinct equations of state for solid reactant and gaseous products, calibrated using MD simulations, to account for thermoelastic effects. Statistical approach is used for the representation of the embedded hot spots (in terms of their size, temperature, and spatial distributions) and other microstructure features. The critical temperature of hot spots is taken to be size-dependent, based on a separate investigation of the criticality of single thermal hot spots. The impact of loading conditions and crack orientations on shock wave propagation are also guided by the results of macroscale simulations that uses stochastic approach to resolve different microstructures. A two-step chemical decomposition sub-model is parameterized by MD simulations. In addition, quantum-corrected and length-dependent thermal diffusivity is integrated into the model. The model is implemented and solved within the framework of the finite element method via MOOSE framework simulation package.

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Title: Material Modeling Parameter Identification of Solid Phase in Cementitious Materials through Combining Real and Virtual Experiments

Author(s): *Tong-Seok Han, *Yonsei University*; Ji-Su Kim, *Yonsei University*;

Virtual experiments can help reduce the number of effort- and time-consuming real experiments in developing new materials and in evaluating performance of existing materials. However, microstructures of cementitious materials are quite complex, and it is difficult to determine the input material modeling parameters for inhomogeneous solids for virtual experiments. When complex and large pore microstructures are present, as in the case of cementitious materials, conducting small scale experiments such as nano-indentation are also difficult. Here, the combined approach of real and virtual experiments is proposed to identify the input material modeling parameters for virtual samples of a cementitious material. The synergistic framework of combing a phase field fracture model [1] and microstructures obtained from micro-CT is investigated. A foamed concrete, which is designed to possess a large amount of pores to reduce thermal conductivity while maintaining load bearing capacity, is used as an example in this study. Foamed concrete specimens with three densities were prepared. The macro-scale properties of the foamed concrete are experimentally determined and microstructures are obtained. The solid phase of microstructures obtained from micro-CT is first homogenized as a single phase, and input material parameters to reproduce the macro-scale stiffness and tensile strength are calibrated for the specimens. The grayscale information in the virtual samples from micro-CT are correlated with the calibrated input material modeling parameters. The relations between the grayscale values from the micro-CT specimens and the input material modeling parameters can be used to determine the input material parameters for multi-phase solid microstructures.
[1] C. Miehe, L.-M. Schänzel, H. Ulmer, Phase field modeling of fracture in multi-physics problems. Part I: Balance of crack surface and failure criteria for brittle crack propagation in thermo-elastic solids, Comput. Meth. Appl. Mech. Eng. 294 (2015) 449–485.

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Title: A Hybrid Approach Using Deep Learning Convolutional Neural Networks for the Solution of Multiphysics Problems in Soft Tissue Electrosurgery

Author(s): *Zhongqing Han, *Rensselaer Polytechnic Institute*; FNU Rahul, *Rensselaer Polytechnic Institute*; Suvranu De, *Rensselaer Polytechnic Institute*;

Electrosurgical procedures are widely used to simultaneously dissect and coagulate soft hydrated tissues [1]. Yet, the understanding of underlying mechanisms of tissue damage in electrosurgery remain limited, causing a large number of accidental burns and tissue injuries each year [1]. Many models have been proposed to study the effects of biophysics of radiofrequency current on the thermo-mechanical response of soft tissue [1][2]. However, efficient modeling of such procedures considering multiphysics electro-thermo-mechanical interactions with high physical fidelity remains a challenging problem, for which state-of-the-art methods [2] require heavy computational resources, limiting their application to simplistic loading conditions. We propose a data-driven hybrid approach that leverages the regressive capabilities of deep learning convolutional neural network (CNN) with the precision of conventional iterative solvers to accelerate multiphysics computations. The electro-thermal problem is solved using standard finite element method (FEM) in conjunction with Krylov subspace based iterative solver with a recently developed an efficient deflation-based block preconditioner [3]. The mechanical deformation induced by evaporation of intra- and extracellular water is obtained using a CNN model with a highly tailored architecture. The CNN is trained using a supervised learning framework that maps a nonlinear relationship between the micropore pressure and deformation field for the given tissue topology. The simulation results show significant improvement in the computational time for the hybrid approach when compared to standard FEM based solution approach using block-preconditioned Krylov solver. The accuracy is shown to be comparable to the ground truth obtained using standard multiphysics solution approach. REFERENCES [1] G. Sankaranarayanan, R. Resapu, D. Jones, S. Schwaitzberg, and S. De, “Common uses and cited complications of energy in surgery”, Surg. Endosc. Vol. 27, pp. 3056–3072, (2013). [2] Z. Han, Rahul, and S. De, “A multiphysics model for radiofrequency activation of soft hydrated tissues”, Comput. Methods Appl. Mech. Eng. Vol. 337, pp. 527–548, (2018). [3] Rahul and S. De, “An efficient block preconditioner for Jacobian?free global–local multiscale methods”, Int. J. Numer. Methods Eng. Vol. 87, pp. 639–663, (2011).

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Title: Propagating Uncertainty in a Calibrated Material Model Using Bootstrapping and DAKOTA

Author(s): *Alexander Hanson, *Sandia National Laboratories*; Kyle Karlson, *Sandia National Laboratories*;

Material model parameters are often calibrated to experimental data sets that include repeats such that the calibration captures the average behavior of the material. However, this results in no information regarding the uncertainty of the material model parameters. It is both time and cost prohibitive to provide the number experimental data sets necessary to generate sufficient independent calibrations to determine parameter uncertainty. Conversely, using the statistical approach of bootstrapping, sets of experiments with limited repeats can be used to estimate the variance in the material model calibration parameters through re-sampling. A large number of calibrations, limited only by the number of unique re-samples, can then be processed to provide statistical distributions for each material parameter. This was applied using a multi-step calibration process with DAKOTA for a temperature and rate-dependent elasto-viscoplasticity material model. Due to its complexity, the material model calibration required an initial global optimization search using a genetic algorithm before refinement with a non-gradient local optimization algorithm. Subsequently, the refinement process was re-run over five-hundred times with bootstrap re-samples, which provided the means to describe the variability in the material model parameters. Using a sampling and surrogate approach, the material model variability was propagated with DAKOTA to a simulation of a pressurized cylinder to determine how the variability in the material behavior effected the failure pressure.

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Title: Spectral Performance of Nitsche's Method

Author(s): *Isaac Harari, *Tel Aviv University*; Uri Albocher, *Tel Aviv University, Afeka College*;

Embedded methods that are based on Nitsche's approach can facilitate the task of mesh generation in many configurations. The basic workings of the method are well understood, in terms of a bound on the stabilization parameter. However, its spectral behavior has not been explored in depth. In addition to the eigenpairs which approximate the exact ones, as in the standard discrete formulation, Nitsche's method, working with a larger solution space, gives rise to complementary pairs. The quotient space is handy for determining the number of eigenpairs and complementary pairs. The complementary solutions approximate functions in the orthogonal complement of the kinematically admissible subspace. These mesh- and stabilization-dependent quantities provide the mechanism for weak enforcement of boundary or interface constraints. The dependence of the scalar values on the Nitsche parameter is related to a boundary quotient of the functions, explaining the manner in which stabilization engenders coercivity without degrading the accuracy of the discrete eigenpairs. The boundary quotient proves to be useful for separating the two types of solutions. A global result for errors in the Galerkin approximation of the eigenvalue problem that pertains to all modes of the discretization, is extended to the Nitsche formulation. Numerical studies on non-conforming aligned meshes confirm the dependence of the eigenvalues on the parameter, in line with the corresponding boundary quotients. The spectrum of a reduced system obtained by algebraic elimination of the added Nitsche degrees of freedom is free of complementary solutions, improving conditioning and warranting its use in the solution of boundary-value problems. The reduced system offers an incompatible discretization of eigenvalue problems that is suitable for engineering applications. Using Irons-Guyan reduction yields a spectrum that is virtually insensitive to stabilization, with high accuracy in both eigenvalues and eigenfunctions.

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Title: Modeling Breakage Using LS-DEM

Author(s): *John Harmon, *Caltech*; Jose Andrade, *Caltech*;

Breakage is a critical aspect of materials for wide ranging applications such as in mining, earthquake mechanics, and mechanics of inhomogeneous materials to name a few. Despite this, many aspects of this phenomenon remain unknown due to the complexity of fracture driving modelers to make compromises for efficiency. In this talk, a development in grain-scale breakage modeling will be discussed that combines the recent capability of exact particle shape in discrete element modeling with a novel breakage method that together maintain the efficiency of sphere based methods while adding the accuracy from exact particle shape and complex fracture surface geometry. We will begin with an overview of how this technique is made possible due to revolutionary advancements in imaging techniques that opened the door for the creation of the Level Set Discrete Element Method (LSDEM). We will then show simulations using the technique and how those simulations compare with experiments both with constitutive relations and key breakage properties such as the evolution of grain size distribution.

15th U.S. National Congress on Computational Mechanics
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Title: Multi-physics Modeling with Multiresolution Wavelets

Author(s): *Cale Harnish, *University of Notre Dame*; Luke Dalessandro, *University of Washington*; Karel Matouš, *University of Notre Dame*; Daniel Livescu, *Los Alamos National Laboratory*;

We present the Multiresolution Wavelet Toolkit (MRWT), an n-dimensional algorithm for multi-physics modeling. This numerical method leverages the multiresolution nature of wavelets to provide significant data compression and explicit error control for solutions to coupled systems of nonlinear partial differential equations (PDEs) with features evolving on a wide range of spatial and temporal scales. We use differentiable wavelet basis functions and second generation wavelets, to solve initial-boundary value problems on finite domains. Moreover, we provide a priori error estimates for the wavelet representation of fields, their derivatives, and the aliasing errors associated with the nonlinear terms in the PDEs. Then, by projecting fields and spatial derivative operators onto the wavelet basis, our estimates are used to construct a sparse multiresolution spatial discretization which guarantees the prescribed accuracy for each field. Additionally, MRWT utilizes a predictor-corrector procedure within the time advancement loop to dynamically adapt the computational grid, maintaining the prescribed accuracy of the solutions of the PDEs as they evolve. We show verification of the MRWT algorithm, demonstrating mathematical correctness and physics simulation capabilities. Furthermore, spatial convergence is achieved at a rate which is in agreement with the a priori estimates.

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Title: Uncertainty Quantification and Stochastic Modeling of Hyperelastic Constitutive Models for Soft Biological Tissues

Author(s): *Md Mehedi Hasan, *Duke University*; Johann Guilleminot, *Duke University*;

Modeling the uncertainties in the constitutive behavior of soft biological tissues is an important aspect in computational biomechanics and related applications (such as computer-aided surgeries and clinical decision making). In this presentation, we address the stochastic modeling, simulation and identification of uncertainties in arterial walls. This is specifically achieved by modeling the anisotropic strain energy function describing the nonlinear response of the biological composite as a random field. An algorithm to sample the model on real patient-specific geometries is also detailed. The overall computational framework is finally demonstrated by performing virtual mechanical tests on arterial strips.

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Title: A Peridynamics (PD) Correspondence Model for Steel Reinforced Concrete Structures

Author(s): *Gabriel Hattori, *University of Cambridge*; John Orr, *University of Cambridge*; Mark Hobbs, *University of Cambridge*; David Miranda, *University of Cambridge*;

Concrete is the most widely used construction material, responsible for a significant percentage of global carbon dioxide emissions [1]. Reducing emissions is a key goal, and for concrete this may be partly satisfied through structural optimisation. Such work requires a reliable understanding of material behaviour under all possible loading. This knowledge has not yet been fully realised, particularly for complex brittle behaviour such as shear. Part of these problems come from the heterogeneity of the concrete at the microscale. It is formed by different materials (sand, aggregate, cement) that can greatly differ in size, which means that microcracks are likely to appear among the larger aggregate. Additionally, concrete is weak in tension, so reinforcements (such as steel) need to be incorporated to concrete structures to increase its resistance for tensile loading. Conventional models for concrete try to take these factors into account, but they still have limited use. Peridynamics (PD) [2] presents a promising numerical model to study reinforced concrete structures. PD is a non-local particle-based method, where each particle has an area of influence with respect to the other particles. It has been shown to be particularly interesting in applications for fracture mechanics, since there is no need for additional assumptions in the presence of discontinuities due to cracks. Additionally, it can consider non-linear behaviour such as crack initiation. In this work we propose a PD model toinvestigate steel reinforced concrete structures based on the work of [3] for anisotropic materials. We analyse different loading cases (bending, shear) and the arising crack patterns in the regions under tension. A simple contact formulation is introduced to model the supports of the structure. We show that PD can be used to capture the behaviour of prismatic and non-prismatic reinforced concrete structures. References [1] D. J. M. Flower and J. G. Sanjayan. Green house gas emissions due to concrete manufacture. The international Journal of life cycle assessment, 12(5):282–288, 2007. [2] S. A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. Journal of the Mechanics and Physics of Solids, 48(1):175–209, 2000. [3] G. Hattori, J. Trevelyan, and W. M. Coombs. A non-ordinary state-based peridynamics framework for anisotropic materials. Computer Methods in Applied Mechanics and Engineering, 339:416–442, 2018.

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Title: Measured Mitochondrial Oxygen Consumption Predicts Right Ventricular Adaptation to Mild Pulmonary Hypertension in Multi-scale Framework of Cardiovascular System

Author(s): *Madison Haugen, *University of Wisconsin - Madison*; Byron Zambrano, *Texas A&M University*; Daniel Beard, *University of Michigan - Ann Arbor*; Naomi Chesler, *University of Wisconsin - Madison*;

In pulmonary hypertension (PH), increased pulmonary vascular resistance and decreased arterial compliance cause structural and functional remodeling of the right ventricle (RV), leading to RV failure (RVF). The capacity for mitochondrial oxidative phosphorylation, the primary source of ATP to drive cellular contraction, is diminished in failing compared to normal right ventricular myocardium. Yet in animal models of mild PH, both mitochondrial and RV mechanical function are preserved (1), suggesting that loss of density and function are key to RVF. However, the impact of mitochondrial dysfunction on RV mechanics is difficult to isolate in vivo. We hypothesized that a computational model of the heart and cardiovascular system (CVS) developed to study left ventricular mechanoenergetics (3) could be adapted to study RV mechanoenergetics, and could uncover the impact of mitochondrial dysfunction on RV contractile function. The mitochondrial/energetic model component is used to determine the myocardial energetic status (ATP, ADP, inorganic phosphate, creatine, and phosphocreatine concentrations) as a function of ATP demand (2). The myocardial mechanics part of the model is used to simulate the influence of energetic status on muscle dynamics and ventricular contraction (3). The heart model is integrated with a simple lumped-parameter model of the systemic and pulmonary circulations (3). In vivo experimental oxygen consumption from rats with PH was input to the mitochondrial module, resulting in decreased ATP and increased ADP and inorganic phosphate concentrations. These concentrations resulted in silico organ-level outputs that matched the reduced end diastolic volume and increased end systolic pressure from the in vivo study after calibrating properties of the vasculature. We conclude that this framework can predict RV multi-scale behavior and will be used for further analysis of mitochondrial mechanisms of RVF. Importantly, the model enabled investigation of multi-scale relationships between RV organelle, cellular, tissue, and organ function that cannot be studied in vivo.
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Title: Compression Molding Simulation and Component Strength Analysis for Long Fiber Reinforced Plastics Using Meshfree and Particle Methods in LS-DYNA

Author(s): *Shinya Hayashi, *JSOL Corporation*; C.T. Wu, *Livermore Software Technology Corporation*; Wei Hu, *Livermore Software Technology Corporation*; Hao Chen, *Livermore Software Technology Corporation*; Youcai Wu, *Livermore Software Technology Corporation*; Xiaofei Pan, *Livermore Software Technology Corporation*;

Composite materials like fiber reinforced plastics (FRP) are becoming more widely used in the automotive industry and have been found very effective in reducing vehicle weight. Recently, long carbon fiber reinforced thermoplastics are increasingly being used for lightweight structural parts with high stiffness, strength and energy absorption performance. Compression molding is considered one of the most efficient manufacturing processes to mass produce FRP parts for automotive applications. Compression molding can form FRP into complex shapes with relatively low manufacturing cost and short process time. However, this often generates unwanted fiber orientation, uneven distribution of fibers, weld lines and matrix rich regions. These forming effects strongly affect mechanical strength. To analyze these complex phenomena, LSTC and JSOL developed new compression molding simulation techniques for long fiber reinforced plastics using a beam-in-adaptive EFG (Element Free Galerkin) coupling function in LS-DYNA. Furthermore, new component strength analysis method with a beam-in-SPG (Smoothed Particle Galerkin) coupling model using deformed beams calculated in the compression molding simulation was developed.

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Title: Multi-Scale Fracture Modeling of Heterogeneous Porous Media

Author(s): *Bang He, *The University of Utah*; Pania Newell, *The University of Utah*;

Most porous media, including geomaterials and bio-materials, are highly heterogeneous in nature, and they contain large variations of micro-pore structures, such as pore size, pore distribution, and pore shape. The oscillation of microstructures is a big challenge in theoretical characterization and is usually ignored in continuous modeling. Thus, continuous models are not exact representations of such porous media, even though in some cases the micro-heterogeneity could be ignored. Considering that the porosity of porous media plays an important role in the mechanical properties (e.g. toughness), it is important to investigate the impact of pore network structures on the fracture behavior in such media. With this in mind, this research work aims to establish a numerical framework with the capability of modeling the micro-scale heterogeneity's effect on the macro fracture behaviors in porous media by using state-of-the-art research achievements on the fracture mechanics (micro and macro) of porous media, combined with the phase-field fracture modeling technique. This numerical modeling strategy solves two Boundary Value Problems (BVPs) at a micro- and a macro-domains, where the propagation of macro fractures will be updated based on the deformation of the micro-pore structure. Therefore, the micro-pore structure's effect on the fracture behavior can be taken into account. This multi-scale technique will be benchmarked against classical problems of single edge crack and three-point bending.

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Title: In Situ Adaptive Reduction of Nonlinear Multiscale Structural Dynamics Models

Author(s): *Wanli He, *Stanford University*; Philip Avery, *Stanford University*; Charbel Farhat, *Stanford University*;

Heterogeneous materials are encountered in solid mechanics and structural dynamics problems. The standard Finite Element (FE) modeling of such problems usually requires extremely fine meshes and leads to prohibitively expensive numerical simulations. Hence, alternative approaches such as the multiscale FE2 have been developed. Typically, these assume that the material configuration is homogeneous at the macroscale but heterogeneous at the smallest represented scale, and couple the sequence of scales using localization and homogenization procedures. For many problems however, they remain computationally unaffordable. This is because they require at each but the finest scale, the solution of a unit cell problem at each quadrature point of the associated FE mesh. Therefore a model order reduction framework was recently presented in [1] for dramatically accelerating the solution of nonlinear dynamic multiscale problems. In this framework, the dimensionality of the governing equations is reduced using the POD method, and computational efficiency is achieved using the ECSW hyperreduction method. Training is performed in two steps: a microscale hyperreduced model is first constructed in-situ in order to achieve significant speedups, even in non-parametric settings; then a classical offline-online training approach is performed to build a parametric hyperreduced macroscale model. A notable feature of this approach is the minimization, at the macroscale level, of the training cost using the in-situ hyperreduced microscale model to accelerate snapshot acquisition. A weak spot however is the in-situ training itself, which, for sufficiently large macroscale models, requires an adaptive reduction process to keep the global ROB accurate and economical at all times. This talk will present such an adaptive process based on the concept of a database of local ROBs that is constructed and updated on-the-fly. This process treats the deformation gradient as a vector parameter, which enables it to locate each unit cell problem in the database and assign to it online the most appropriate local ROB. Its accuracy is optimized by collecting new snapshots as needed and updating accordingly the local ROBs. The resulting adaptive nonlinear model reduction framework is illustrated with the fast solution of several nonlinear dynamic multiscale problems. Reference [1] M. J. Zahr, P. Avery, and C. Farhat, A Multilevel Projection-based Model Order Reduction Framework for Nonlinear Dynamic Multiscale Problems in Structural and Solid Mechanics, International Journal for Numerical Methods in Engineering, vol. 112, pp. 885-881, 2017.

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Title: A Parallel Dynamic Overset Grid Framework for Simulations of Biological Flows

Author(s): *Mohammadali Hedayat, *Texas A&M*; Iman Borazjani, *Texas A&M*;

The overset grid technique is one of the most popular algorithms in computational fluid dynamics which enables the flow solvers to handle complex geometries, or unsteady moving grid simulations. However, the task of overset grid assembly on parallel distributed systems still remains challenging. A new scalable parallel grid assembly and interpolation framework is developed to performing overset grid connectivity among multiple structured meshes which are in a distributed computing environment. This framework is integrated with a sharp interface curvilinear immersed boundary (CURVIB) flow solver to handle multiple overlapping domains along with arbitrarily complex geometries in the fluid domain. The grid connectivity is fully parallel and all operations are performed on the distributed grid data. A successful, scalable parallel implementation of overset grid framework requires an efficient data structure for storage of connectivity information and minimizing the communication cost between processors. In order to achieve to this goal several steps are implemented in our framework: 1) oriented bounding boxes (OBB) are constructed instead of axis-aligned bounding boxes to minimize the search space and consequently memory allocation; 2) Gradient search for identifying the donor; 3) Removing the I/O file for communication with flow solver; and 4) Efficient vectorized implementation for velocity interpolation. The moving grids are handled using a conservative general non-inertial frame of reference flow solver to prevent the recomputation of curvilinear grid metrics during grid rotation/translation. The framework verified and validated against experimental and analytical data. Our results show a good scalability and accuracy for this new framework. In addition, its capabilities are demonstrated by simulating real-life biological flows. This work is supported by the American Heart Association Grant 13SDG17220022, and the computational resources were partly provided by the high-performance research computing (HPRC) at Texas A&M.

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Title: Data-driven Validation of Bishop's Effective Stress Principle through Deep Reinforcement Learning

Author(s): *Yousef Heider, *Columbia University*; Kun Wang, *Columbia University*; Hyoung Suk Suh, *Columbia University*; WaiChing Sun, *Columbia University*;

In analogy to Terzaghi's effective stress principle in fully-saturated porous media, Bishop's effective stress principle presents a partition of the total stress in unsaturated porous media between suction and effective stress contributions. Although widely applied in Geomechanics, the validity and generality of Bishop's principle across saturation regimes still a matter of debate, especially for path-dependent materials that exhibit hysteresis retention behaviors. The proposed meta-modeling automated learning approach makes use of data-based constitutive modeling, generated via reinforcement learning, to evaluate the validity and generality of Bishop's effective stress principle for various types of blind predictions involving material failures, such as strain localization and brittle fracture. Synthetic micro-structural-based data of unsaturated granular materials (such as coordination number, fabric tensor, porosity, saturation, suction, and intrinsic permeability) are generated using the discrete element method DEM together with the pore-network approach, applied to a representative volume element (RVE). Data set generated from sub-scale simulations are used to automatically create, train, calibrate and validate plausible alternative stress partition theories represented by directed graphs until an optimal knowledge graph is formed. The blind prediction performance of the data-driven discovery will then be compared with predictions based on different variations of the effective stress principle for unsaturated porous media.

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Title: A DPG Maxwell Approach for Studying Nonlinear Thermal Effects in Active Gain Fiber Amplifiers

Author(s): *Stefan Henneking, *The University of Texas at Austin*; Leszek Demkowicz, *The University of Texas at Austin*; Jacob Grosek, *Air Force Research Laboratory*;

Fiber lasers that are operated at high power levels suffer from undesired nonlinear effects such as Transverse Mode Instability (TMI). Indeed, TMI is a major obstacle in power-scaling of continuous-wave, weakly guided, large mode area, active gain, silica fiber amplifiers. A better understanding of these relevant nonlinear coupling effects is beneficial in the design of new fibers. To that end, we propose a three-dimensional Discontinuous Petrov-Galerkin (DPG) finite element approach for studying a novel nonlinear full vectorial Maxwell model. The model incorporates both amplification (or laser gain) as well as thermal effects via coupling with the heat equation. The high-frequency nature of this nonlinear wave propagation problem requires the use of high-order discretizations to effectively counter numerical pollution. The DPG methodology provides a suitable framework for this. In particular, we apply the ultraweak DPG formulation to the Maxwell system, carrying desirable properties in the high-frequency regime. The ultraweak Maxwell system is then coupled with the primal DPG formulation of the heat equation. The derived DPG formulation comes with a host of advantageous properties, including mesh-independent stability and a reliable built-in a-posteriori error estimator enabling adaptivity. We present numerical results for this coupled system, modeling fibers with up to 100 wavelengths. For that, we emphasize the importance of high-order discretization. Our qualitative results provide new insight into the nonlinear effects of laser gain and thermal fluctuations on the propagation of guided modes in the fiber amplifier. [1] C. Carstensen, L. Demkowicz, and J. Gopalakrishnan. "Breaking Spaces and Forms for the DPG Method and Applications Including Maxwell Equations." Computers & Mathematics with Applications 72, no. 3 (2016): 494-522. [2] S. Nagaraj, J. Grosek, S. Petrides, L. Demkowicz, and J. Mora. "A 3D DPG Maxwell Approach to Nonlinear Raman Gain in Fiber Laser Amplifiers." arXiv preprint arXiv:1805.12240 (2018), accepted for publication in Journal of Computational Physics: X.

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Title: An Immersed Volumetric Nitsche's Approach for Meshfree Analysis of Composites

Author(s): *Michael Hillman, *Penn State*; Guohua Zhou, *Optimal Inc*;

It is difficult to generate body fitting discretizations for interface problems such as modeling inclusions in solid mechanics. Among the methods available, immersed boundary methods that discretize bodies independently provide potential for tackling these type of problems since a matching discretization is not needed. However, for meshfree methods the associated strong enforcement of kinematic conditions on boundaries is non-trivial [1], particularly for arbitrary interior interfaces [2]. Volumetric approaches are available such as the Lagrange multiplier and penalty methods which can circumvent this issue [3], yet have the well-known inherent shortcomings of LBB instability and sensitivity to tunable parameters, respectively. In this work, an immersed framework is proposed that imposes interface continuity with a volumetric Nitsche's approach, which precludes the issues of imposing boundary constraints, and avoids the issues with penalty- or Lagrange multiplier-based volumetric approaches. The higher-order continuity required in the method is easily attained using the flexibility of meshfree approximations. The effectiveness of this method is examined by solving composite benchmark problems, where high accuracy and optimal convergence are obtained. [1] S. Fernández-Méndez, A. Huerta, "Imposing essential boundary conditions in mesh-free methods," Comput. Methods Appl. Mech. Eng. (193) 12, 1257–1275, 2004. [2] C.T. Wu, Y. Guo, E. Askari, "Numerical modeling of composite solids using an immersed meshfree Galerkin method," Compos. Part B Eng. (45) 1, 1397–1413, 2013. [3] P.J. Blanco, R.A. Feijóo, E.A. Dari, "A variational framework for fluid-solid interaction problems based on immersed domains: Theoretical bases," Comput. Methods Appl. Mech. Eng. (197) 25–28, 2353–2371, 2008.

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Title: Integration of CAE and AI on the Cyber Physical Systems for the Foudation of Society5.0

Author(s): *Tohru Hirano, *Daikin Information Systems*;

Japanese government has formulated Society 5.0 as a measure to balance economic advancement with the resolution of the social issues such as declining population and aging society. This is aimed at a human-centered society with systems that highly combine cyber spaces and physical (real) spaces. Integrating information science (IoT, AI, 5G, etc.), computational science (FEM, FDM, MBD, UQ, HPC, etc.) and behavioral economics (Bounded Rationality, Prospect Theory, Nudge theory, etc.), which are the academic background to realize Society 5.0, the foundation of "Computational Information Science" is introduced incorporating human and society into the system models. Uncertainty Quantification of the CPS process is classified into two different objects, one is concerning to physical spaces and related cyber models such as devices, sensing data and physical system models (Digital Twins), and the other is concerning to human behavior and the social decision making which should be incorporated into the Smart Services. We also define separately for Deep Learning capability on the platform and Reasoning capability on the edge, and present the application of Transfer Learning for the intelligence sharing on the CPS process .

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Title: Treatment of Discrete Events in Embedded Boundary Methods for CFD and Fluid-structure Interaction

Author(s): *Jonathan Ho, *Stanford*; Charbel Farhat, *Stanford*;

Embedded boundary methods (EBMs) are often preferred over body-fitted approaches for fluid-structure interaction (FSI) problems with complex geometries, large deformations and/or topological changes. When the boundary treatment characterizing an EBM attempts to sharply capture the material interface ? and the fluid state at this interface, it tends to generate an oscillatory numerical solution for at least two different reasons. The first one is the ill-conditioning generated by extrapolation in the vicinity of ?, which is a source of spatial oscillations. This has been previously addressed for both incompressible and compressible flows [1]. The second reason is the sudden status change of an embedding CFD grid point – from real (active) to ghost (inactive), or vice-versa -- when this point is traversed by a moving interface ?. This discrete event is a source of spurious, temporal oscillations. It has been previously discussed but only for incompressible flows [2]. For some problems, the source of spatial oscillations tends to be the dominant one. For other problems – for example, for gradient-base shape optimization problems where the gradients of the flow solution with respect to ? must be computed – the source of temporal oscillations becomes more significant. Hence, both sources of spurious oscillations must be mitigated. Accordingly, this lecture presents a novel approach for the treatment of discrete events in compressible flows. This approach evolves the concept of the status of a fluid grid point to that of a fluid edge, by introducing: two additional fluid edge types besides the conventional fluid-fluid and fluid-structure types; and an interpolatory algorithm to effectively enforce a smooth transition. It also incorporates an enhanced moving least-squares scheme to address discrete events associated with the computation of quantities of interest. While the proposed approach is applicable to any EBM, it is presented in the context of the FIVER EBM [1] for compressible flows. References [1] Daniel Z. Huang, Dante De Santis, and Charbel Farhat. A family of position- and orientation-independent embedded boundary methods for viscous flow and fluid-structure interaction problems. Journal of Computational Physics, 365:74-104, 2018. [2] Haoxiang Luo, Hu Dai, Paulo J.S.A. Ferreira de Sousa, and Bo Yin. On the numerical oscillation of the direct-forcing immersed-boundary method for moving boundaries. Computers & Fluids, 56:61-76, 3 2012.

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Title: Computational Modelling of Reinforced Concrete Members with Peridynamics

Author(s): *Mark Hobbs, *University of Cambridge*; John Orr, *University of Cambridge*; David Miranda, *University of Cambridge*; Gabriel Hattori, *University of Cambridge*;

There is a pressing need to address the overdesign of reinforced concrete structures. The utilisation of structural concrete members is often very low and structural material wastage in the order of 50% is common. Orr (2011) showed that it is possible to design and build optimised non-prismatic concrete members that use up to 40% less concrete than prismatic members of equivalent strength. Ensuring the safety and reliability of highly efficient structural members requires accurate analysis methods. Predicting the shear behaviour of reinforced concrete members is notoriously difficult and codified design methods are generally based on empirical formulas derived from the testing of prismatic beams. Non-prismatic members fall outside of conventional design codes and current methods for determining their structural response and ultimate limit state behaviour are inadequate. Robust and accurate numerical models are needed for predicting the behaviour of optimised reinforced concrete structural members. This work utilises the peridynamic theory of solid mechanics (Silling, 2000) to develop numerical models for the analysis of three-dimensional reinforced concrete members. The peridynamic theory does not include spatial derivatives and remains valid across discontinuities, allowing for the natural inclusion of fracture behaviour. The presented work examines the suitability of numerical models based on the peridynamic theory for simulating the complex ultimate limit state behaviour of reinforced concrete, when little or no a priori knowledge is available on possible fracture behaviour. The developed numerical model is applied to the simulation of reinforced concrete members failing in flexure and shear. It is demonstrated that the numerical model can capture the failure mode and load capacity of reinforced concrete members and the observed fracture behaviour is generally in agreement with experimental results. Using only a simple linear damage model it is possible to simulate different types of shear failure in reinforced members. Numerical models based on the peridynamic theory could be utilised to help facilitate the design and construction of efficient structural members. Orr, J., Darby, A., Ibell, T., Evernden, M., Otlet, M., 2011. Concrete structures using fabric formwork. Struct. Eng. 89, 20–26. Silling, S.A., 2000. Reformulation of elasticity theory for discontinuities and long-range forces. J. Mech. Phys. Solids 48, 175–209. https://doi.org/10.1016/S0022-5096(99)00029-0

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Title: Observations Regarding the Possibilities of Handling "the Time Situation" for Part Scale LPBF Modeling

Author(s): *Neil Hodge, *Lawrence Livermore National Laboratory*; Robert Ferencz, *Lawrence Livermore National Laboratory*;

Laser powder bed fusion (LPBF) is a manufacturing process which can realize significant benefits over traditional manufacturing processes, including significantly shortened time between design and manufacture of parts, and the ability to create parts with much more geometric complexity than has previously been tenable, or in some cases, even possible. In order to understand the nature of these processes, many researchers and end users have turned to modeling to predict quantities such as microstructure and residual stress as a function of the process parameters. However, the complex nature of these models, and in particular, the extreme spatio-temporal scales over which they operate, makes it difficult to calculate high quality solutions in reasonable wall clock times. While both the spatial and temporal problems in LPBF are clearly "multi-scale", the temporal scales often span more orders of magnitude than the spatial scales. Many existing finite element codes employ various strategies to speed the calculation of the spatial problem; indeed, some highly parallel codes are far past the point of diminishing returns for this aspect of the problem. However, the temporal problem has received much less attention. These two facts result in a situation where there are clear performance gains to be made regarding the temporal portion of the calculation. This presentation will discuss certain aspects of the physical problem and the implications on model definition and performance, comment on why this portion of the problem space has been largely neglected by the modeling community, and present some initial results of one possible solution to "the time situation" for part-scale LPBF modeling.

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Title: Image-Based Analysis of Cortical Thickness Patterns

Author(s): *Maria Holland, *University of Notre Dame*; Mohsen Darayi, *University of Notre Dame*; Mia Hoffman, *University of Notre Dame*; Kyra Twohy, *University of Notre Dame*; Antonio Hardan, *Stanford University*; Alain Goriely, *University of Oxford*; Ellen Kuhl, *Stanford University*;

The outer surface of the human brain, the cerebral cortex, is deeply wrinkled. The thickness of this cortical layer varies throughout the brain in a consistent way - thicker on the outside peaks, thinner in the buried valleys. As alterations in cortical thickness have been associated with neurodevelopmental disorders including epilepsy, schizophrenia, and Autism Spectrum Disorders (ASD) [1], cortical thickness is an important biomarker for a wide variety of neurological disorders. Conveniently for clinical purposes, MRI allows for the reliable measurement of cortical thickness noninvasively. We have recently presented evidence for a mechanical role in the creation of this characteristic thickness pattern [2], showing that thickness differences emerge in nonbiological materials as well. That study included an analysis of 120 regions in over 500 typically-developing adult human brains. Here we expand on that initial work by expanding the scope to include individuals with neurological disorders and primates. At the same time, we refine our imaging analysis to examine cortical thickness patterns at a smaller scale. This work relies on imaging analysis techniques to uncover patterns of cortical thickness variations in brains that vary in size, shape, foldedness, etc. Comparison of typically-developing individuals and those with ASD is hoped to lead towards objective diagnosis via noninvasive medical imaging. [1] Hardan AY, Muddasani S, Vemulapalli M, Keshavan M, Minshew N (2006) An MRI study of increased cortical thickness in autism. Am J Psychiatry 163:1290-1292. [2] Holland MA, Budday S, Goriely A, Kuhl E (2018) Symmetry Breaking in Wrinkling Patterns: Gyri Are Universally Thicker than Sulci. Phys. Rev. Lett. 121:228002

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Title: Efficient Quantification of Left Ventricular Function During the Full Cardiac Cycle Using a Characteristic Deformation Model

Author(s): *Brian Hong, *University of Nebraska Medical Center*;

Heart failure is a significant source of morbidity and the prevalence of heart failure continues to rise. Quantification of cardiac function beyond standard clinical indices is essential to improving heart failure diagnosis specificity. Patient-specific computational models of the heart offer detailed descriptions of cardiac function suitable for this purpose. Such models are typically constructed using 0D “varying elastance” or 3D Finite element method (FEM) approaches. While both methods have been successfully applied to many patient-specific applications, each has limitations. Varying elastance models are limited by their simplified representation of the myocardium while FEM models have a high computational cost that is restrictive in applications that require the simulation of many cardiac cycles. As an alternative to these approaches, we describe a computationally efficient method for simulating the dynamics of the left ventricle (LV) in three dimensions using characteristic deformation modes (CDM). In the CDM-LV model, LV motion is represented as a combination of a limited number of deformation modes, chosen to represent observed cardiac motions. A variational approach is used to incorporate a mechanical model of the myocardium. Passive stress is governed by a transversely isotropic elastic model. Active stress acts in the fiber direction and incorporates length-tension and force-velocity properties of cardiac muscle. We apply this model to quantify LV function in three cases. First, we quantify the passive stiffness of a mouse heart. The stiffness parameters of the mouse LV calculated with the CDM model are similar to those identified using a FEM approach. Second, we quantify LV function during the full cardiac cycle from 3D echocardiogram data. We estimate parameters for the myocardial passive stiffness and active contractile function using a bounded quasi-newton numerical optimization algorithm. We demonstrate that this method is capable of recapitulating the observed aggregated motion of the LV and provides reasonable estimates for the mechanical parameters. Finally, to illustrate the computational efficiency and broad applicability of this method, we present preliminary results of a study of heart failure with preserved ejection fraction (HFpEF). In this study we apply the CDM-LV to clinical echocardiogram data to estimate cardiac function in ten normal volunteers and ten HFpEF patients. Collectively, these applications demonstrate that this approach provides reasonable estimates for the mechanical parameters that determine LV function on a clinically relevant time-scale.

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Title: Multi-material Topology Optimization for Reduction of Dynamic Structural Response

Author(s): Takuma Endo, *Tohoku University*; Junji Kato, *Nagoya University*; *Hiroya Hoshiba, *Nagoya University*;

One of the innovative and possible developments in additive manufacturing may be the products based on multi-materials. In this context, the development of multi-material topology optimization receives a lot of attention for the future products. However, the design methods for multi-material structures have yet to be well investigated, which make the most of the advantage/performance of each constituent. From these circumstances, the present study focuses on a problem in dynamics and proposes a multi-material topology optimization method to reduce the dynamic response of structures. The density, Young's modulus and viscosity coefficient in the multi-material are controlled by material volume fraction at the finite element based on the SIMP-like interpolation scheme. In particular, the interpolation of elemental viscosity is proposed and its effectivity is discussed in the research. Adjoint sensitivity analysis is applied to obtain the accurate sensitivities of variables. The performance of the proposed method is verified by the series of numerical examples.

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Title: Mixed Precision Conjugate Gradient Iterations Considering Hierarchical Memory Configurations

Author(s): Hiroshi Okuda, *The University of Tokyo*; *Hiroki Hosokawa, *The University of Tokyo*;

Solving large systems of linear equations represents the most time consuming part of a finite element code. For very large and sparse matrices, Krylov solvers are usually preferred over direct solvers. From these, the most popular ones are the Conjugate Gradients (CG) method and GMRES. Composed of vector -vector (dot products, vector updates) and sparse-matrix vector multiplications (SpMV), such solvers have been historically running at less than in 10% CPU peak. In using current generation CPUs equipped with GPUs as promising accelerators, in order to enjoy their potential, optimized mixed-precision programming and low energy consumption computation are the promising strategies. In this study, among the mixed-precision strategies, the iterative refinement technique, which makes use of single precision as much as possible and only little in higher precision, has been devised in order to accelerate the computation and to reduce the energy consumption.

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Title: The Effect of 3D Shape on Plaque Vulnerability and Targeted Nanomedicine Delivery

Author(s): *Shaolie Hossain, *Texas Heart Institute*; Michael Johnson, *The University of Texas at Austin*; Travis Sanders, *The University of Texas at Austin*; Thomas Hughes, *The University of Texas at Austin*;

Roughly 70% of heart attacks occur when vulnerable plaques in the coronary arteries rupture releasing their lipid content into the blood stream forming a thrombus. This restricts blood flow to the heart muscle, inducing myocardial infarction. Hemodynamic features near vulnerable plaques are known to affect plaque instability. For instance, plaque ulcerations are known to occur in areas of high wall shear stress (WSS), while highly positive wall shear stress gradients (WSSG) are known to affect the endothelial cell alignment on the plaque cap, weakening its fracture toughness and increasing rupture risk. The effect of plaque aspect ratio, axial symmetry, and differing distal and proximal shape on local WSSG is not well understood. In addition, there have been no reports on the influence of plaque shape on the level of local inflammation (e.g., VCAM-1 expression), a known precursor to plaque rupture. A computational workflow has been developed within an isogeometric analysis (IGA) framework to enable a comprehensive parametric study of plaques of arbitrary shape in conjunction with patient-specific attributes in order to gain predictive insights into plaque instability. Parameterized 3D plaque models are created within a coronary artery tree using an in-house vascular NURBS (Non-Uniform Rational B-Splines) modeling pipeline that leverages a robust algorithm development plugin called Grasshopper within the CAD software package Rhinoceros. By adjusting the axial and proximal/distal symmetry parameters while keeping the plaque length and degree of stenosis fixed, 9 representative solid plaque models are created for the purposes of this study. A Navier-Stokes solver, coupled to an experimentally-validated particle adhesion model, and subjected to appropriate boundary conditions, is utilized to simulate realistic bulk flow features and near wall quantities including WSS and WSSG. Vascular distribution of inflammation-targeted nanomedicine is also quantified. Results show that while the maximum velocity is unaffected by plaque shape for the same degree of stenosis, WSS and WSSG are varied by as much as 22.8% and 57.7%, respectively, among the cases considered. The proximally skewed model with an axial offset has the most vulnerable combination of high WSS, high positive WSSG and elevated inflammation. The presented approach, if confirmed in a large study of patient data, can identify hemodynamic quantities (WSS WSSG, etc.) as surrogate marker(s) of plaque instability, potentially leading to a non-invasive diagnosis and treatment of vulnerable plaques. REFERENCES [1] B Urick, TM Sanders, SS Hossain,Y Zhang, TJR Hughes, Archives of Computational Methods in Engineering, Published online December 12, 2017.

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Title: A Computational Study of the Biomechanical Response of the Human Lower Extremity Subjected to High Rate Vertical Accelerative Loading

Author(s): *Zachary Hostetler, *Wake Forest University School of Medicine, Virginia Tech -Wake Forest University Center for Injury Biomechanics*; Jazmine Aira, *Wake Forest University School of Medicine, Virginia Tech -Wake Forest University Center for Injury Biomechanics*; Joel Stitzel, *Wake Forest University School of Medicine, Virginia Tech -Wake Forest University Center for Injury Biomechanics*; F. Scott Gayzik, *Wake Forest University School of Medicine, Virginia Tech -Wake Forest University Center for Injury Biomechanics*;

Introduction Vertical loading in the underbody blast (UBB) condition generates high accelerative loading at the point of contact of the human-machine interface, particularly the lower extremity. Computational human body models have not been fully leveraged to explore such events. The objective of this study is to use the Global Human Body Models Consortium (GHBMC) average male lower extremity to quantify the resulting loads (both gross and local) experienced in representative UBB conditions. A secondary aim is to evaluate the stability and robustness of the model in these conditions. Methodology A design of experiments (DOE) was conducted using the GHBMC M50-O v. 4.5 leg (proximal tibia through foot) in a range of UBB loading conditions. The booted GHBMC leg in a 90-90-90 posture was mounted on a cantilevered arm and loaded vertically via an instrumented plate with prescribed motion. Data were extracted from virtual load cells at the knee, tibia, and calcaneus. Simulations were conducted varying the time-to-peak (TTP), acceleration, jerk, and pulse duration commensurate with previously published data of UBB events (Kulkarni et al 2014). The design space of the DOE was sampled uniformly to generate 49 loading conditions. Peak forces, moments, displacements, accelerations, and strains were output. The Tibia Index criteria, energy absorbed by the leg, leg compression, leg shaft fracture and calcaneus fracture were calculated from published risk curves. Results All 49 simulations normal terminated. Pulse durations varied from a minimum of 4 milliseconds to 30 milliseconds. Acceleration at the loading plate ranged from 45 g’s to 1665 g’s with TTP values of 15 and 2 ms respectively. The peak force observed in the knee, tibia, and calcaneus was 11.3, 14.6, and 14.8 kN respectively. Furthermore, 32 of the 49 simulations resulted in a Tibia Index > 1. The peak leg compression was 9.7 % of total leg length and the maximum energy absorbed by the leg was 515 J. Finally, 31 and 27 simulations resulted in greater than 50% risk probability of leg shaft fracture and calcaneus fracture respectively. Conclusions The majority of the simulated trials, which align with peak forces and accelerations previously reported from UBB experiments, indicated the presence of injury. The GHBMC M50-O lower extremity model was stable and robust in simulated UBB environments. The model can provide insight and guidance on the lower extremity injury risk from severe vertical loading.

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Title: Model Order Reduction for Finite Element Analysis with Geometry and Materials Variations

Author(s): *Jie Hou, *University of Massachusetts Dartmouth*; Jun Li, *University of Massachusetts Dartmouth*; Alfa Heryudono, *University of Massachusetts Dartmouth*; Wenzhen Huang, *University of Massachusetts Dartmouth*; Jing Bi, *Dassault Systemes SIMULIA Corp*;

Additive manufacturing (AM) has revolutionized the making of engineering products and relevant standards/methodologies. With more freedom in design space, one can create more design variants in geometry and material distributions. During AM process, part distortions and material defects may also lead to geometry and materials variations. Finite element analysis (FEA) is a powerful tool for physics-based high-fidelity simulations while may be time- consuming. A data-driven approach using Machine Learning has the promise to rapidly predict reliable results for real-time design evaluation and AM process quality control with improved decision-making capability. Two examples were investigated in this study: the first one considers the stress field predictions of a 3D cuboid model with varying sizes subjected to bending; the second one predicts the strain field of a 2D panel under uniaxial tension with a material defect varied in location and sizes. The model order reduction techniques of both POD (Proper Orthogonal Decomposition) and PGD (Proper Generalized Decomposition) are studied for the two examples. They both enable the representation of full FEA stress/strain field outputs with much less number of variables at an acceptable accuracy.

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Title: An Agglomeration-Based, Massively Parallel Non-Overlapping Additive Schwarz Preconditioner for High-Order Discontinuous Galerkin Methods on Polytopic Grids

Author(s): *Paul Houston, *University of Nottingham*; Paola Antonietti, *Politecnico di Milano*; Giorgio Pennesi, *Politecnico di Milano*;

In this talk we design and analyze a class of two-level non-overlapping additive Schwarz preconditioners for the solution of the linear system of equations stemming from high-order/hp-version discontinuous Galerkin discretizations of second-order elliptic partial differential equations on polytopic meshes. The preconditioner is based on a coarse space and a non-overlapping partition of the computational domain where local solvers are applied in parallel. In particular, the coarse space can potentially be chosen to be non-embedded with respect to the finer space; indeed it can be obtained from the fine grid by employing agglomeration and edge coarsening techniques. We investigate the dependence of the condition number of the preconditioned system with respect to the diffusion coefficient and the discretization parameters, i.e., the mesh size and the polynomial degree of the fine and coarse spaces. Numerical examples are presented which confirm the theoretical bounds.

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Title: HPC Techniques for Multi-physics Coupling

Author(s): *Guillaume Houzeaux, *Barcelona Supercomputing Center, Spain*; Marta Garcia-Gasulla, *Barcelona Supercomputing Center, Spain*; Frédéric Magoulès, *Centrale Supélec (Ecole Centrale Paris), France*; Juan Carlos Cajas, *ENES Mérida, UNAM, Mexico*; Ricard Borrell, *Barcelona Supercomputing Center, Spain*; Mariano Vázquez, *Barcelona Supercomputing Center, Spain*;

The setting-up of numerical simulations requires physical, numerical and computational decisions that impact the accuracy, the duration and the cost of the simulation. When multi-physics problems involve different sets of equations to be solved on different computational domain, like e.g. fluid-structure interactions, several additional numerical and computational decisions must be taken. On the algorithmic side, one must select a coupling algorithm, basically between a monolithic and a partitioned approach. The partitioned approach is usually preferred as it enables the reuse of existing codes for each of the physics to be coupled. If this is the case, then one has to select between a block Jacobi and block Gauss-Seidel algorithm to converge (or to approximately converge) to the monolithic solution. Therefore, before starting the simulation, several computational choices must then be made: 1) Given a certain number of available CPUs, how do we optimally distribute the resources between the physics? 2) Disregarding acceleration methods (Quasi-Newton, under-relaxation, etc.) to accelerate the convergence of both algorithms, it is well known that Gauss-Seidel method has better convergence properties than the Jacobi method. However, such a method solves the different physics alternatively, and thus the computational resources are not fully exploited, the CPUs of the physics being alternatively idle. On the other hand, if the CPU time to solve one iteration for all the physics is the same, then the Jacobi method exhibits prefect efficiency. Gauss-Seidel converges better than Jacobi but as poor computational efficiency compared to the Jacobi method. So whom do you want to upset? The engineer who's waiting for the results, or your system manager because you are throwing away resources? In this work, we will study the impact of both algorithms on the convergence and on the computational efficiency for solving partitioned problems. We will then analyze the performance of different techniques to enhance the computational efficiency of both Jacobi and Gauss-Seidel methods. These techniques will include assignment of computational resources, tuning of MPI parameters and dynamic load balancing. D.E. Keyes. Multiphysics simulations: Challenges and opportunities, Int. J. High Performance Computing Application, 27(1): 4-48, 2012. G. Houzeaux, J.C. Cajas, M. Discacciati, B. Eguzkitza, A. Gargallo-Peiró, M. Rivero, and M. Vázquez. Domain decomposition methods for domain composition purpose: Chimera, overset, gluing and sliding mesh methods Arch. Comp. Meth. Eng., 24(4):1033-1070, 2017.

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Title: Tent Pitching Meshes for Asynchronous Spacetime Discontinuous Galerkin Solvers in 3d×time

Author(s): *Christian Howard, *University of Illinois at Urbana-Champaign*; Amit Madhukar, *University of Illinois at Urbana-Champaign*; Jeff Erickson, *University of Illinois at Urbana-Champaign*; Robert Haber, *University of Illinois at Urbana-Champaign*; Reza Abedi, *University of Tennessee Knoxville (UTK) / Space Institute (UTSI)*;

The asynchronous Spacetime Discontinuous Galerkin (aSDG) method [1] is a powerful solution scheme for hyperbolic systems. In lieu of traditional implicit or explicit time-marching procedures, aSDG solvers implement a locally implicit solution scheme on fully unstructured and asynchronous spacetime grids. The locality property, critical to the computational efficiency of aSDG solvers, derives from discontinuous spacetime basis functions defined on spacetime meshes that satisfy a so-called causality constraint. The resulting aSDG solution schemes feature unconditional stability, conservation over every spacetime cell, linear computational complexity, support for arbitrarily high-order elements, a rich structure for parallel implementations, and dynamic adaptive spacetime meshing. The Tent Pitcher algorithm with adaptive extensions [2] is the key technology for generating causal spacetime meshes for aSDG solvers. Let d be the spatial dimension of the analysis domain. Tent Pitcher's main procedure advances a front mesh of d-simplices through the spacetime analysis domain. In addition to spatial coordinates, each front-mesh vertex is assigned a private time coordinate that is initialized to zero. Tent Pitcher advances the front locally and asynchronously by incrementing the time coordinate of one vertex at a time. The causality constraint limits the vertex's time increment to ensure that the updated front remains space-like with respect to the characteristics of the target hyperbolic system. We generate a new spacetime patch, comprised of a small set of (d+1)-simplices that covers the spacetime volume between the old and new fronts, every time a vertex advances. Previously, robust adaptive meshing for aSDG solvers has only been available for meshes in up to 2d×time. However, robust meshing in up to 3d×time is essential for the aSDG method to achieve its full potential. This presentation describes recent progress toward a new meshing implementation that meets that requirement. A new dimension-independent version of the basic Tent Pitcher algorithm is enhanced with dimension-dependent h-adaptive extensions. Examples will demonstrate meshing and solution capabilities in 3d×time; directions for continuing development will be discussed. References: [1] R. Abedi, R. B. Haber, B. Petracovici. A spacetime discontinuous Galerkin method for elastodynamics with element-level balance of linear momentum, ?Comput. Methods Appl. Mech. Eng. 195 (2006) 3247–3273. [2] R. Abedi, S. H. Chung, J. Erickson, Y. Fan, M. Garland, D. Guoy, R. B. Haber, J. Sullivan, S. White, Y. Zhou. Space-time meshing with adaptive refinement ?and coarsening, in: Proc. 20th Annual ACM Symposium on Comp. Geometry, ACM, (2004) 300–309.

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Title: Integrating Cell Mechanics and Signaling to Quantify Mechanical Information Processing by Valve Interstitial Cells

Author(s): *Daniel Howsmon, *The University of Texas at Austin*; Michael Sacks, *The University of Texas at Austin*;

Cells are able to recognize and respond to a variety of proteins and small molecules in their microenvironment, triggering complex signaling cascades that modify cell behavior. Additionally, cells can directly respond to their mechanical environment via mechanically-activated bonds, binding sites, and ion channels. Valve interstitial cells (VICs), the primary resident cells in the four heart valves, transition from a quiescent to activated phenotype in response to changes in material stiffness alone (i.e., without biochemical stimulation). This transition is often associated with the emergence of valvular disease; however, the processes that govern this mechanically-activated transition are not fully characterized and have yet to be completely modeled. This work describes our initial investigation the dynamics of VIC activation on hydrogels of different stiffnesses, connecting models of traditional signal transduction networks with mechanically-dependent processes. Material stiffness alters force-sensitive bonds in molecular clutches, structural complexes that connect the extracellular matrix to the cytoskeleton of the cell via integrins and adaptor proteins talin and vinculin. With enough force, the bond between integrins and extracellular matrix will break and the entire complex dissociates. Signaling proteins also bind to these molecular clutches and the evolution of the signaling cascade is regulated by the dissociation of the clutches. These simulations promise to provide a systems-level view of how VICs process mechanical information, identifying key parameters and events responsible for the transition from a quiescent to activated phenotype.

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Title: Fluid-Structure Interaction Modeling of Transcatheter Aortic Valve Replacement Using Immersogeometric Analysis

Author(s): *Ming-Chen Hsu, *Iowa State University*; Michael C.H. Wu, *Iowa State University*; Heather Muchowski, *Iowa State University*; Manoj Rajanna, *Iowa State University*; Emily Johnson, *Iowa State University*;

Transcatheter heart valves (THVs) have emerged as a minimally invasive alternative to surgical bioprosthetic heart valves therapy. THVs offer advantages such as less postoperative pain, faster rehabilitation, and better pressure gradients. However, issues such as paravalvular leakage, leaflet fatigue, and valve migration limit the widespread use of THV in the younger population, especially due to the lack of data concerning its long-term performance and durability. In this work, we develop a novel computational fluid-structure interaction (FSI) framework for the modeling and simulation of THVs. To account for physiological realism, methods are proposed to model and couple the main components of the system, including the arterial wall, blood flows, heart valve leaflets, and the stent frame. For a better integration between design and analysis, the computational framework is developed based on the isogeometric and immersogeometric methods. The proposed framework is applied to study the performance of various transcatheter valve designs. The accuracy and effectiveness of the FSI model will be discussed.

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Title: FEM Simulation on Frequency-temperature Behavior of SAW Devices

Author(s): *Hongping Hu, *Department of Mechanics, Huazhong University of Science and Technology, Wuhan 430074, P. R. China*; Yanming Zhang, *Department of Mechanics, Huazhong University of Science and Technology, Wuhan 430074, P. R. China*; Qin Qian, *Department of Mechanics, Huazhong University of Science and Technology, Wuhan 430074, P. R. China*;

SAW devices, such as Resonator, filter, duplexer, are widely used in communication electronics. SAW devices are developing toward higher frequencies and smaller sizes[1]. As the increasing of the operation frequency, the performance of SAW devices is seriously affected by the temperature fluctuation. To achieve steep cutoff and stable characteristics, a SAW resonator is required that not only has a high quality factor (Q) but also own a small temperature coefficient of frequency (TCF) [2, 3]. Most of temperature compensation researches focus on bulk acoustic wave (BAW) devices, but only a few research on SAW devices. The TCF is usually regarded as the level of temperature-frequency behavior. To get a small and even zero temperature coefficient, a SAW resonator with a double-layer IDT is built. The temperature variation is applied on the structure of the SAW as a steady-state uniform field. The motion of the structure is described by incremental Lagrangian equations. The optimal structural size is found. The numerical results show that an excellent temperature coefficient of frequency of the SAW resonator is approximately equal to zero (0 ppm/?) at 25? and the resonant frequency is 1214.9MHz with the wavelength being 4um on the optimal situation. References [1] Wang, L., Chen, S., Zhang, J., Xiao, D., Han, K., Ning, X., Liu, J., Chen, Z., and Zhou, J. Enhanced performance of 17.7 GHz SAW devices based on AlN/diamond/Si layered structure with embedded nanotransducer. Applied Physics Letters, 111, 253502 (2017) [2] Takai, T., Iwamoto, H., Takamine, Y., Yamazaki, H., Fuyutsume, T., Kyoya, H., Nakao, T., Kando, H., Hiramoto, M., and Toi, T. High-performance SAW resonator on new multilayered substrate using LiTaO3 crystal. IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, 64, 1382-1389 (2017) [3] Iwamoto, H., Takai, T., Takamine, Y., Hiramoto, M., and Koshino, M. A novel SAW resonator with incredible high-performances. In 2017 IEEE International Meeting for Future of Electron Devices, Kansai (IMFEDK), 2017; 102-103.

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Title: The Friction Effect on the Buckling of Soft Mechanical Metamaterials under Compression

Author(s): *Jianying Hu, *Ningbo University*; Zishun Liu, *Xi'an Jiaotong University*;

ABSTRACT: By introducing a periodic array of pores with different shapes in an elastic matrix, elastic instabilities can be triggered. These instabilities can be utilized to rationally design a series of mechanical metamaterials with unusual properties such as negative Poisson's ratio and adjustable flexural rigidity. Previously we've already investigated the non-linear response of periodic materials with different shape holes and researched the effect of the friction on periodic materials with circular holes, but how the friction on soft mechanical metamaterials with different designed holes is still an unresolved mystery. In this work, we theoretically calculate the critical buckling force for the buckling or pattern transformation of soft mechanical metamaterials. Meanwhile, we also numerically analyze the effect of friction on the buckling behavior of these cellular structures. We find out that, with the effect of friction, new buckling modes arise for holey columns with different shape holes, in which holes of mechanical metamaterials collapse into various patterns. We expect our study could provide future perspectives for mechanics of buckling or optimal design for soft mechanical metamaterials. Keywords: Soft Mechanical Metamaterials; Instabilities; Buckling; Friction Effect This work was supported by Research Foundation (No. SV2018-KF-24) of State Key Laboratory for Strength and Vibration of Mechanical Structure, Xi'an Jiaotong University.

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Title: A New Decomposition to Obtain Traction-Free Crack Surfaces in a Cohesive Phase-Field Model of Fracture, with Application to Soil Networks

Author(s): *Tianchen Hu, *Duke University*; Yingjie Liu, *Duke University*; Rudy Geelen, *Duke University*; John Dolbow, *Duke University*;

Most phase-field formulations for brittle fracture tie the regularization length to the critical strength of the material and other properties. However, certain materials, i.e. a typical mud specimen, have process zone sizes that are significantly larger than specimen dimensions of interest. Hence, a cohesive phase-field formulation for fracture that requires a material-property-independent length scale is necessary to produce reasonable results. Phase-field for fracture models also typically employ a decomposition of the constitutive relations to preclude damage growth under compression. Two of the most widely used decompositions are the spectral decomposition and the volumetric-deviatoric decomposition, either of which is suitable for a range of materials. A decomposition that is both variationally consistent and allows for the regularized fracture surfaces to be completely traction-free has proven to be elusive. In this work, we propose a variational decomposition that splits the local strain energy into normal and tangential parts with respect to the estimated crack surface orientation, and we show that traction-free boundary conditions can be obtained as the regularization length vanishes. We present several numerical examples to demonstrate the differences between various decompositions and the utility of enforcing the traction-free boundary condition. The phase-field model for cohesive fracture with the new decomposition is used to examine soil desiccation and the formation of crack networks. This is a problem that has been extensively studied using traditional approaches to fracture. The phase-field approach for fracture enables us to extend simplified 2D simulations to full-scale 3D simulations, and the new decomposition establishes a linkage between the degradation functions in a phase-field model of fracture and the traction-separation laws in cohesive zone method. Soil cracks are sedimentary structures formed as wet, muddy sediment dries up and contracts. We aim to understand the process of crack formation under controlled environmental conditions, and analyze the impact of different factors (e.g. soil thickness, soil type, boundary conditions). For each realization of the numerical model, a spatially correlated random field of material strength is generated and projected onto the mesh, evaporation is controlled to continuously build up volumetric strains throughout the specimen, and cracks nucleate at weak points and evolve from there. An extensive suite of simulations are then used to quantify the relationship between the characteristic size of the fragments and various model parameters.

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Title: Peridynamic Modeling of Delamination Growth in MMB Test

Author(s): *Yile Hu, *Aerospace Structure Research Center, School of Aeronautics and Astronautics, Shanghai Jiao Tong University, 200240, China*; Yin Yu, *Aerospace Structure Research Center, School of Aeronautics and Astronautics, Shanghai Jiao Tong University, 200240, China*;

Abstract: Resin-rich interface between adjacent plies can be considered the weakest link in fiber-reinforced polymer composites. Composites often contain manufacturing defects and microcracks in these interfaces. Upon loading these defects and microcracks can grow and coalesce leading to delamination. Accurate modeling and evaluation of the influence of a delamination on damage initiation and growth in fiber-reinforced composite laminates under complex loading conditions is a primary design concern. In the previous study in peridynamics, Mode-I and Mode-II delamination are of primary concern [1]. However, composite laminates are subjected to mixed-mode deformation in a general loading condition. In order to model MMB (Mixed-Mode Bending) test, two technical issues are working as the fundamental blocks: (i) frictional contacts between adjacent plies and (ii) accurate bending behaviors. In the present study, a point-to-surface contact model accounting for frictions between adjacent plies is proposed and solved by Lagrange multiplier method. In addition, Mindlin plate theory is employed to model bending and transverse deflections in composite laminates by using peridynamics [2]. Mixed-mode delamination failure is governed by Benzeggagh-Kenane criteria. In the numerical implementation, an implicit algorithm is applied to solve the nonlinear system. The computational model of a MMB specimen is made of AS4/PEEK composite system, it is loaded under five different mixed ratios (0.0, 0.2, 0.5, 0.8 and 1.0), ranging from Mode-I to Mode-II. Peridynamic predictions are compared with FE predictions and experimental results [3]. Detailed modeling approach and comparison results are presented in this study. [1] Y.L. Hu, N.V. De Carvalho, E. Madenci. Peridynamic modeling of delamination growth in composite laminates. Composite Structures, Vol. 132, 2015, 610-620. [2] C. Diyaroglu, E. Oterkus, S. Oterkus, E. Madenci. Peridynamics for bending of beams and plates with transverse shear deformation. [3] P.P. Camanho, C.G. Davila, M.F. De Moura. Numerical Simulation of Mixed-Mode Progressive Delamination in Composite Materials. Journal of Composite Materials, 2003, Vol. 37(16), 1415-1438.

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Title: Applications of B-Differential Equations Methods for the Frictional Contact Problems with Non-matching Meshes

Author(s): *Zhiqiang Hu, *Faculty of Infrastructure Engineering, Dalian University of Technolgy*;

Applications of B-Differential Equations Methods for the Frictional Contact Problems with Non-matching Meshes HU Zhiqiang Faculty of Infrastructure Engineering , Dalian University of Technology , Dalian 116024 , Liaoning , China The Mortar Segment-to-Segment method[1] is efficiently used to solve the frictional contact problem in which the meshes on the potential contact boundaries are non-matching. The work done by the contact stresses on the contact boundaries can be modeled with high accuracy. The over-constraints are eliminated and the contact patch tests passes. In the B-Differential Equations methods[2] (simply denoted as BDE), the frictional contact conditions are written in the form of B-differentiable equations and satisfied accurately, which are solved by B-differentiable Newton method. Due to the nonsmooth property of potential energy in the frictional contact system resulted from the nonsmooth contact constraints, the traditional trial-and-error iteration method in which the tangent stiffness is updated according to the contact status, is difficult to guarantee the convergence of solution. For the BDE method, the B-differentiable Newton algorithm has the advantage of proven convergence property, which improve the robustness of the solution for the engineering practice involving the frictional contact behavior. However, the original BDE method is used for node-to-node contact model in which the discretizations are the same on the contact surfaces. In this work, the BDE method combined with Mortar Segment-to-Segment methods, is proposed to solve the frictional contact problem in which the discretization of two contact surfaces are not matched with each other. The contact constraints are implemented at the non-mortar nodes by the traction on the non-mortar side and the relative displacements at the non-mortar nodes. The proposed method will increase the accuracy of implementation of contact constraints and guarantee the convergence of solution for the contact problems with non-matching meshes. The numerical examples will demonstrates contact patch test results and the accuracy of the combined method. Reference 1. M. A. Puso, T. A. Laursen, A mortar segment-to-segment frictional contact method for large deformations, Comput. Methods Appl. Mech. Engrg., 2004, 193(4-5): 4891–4913 2. Christensen P., Klarbring A., Pang J. S. and Stromberg N., Formulation and comparison of algorithm for frictional contact problems, Int. J. Numer. Methods Eng., 1998, 42(1): 145-173

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Title: Linear Experimental Design for Optimal Control Variate Based Surrogate Models

Author(s): Alex Gorodetsky, *University of Michigan*; Gianluca Geraci, *Sandia National Laboratories*; *Xun Huan, *University of Michigan*;

Optimal experimental design (OED) finds experiments that produce the most useful data for improving models of physical systems. With multiple models of different fidelity often available in engineering and science applications, and control variate frameworks that can leverage correlation and cost trade-offs among models to achieve efficient predictions, it is important to consider settings where experiments, data, and learning are geared towards these multifidelity (MF) systems. While many existing OED approaches focus on a single model, we seek to develop OED capability that accommodates an arbitrary number of models linked under a control variate structure. We start by studying linear designs where model response is linearly dependent on the unknown parameters but can be nonlinear in the design variables, such as for linear regression surrogates with nonlinear features. The single fidelity setting has established optimality criteria, including the popular D-optimal design that maximizes the determinant of the information matrix. We derive the Fisher information matrix in the MF setting for the optimally weighted multivariate control variate surrogates, and illustrate the relationship with its single fidelity counterpart. We then present numerical algorithms to optimize this quantity for batch design of multiple experiments, considering gradient-based methods on continuous design spaces and rank-revealing QR factorization on randomly discretized design variables. Results are shown for a MF dynamical system, and the quality of designs are compared to when independent OED are conducted for each model separately.

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Title: An Embedded Boundary Approach for the Direct Computation of Cable-Driven Flow-Structure Interactions

Author(s): *Daniel Huang, *Stanford*; Charbel Farhat, *Stanford*;

When immersed in a flow, cable structures can be responsible for strong fluid-structure interactions that may significantly affect the performance of the system they are attached to. In CFD computations, the brute force approach for accounting for the presence of a cable can be challenging, particularly when the size of its cross section is small compared to the characteristic length of the host system. In FSI computations, this issue is exacerbated by the fact that from a structural dynamics viewpoint, the geometry of a cable is typically modeled using line elements, which complicates the task of transferring information between its structural and fluid representations. For body-fitted CFD meshes, a "dressing" approach based on phantom surface elements and massless rigid elements was proposed in [1] to address this issue. While it can also be used in non body-fitted CFD frameworks, this approach has computational disadvantages that are identified and discussed in this lecture. For this reason, an alternative, embedded boundary approach is proposed for computing cable-driven flow-structure interactions. This approach is more robust than the ``dressing'' approach and is characterized by a superior computational performance. It is based on: master/slave kinematics between the line representing the geometry of a cable typically found in finite element structural models, and a discretization of its true surface that is embedded in the CFD mesh; a highly accurate algorithm for computing the flow-induced forces and moments on a discrete surface embedded in a CFD mesh; and an energy-conserving method for transferring distributed forces and moments acting on the nodes of a discrete surface to the nodes of a discrete line enclosed by that surface. This proposed approach for computing cable-driven flow-structure interactions is incorporated in the FIVER (Finite Volume method with Exact two-phase Riemann problems) method [2] and demonstrated for a flexible riser problem and a supersonic parachute inflation dynamics problem. References [1] V. Lakshminarayan, C. Farhat, A. Main, An Embedded Boundary Framework for Compressible Turbulent Flow and Fluid-Structure Computations on Structured and Unstructured Grids, International Journal for Numerical Methods in Fluids, vol. 76, pp. 366-395, 2014. [2] C. Farhat, J.F. Gerbeau, A. Rallu, FIVER: A Finite Volume Method Based on Exact Two-Phase Riemann Problems and Sparse Grids for Multi-Material Flows with Large Density Jumps, Journal of Computational Physics, vol. 231, no. 19, pp. 6360-6379, 2012.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Hybridized discretization techniques for incompressible and compressible flow problems

Author(s): Matteo Giacomini, *LaCàN/UPC*; Rubén Sevilla, *Swansea University*; *Antonio Huerta, *LaCàN/UPC*;

Low and high-order strategies are still competing for accurate numerical evaluation of quantities of engineering interest in complex flows. Lately, hybridization techniques have unveiled new possibilities to devise efficient low and adaptive high-order strategies capable of treating large-scale engineering problems in a competitive way. A novel approach for viscous incompressible flows based on hybrid mixed formulation strongly-enforcing symmetry of the stress tensor will be discussed [1]. The symmetry of a second-order tensor (e.g. the Cauchy stress tensor) represents the enforcement of the balance of angular momentum. It follows that a weak imposition of this property leads to a numerical approximation of the balance equation and, consequently, to a violation of the equilibrium to rotations. This is especially critical in the context of flow problems in which quantities of engineering interest have to be evaluated starting from the stress tensor. Some methods lead to a suboptimal convergence of the mixed variable, especially for low-order approximations. This is not the case for the proposed approach, which also presents superconvergence of the post-processed primal field. Thus, an inexpensive local error indicator can be used to drive degree adaptivity [2] accounting for exact geometries. Moreover, since optimal convergence of order k+1 (including the mixed variable) is obtained for any k (degree of the polynomial discretization), including k=0, fast and robust computations of large-scale problems are performed with order zero. This is a face-centered finite volume method (FCFV) [3,4]. It is able to perform efficiently large-scale simulations on complex unstructured meshes. It is robust to cell distortion and stretching. It provides first-order accurate approximations for stresses/fluxes without the need of flux reconstruction procedures. It is locking-free in the incompressible limit and does not require any shock-capturing technique to compute non-oscillatory approximations of shock waves. References M. Giacomini, A. Karkoulias, R. Sevilla, and A. Huerta."A superconvergent HDG method for Stokes flow with strongly enforced symmetry of the stress tensor," Journal of Scientific Computing, 77(3):1679-1702 (2018). R. Sevilla, and A. Huerta. “HDG-NEFEM with degree adaptivity for Stokes flows,” Journal of Scientific Computing, 77(3):1953-1980 (2018). R. Sevilla, M. Giacomini, and A. Huerta. "A face-centred finite volume method for second-order elliptic problems." Int. J. Numer. Methods Eng., 115(8):986-1014, (2018). R. Sevilla, M. Giacomini and A. Huerta. "A locking-free face-centred finite volume (FCFV) method for linear elastostatics," Comput. Struct., 212:43–57, (2019).

15th U.S. National Congress on Computational Mechanics
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Title: Mechanical Properties of the Murine Thoracic Aorta in Health and Disease

Author(s): *Jay Humphrey, *Yale University*; Matthew Bersi, *Vanderbilt University*; Chiara Bellini, *Northeastern University*; Stephane Avril, *Mines-St. Etienne*;

Thoracic aortic aneurysms are responsible for significant morbidity and mortality, thus there is a pressing need to quantify the associated multiaxial mechanical properties. Although data are available from patients, diverse mouse models provide a unique opportunity to study biomechanical mechanisms associated with disease initiation and progression, particularly for different risk factors that include diverse genetic mutations. We have developed two unique, complementary experimental systems to quantify the multiaxial mechanical properties of the murine aorta. The first system subjects nearly cylindrical samples to biaxial loading (cyclic distension and extension) whereas the second system enables full-field characterization for more complex shaped samples using a panoramic digital image correlation method with inverse characterization. Best-fit values of the associated material parameters are determined using nonlinear regression of the data for a "four-fiber family" constitutive model, which in turn allows calculations of multiaxial wall stress and stiffness as well as elastic energy storage. Importantly, our studies revealed that the circumferential material stiffness is elevated significantly in vessels that either have a propensity to aneurysmal dilatation or are already aneurysmal. This finding is consistent with an emerging hypothesis that aneurysms develop in part due a dysfunctional ability of the intramural cells to correctly mechano-sense and mechano-regulate the extracellular matrix. Of particular importance, we have been able to compare results for multiple mouse models of thoracic aneurysm, thus providing the first direct comparison of changes in mechanical properties with disease severity in cases resulting from hypertension or genetic mutation. These findings are also important for they promise to inform computational models of aneurysmal growth and remodeling, which in turn can provide unique information on the mechanical mechanisms of lesion enlargement. The interested reader is referred to two recent publications for further details [1,2]. [1] Bellini, C. et al. J R Soc Interface 14: 20160995, 2017 [2] Bersi, M.R. et al., Biomech Model Mechanobiol, 2019 (in press)

15th U.S. National Congress on Computational Mechanics
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Title: A Pseudo Direct Numerical Simulation to solve Turbulent CFD Problems

Author(s): *Sergio Idelsohn, *CIMNE*; Eugenio Oñate, *CIMNE*; Norberto Nigro, *CIMEC*; Axel Larreteguy, *UADE*; Juan Gimenez, *CIMEC*; Pavel Rytzhakov, *CIMNE*;

Although the Navier-Stokes equations are equivalently applicable to both laminar and turbulent fluid flows, the current computing power generally precludes employing fine meshes that would allow to simulate turbulent flows without introducing empirical approximations. The prediction power of the models is therefore restricted to problems within the margins of the selected empirical approximation. Solving a problem without such approximations on a mesh sufficiently fine so as to represent the whole expected range of eddy sizes is known as “Direct Numerical Simulation” (DNS). Taking into account that many fluid flow problems of industrial interest are indeed turbulent, it is worthwhile to continue improving the models so that they fit more and more with the physics of the problem. Simulating a CFD problem in a given domain with a “fine enough” DNS mesh introduces an unmanageable number of unknowns for current computers. The project we are working on involves modelling turbulent flow in a DNS fashion, i.e. without any additional turbulence model. However, we strive to develop an approach considerably more computationally efficient than a classical DNS. The basic idea is as follows. The global (macro) domain, can be subdivided into many equally-shaped small domains, the so-called RVEs, “Representative Volume Elements” (micro problems). These RVEs, in principle, can be solved individually and independently from each other. The RVEs may even be previously solved off-line for different time-dependant loads. The micro and macro problems require to be coupled. This will be performed via the theory known as “homogenization”. Another important aspect of the solution process in our approach is the use of a Lagrangian particles at the macro level [1]. The Lagrangian particles will take care of the transport of the macro-velocity and also of the micro-eddies, thus convecting the turbulent energy. This is a very important feature in turbulent flows where turbulence is produced in some high gradient regions and is then convected to other regions. This presentation is a work in progress, aimed more at opening a discussion on the topic, rather than presenting elaborate results. REFERENCES [1] Lagrangian versus Eulerian integration errors; S.R. Idelsohn; E. Oñate, N. Nigro, P. Becker, J. M. Gimenez; Comput. Methods Appl. Mech. Engrg. (2015).

15th U.S. National Congress on Computational Mechanics
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Title: A New Numerical Approach to the Solution of Partial Differential Equations with Optimal Accuracy on Irregular Domains and Cartesian Meshes. Application to the Wave, Heat, Helmholtz and Poisson Equations

Author(s): *Alexander Idesman, *Texas Tech University*;

A new numerical approach based on the minimization of the local truncation error is suggested for the solution of partial differential equations. Similar to the finite difference method, the form and the width of the stencil equations are assumed in advance. A discrete system of equations includes regular uniform stencils for internal points and non-uniform stencils for the points close to the boundary. The unknown coefficients of the discrete system are calculated by the minimization of the order of the local truncation error. The main advantages of the new approach are a high accuracy and the simplicity of the formation of a discrete (semi-discrete) system for irregular domains. For the regular uniform stencils, the stencil coefficients can be found analytically. For non-uniform cut stencils, the stencil coefficients are numerically calculated by the solution of a small system of linear algebraic equations (20-100 algebraic equations). In contrast to the finite elements, there is no necessity to calculate by integration the elemental mass and stiffness matrices that is time consuming for high-order elements. As a mesh, the grid points of a uniform Cartesian mesh as well as the points of the intersection of the boundary of a complex domain with the horizontal, vertical and diagonal lines of the uniform Cartesian mesh are used; i.e., in contrast to the finite element meshes, a trivial mesh is used with the new approach. Changing the width of the stencil equations, different high-order numerical techniques can be developed. Currently the new technique is applied to the solution of the wave, heat, Helmholtz and Laplace equations. The theoretical and numerical results show that for the width of the stencil equations equivalent to that for the linear quadrilateral finite elements, the new technique yields the fourth-order of accuracy for the numerical results on irregular domains for the considered partial differential equations (it is much more accurate compared with the linear and high-order finite elements at the same number of degrees of freedom). 3-D numerical examples on irregular domains show that at accuracy of 5%, the new approach reduces the number of degrees of freedom by a factor of greater than 1000 compared to that for the linear finite elements with similar stencils. This leads to a huge reduction in computation time for the new approach at a given accuracy. This reduction in computation time will be even greater if a higher accuracy is needed; e.g., 1% or less.

15th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Correction for Reduced Order Modeling of Nonlinear Systems

Author(s): *Traian Iliescu, *Virginia Tech*;

In this talk, we address the following question: Given a nonlinear equation u' = f(u) and a basis of fixed dimension r, find the best Galerkin model of dimension r. We present the answer proposed by our group for reduced order models (ROMs), supporting numerical results, and open questions. Specifically, we propose a data-driven correction ROM (DDC-ROM) framework, which can be formally written as DDC-ROM = Galerkin-ROM + Correction. To minimize the new DDC-ROM's noise sensitivity, we use the maximum amount of classical projection-based modeling and resort to data-driven modeling only when we cannot use the projection-based approach anymore (i.e., for the Correction term). The resulting minimalistic data-driven ROM (i.e., the DDC-ROM) is more robust to noise than standard data-driven ROMs, since the latter employ an inverse problem (which is sensitive to noise) to model all the ROM operators, whereas the former solves the inverse problem only for the Correction term. We test the novel DDC-ROM in the numerical simulation of a 2D channel flow past a circular cylinder at Reynolds numbers Re = 100, Re = 500, and Re = 1000.

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Title: On the Solution of 3D Free Surface Flows during Gas Jet Wiping Process for Continuous Galvanization

Author(s): *Florin Ilinca, *National Research Council Canada*; Kintak Raymond Yu, *National Research Council Canada*; Frank Goodwin, *International Zinc Association*;

In continuous galvanizing line operations, the thickness and the uniformity of the zinc coating are governed by the gas jet wiping process which is a complex multi-phase, multi-scale phenomenon. In this process, a steel strip is passed continuously through a molten zinc bath at around 460°C. When the steel strip exits from the bath, it is coated with a layer of liquid zinc, whose thickness is controlled by a wiping gas jet impinging on both sides of the strip. The dimensional characteristics and stability of the coating depend on various factors such as the jet dimensions and speed, the viscosity of the liquid zinc, the speed of the strip and the height of the gas knifes. This makes the process optimization difficult and the right operating window is hard to achieve, especially when there are changes in the product type or bath operations. To advance the fundamental understanding of such intricate process, an efficient and accurate numerical model would be highly valuable. In this work, we present the development of a finite element method for free surface flows in the presence of surface pressure and shear forces such as those encountered during the wiping process. The method considers the effect of the gravity and the boundary conditions describing the moving strip. Solutions are obtained on a fixed mesh by using the level-set technique for the free surface and a discontinuous pressure gradient approach on elements cut by the liquid/gas interface. The effect of the wiping jet is incorporated through distributed normal and tangential forces on the liquid/gas interface reproducing the pressure and shear stress distribution from the turbulent gas flow. Those forces can be obtained either from experiments or by numerical simulation. The method is first validated for the liquid entrainment inside a cavity, the upper surface being subjected to shear forces. Then, the methodology is applied to solve the flow dynamics in the coating layer under the effect of wiping jets. It is shown that the method is able to tackle the extreme range of length scales encountered, from the one of the moving strip in the order of meters, to that of the coating thickness of only a few microns. The finite element stabilization method capable to handle the high aspect ratio meshes employed for this application is also discussed. Finally, a study of the effect of different parameters on the coating thickness will be presented.

15th U.S. National Congress on Computational Mechanics
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Title: Integration Accuracy with Non-coincident Geometries in the Material Point Method

Author(s): *Austin Isner, *Los Alamos National Laboratory*; Duan Zhang, *Los Alamos National Laboratory*;

The material point method (MPM) has been applied in the simulation of a wide variety of problems involving large material deformations, such as the modeling of granular flows, void growth and material failure, and impact. The MPM employs both Lagrangian material points and a background Eulerian mesh to seek a weak solution of the partial differential equations. Unlike the finite element method (FEM), a material point is not fixed to any one element, but is free to move throughout the mesh, carrying all state information including the deformation history. During each time step, information is mapped between the material points and the mesh nodes. Since the background computational mesh is fixed, the MPM avoids both the issues of mesh entanglement in pure Lagrangian methods in cases of large deformation and numerical diffusion of history-dependent information in Eulerian methods, since there is no projection of the material state variables between particles and the grid. In many applications of the MPM to large-deformation mechanics problems, the material point discretization of the initial problem configuration may be carefully selected. Additionally, a material point region may be constructed such that geometric boundaries or material interfaces align with element boundaries, allowing for unambiguous imposition of boundary conditions at the cell nodes. For large deformations, the initial distribution of material points relative to a fixed element can quickly change as points follow their respective Lagrangian trajectories. In this work, we quantify the errors in the MPM for non-coincident material point geometries, i.e. when the discretized material point domain is not aligned with the background grid. We characterize the effect on order of convergence in non-aligned problems using time explicit integration for different refinement approaches including changing number of material points per cell or changing cell size with a fixed number of material points per cell. To avoid the effect of cell-crossing noise, we only consider small strain problems using either a momentum-based MPM formulation or a velocity-based formulation with distribution coefficients to handle small mass node instabilities, in order to focus on the effect of arbitrarily distributed or misaligned material points within an element on overall solution accuracy.

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Title: Modeling the Deformation of a Four Chamber Cardiac Model with Pericardium

Author(s): *Arian Jafari, *Iowa State University*; Anushrut Jignasu, *Iowa State University*; Adarsh Krishnamurthy, *Iowa State University*;

Four-chamber cardiac models can capture the deformation characteristics of the heart accurately with physiologically equivalent boundary conditions. We have created a four-chamber cardiac model utilizing cubic-Hermite elements and simulated a full cardiac cycle by coupling the biventricular 3D finite element model with a lumped circulation model and passively applying the pressure boundary conditions to the atria. Cubic-Hermite finite element meshes are widely used for simulating cardiac biomechanics due to their superior convergence characteristics and their ability to capture smooth geometries compactly compared to linear tetrahedral meshes. However, such meshes have previously been used only with simple ventricular geometries with non-physiological boundary conditions due to challenges associated with creating cubic-Hermite meshes of the complex heart geometry. The complex geometry of the heart, especially near atrial regions and valves necessitates the appearance of extraordinary nodes (nodes with 3 or >= 5 adjacent elements in 2D) in the mesh. We have developed a four-chamber cardiac model with cubic-Hermite elements with extraordinary nodes. The myocardial fiber orientations were interpolated within the mesh using the Log-Euclidean interpolation to overcome the singularity associated with interpolation of orthogonal matrices. Physiologically equivalent boundary conditions were applied to the nodes along the valve plane. The myocardial wall displacements obtained from the four-chamber cardiac model are comparable to actual patient data without requiring complicated non-physiological boundary conditions usually required in truncated ventricular heart models. We then studied the effect of Pericardium on the deformation of the four-chamber model. The effect of Pericardium was applied as an external pressure to the outer surface without friction or contact. To assess the effect of the pericardium on the heart deformation, we measured the apex-base distance for both the models with and without pericardial pressure. We show that the apex-base distance for the model without pericardial pressure matches well with values reported in literature. References: 1. Adarsh Krishnamurthy, Matthew J. Gonzales, Gregory Sturgeon, W. Paul Segars, Andrew D. McCulloch, Biomechanics simulations using cubic Hermite meshes with extraordinary nodes for isogeometric cardiac modeling, In Computer Aided Geometric Design, 43, 2016. 2. Fritz, T., Wieners, C., Seemann, G., Steen, H. and Dössel, O., Simulation of the contraction of the ventricles in a human heart model including atria and pericardium, In Biomechanics and Modeling in Mechanobiology, 13(3), 2014.

15th U.S. National Congress on Computational Mechanics
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Title: Efficient Computations for Nonlocal Models with a Fourier Spectral Method and Volume Penalization

Author(s): *Siavash Jafarzadeh, *University of Nebraska-Lincoln*; Adam Larios, *University of Nebraska-Lincoln*; Florin Bobaru, *University of Nebraska-Lincoln*;

We introduce a novel efficient numerical method for nonlocal models, in particular for peridynamics, based on the Fourier spectral methods and Brinkman volume penalization [1]. The proposed method reduces the computational complexity to O(N.logN), from O(N^2) with the conventional methods used to discretize peridynamic models, such as the meshfree discretization with one-point Gaussian quadrature or the Finite Element Method. In the proposed method, Fourier transform untangles the convolution integral to a simple multiplication in Fourier space. The major cost of this scheme then is the Fourier transform which is performed via well-known FFT algorithms and only costs O(N.logN). While the assumption of periodicity of the computational domain is necessary to allow for the Fourier transformation, we enforce a penalization technique for arbitrary volume constraints, and, therefore, problems with arbitrary boundary conditions (volume constraints) can be solved easily. The spectral method with penalization introduced here for peridynamic models is efficient and general. We will present several examples that demonstrate the speed-up achieved compared to other discretization methods for diffusion-type problems, in 1D, 2D, and 3D. Remarks on convergence and error estimates will also be made. References: [1] S. Jafarzadeh, A Larios, F. Bobaru. “A spectral method with volume penalization for peridynamic models”, Journal of Peridynamics and Nonlocal Modeling (2019), to be submitted.

15th U.S. National Congress on Computational Mechanics
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Title: A Computational Model for Phase Transformations on Lipid Bilayer Membranes

Author(s): *Eshwar Jagadeesh Savitha, *RWTH Aachen University*; Christopher Zimmermann, *RWTH Aachen University*; Kranthi K. Mandadapu, *University of California at Berkeley*; Roger A. Sauer, *RWTH Aachen University*;

A phase field model for deforming cell membranes is presented. Cell membranes are typically comprised of two layers of lipid molecules that aggregate into surface-like structures. The constitutive behavior of this bilayer can be modeled in general as a two-dimensional visco-elastic continuum which is based on in-plane viscosity and the Helfrich bending model. Since there are various kinds of lipid molecules, the bilayer membrane is dynamically heterogeneous. The heterogeneity fluctuates close to the critical phase transition temperature leading to the development of domains or clusters of correlated lipid molecules [1]. The time scale of cluster formation strongly depends on the length of phase interface and temperature. In this regard, the phase separation of a binary mixture that is elucidated by the Cahn-Hilliard equation is studied on deforming shells using Kirchhoff-Love kinematics. Kirchhoff-Love shell formulations and high-order phase field models require at least C1-continuous spatial discretization across element boundaries. To achieve this, NURBS-based isogeometric finite elements are used [2]. As the deformation of the shell is considered to depend on the local phase state, the phase separation process therefore directly affects the mechanical behavior. The phase field and the mechanical field are coupled monolithically. In addition to that, an adaptive time-stepping algorithm [3] based on the errors of the phase field as well as the mechanical field is utilized. The proposed formulation is illustrated by several numerical examples. [1] Jørgensen, K., Ipsen, J. H., & Mouritsen, O. G. (1997). "Lipid-bilayer heterogeneity." In Principles of Medical Biology (Vol. 7, pp. 19-38). [2] Duong, T. X., Roohbakhshan, F., & Sauer, R. A. (2017). "A new rotation-free isogeometric thin shell formulation and a corresponding continuity constraint for patch boundaries." Comp. Meth. Appl. Mech. Engrg., (Vol. 316, pp. 43-83). [3] Zimmermann, C., Toshniwal, D., Landis, C. M., Hughes, T. J., Mandadapu, K. K., & Sauer, R. A. (2017). "An isogeometric finite element formulation for phase fields on deforming surfaces." arXiv preprint arXiv:1710.02547.

15th U.S. National Congress on Computational Mechanics
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Title: Stochastic Isogeometric Analysis in Elastostatics

Author(s): *Ramin Jahanbin, *University of Iowa*; Sharif Rahman, *University of Iowa*;

Stochastic Isogeometric Analysis in Elastostatics Many elastostatic engineering problems entail uncertainties in the input to the system and henceforth call for the uncertainty quantification for the response of interest. Akin to the existence of various methods for the numerical solution of the governing differential equation, in general, the uncertainty propagation analysis may also be conducted by numerous methods based on the regularity of the response function, number of random variables, and the budget and accuracy desired. The fundamentals of the Isogeometric Analysis (IGA) was established to bridge the gap between design and numerical mechanics frameworks delivering globally smooth basis functions in contrast with those of the classical finite element method [1]. While the IGA is being ubiquitously implemented to geometrical modelling and finite element analysis of problems in engineering, this study aims to broaden the areas of application of this method up to the stochastic analysis to obtain the second moment properties of the response. Oftentimes, the response function exhibits either a non-smooth or a highly oscillatory behavior. This phenomenon makes the uncertainty propagation analysis quite challenging when globally supported basis functions are utilized as with polynomial-based expansions as a higher order of bases is required to accurately capture the function. Moreover, large number of samples is needed in case of the Monte Carlo analysis of such problems. This very common case, however, can be solved by proposing a surrogate model in form of the Non-uniform Rational B-splines (NURBS). By defining the multi-dimentional order vector and set of knot vectors, the domain of the stochastic analysis is discretized to approximate the exact response function. The method intuitively involves projection of the function onto a finite-dimensional subspace of a Hilbert space where B-splines and NURBS spanning the subspace can be used. The dimension reduction technique for calculation of coefficients will also be introduced for efficiency purposes. Numerical examples illustrate the accuracy of the proposed method for approximation of the second moment properties of the response. 1. Hughes TJR, Cottrell JA, Bazilevs Y. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. Comput:Methods:Appl:Mech:Eng. 2005;194 (39-41):4135-4195.

15th U.S. National Congress on Computational Mechanics
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Title: Recent Advances in Multibody and Multiphase Fluid-Structure Interaction

Author(s): *Rajeev Jaiman, *The University of British Columbia, Vancouver*;

In this talk, I will review some of our recent methods and software development on flexible multibody and multiphase fluid-structure interaction (FSI) simulations, with applications to aerospace and marine/offshore engineering. We address three key numerical challenges in the proposed coupled variational formulation: (i) stable and robust coupling of incompressible turbulent flow with a system of nonlinear elastic bodies, (ii) a conservative and positivity preserving two-phase coupling based on the phase-field diffused interface approach, and (iii) stable integration of phase-field model with fluid-flexible multibody solver involving moving boundaries. In the proposed formulation, the modeling of air-water interface is accomplished by the positivity preserving variational method [2] applied to the conservative Allen-Cahn phase-field equation and the turbulence is modeled by hybrid RANS/LES formulation. The structural domain consisting of rigid and flexible bodies with contact constraints is solved using a nonlinear co-rotational method, whereas the fluid domain is discretized by a stabilized Petrov-Galerkin variational method. The proposed fully-coupled multifield formulation consisting of multiphase fluid flow, multibody structural dynamics, turbulence, and ALE mesh field is solved in a partitioned iterative implicit manner, which utilizes the nonlinear iterative force correction [1] at fluid-structure interface for the stability at low structure-to-fluid mass ratios typically found in marine and offshore systems. We assess the accuracy and robustness of our multibody FSI solver on an anisotropic wing with battens and membranes with composite materials. Our hybrid phase-field/ALE variational formulation involving the dynamical interaction of rigid bodies with a free surface is then assessed for the decay test problems of increasing complexity. We next examine the effectiveness of multibody FSI framework to a bat flight dynamics [3] and a practical problem of internal two-phase flow in a flexible circular pipe subjected to vortex-induced vibrations due to external fluid flow. Finally, we demonstrate the applicability of our solver to a large-scale scenario of the offshore vessel-riser system interacting with ocean waves and current flow. References: 1. Jaiman, R.K., N.R. Pillalamarri, and M.Z Guan. A stable second-order partitioned iterative scheme for freely vibrating low-mass bluff bodies in a uniform flow. Computer Methods in Applied Mechanics and Engineering, 301:187–215, 2016. 2. Joshi, V. and Jaiman, R.K, A hybrid variational Allen-Cahn/ALE scheme for the coupled analysis of two-phase fluid-structure interaction, Int J Numer Methods Eng, 117:405-429,2019. 3. Li, G., Law, Y.Z. and Jaiman, R.K., A novel 3D variational aeroelastic framework for flexible multibody dynamics: Application to bat-like flapping dynamics, Computers & Fluids, 2019.

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Title: Topology Optimization of Multi-Body Mechanisms Via Gaussian Layer Connectivity Parameterization

Author(s): Kenneth Swartz, *University of Illinois at Urbana-Champaign*; *Kai James, *University of Illinois at Urbana-Champaign*;

We present a novel technique for computational synthesis of multi-body planar mechanisms. Each component in the mechanism comprises a two-dimensional domain or “layer”, in which the material distribution is determined using SIMP-based topology optimization. The layers are connected by rotational hinges, whose locations are parameterized via a Gaussian distribution function. This function enables us to map the continuously variable hinge locations, to discrete points corresponding to the node locations within the finite element meshes used to model each layer. This mapping is smooth, thereby allowing for analytical sensitivity analysis and subsequent gradient-based optimization. The hinge locations and the layer topologies are optimized simultaneously to achieve maximum mechanical advantage. To allow for rigid body motion of the respective layers, we implement a geometrically nonlinear finite element analysis. The resulting structural displacements are solved iteratively using a Newton-Raphson procedure. We use adjoint sensitivity analysis to compute the design sensitivities used in the gradient-based optimization procedure. The proposed framework is demonstrated using a series of benchmark problems that include the design of multi-body gripper mechanisms, and multi-body mechanical inverters. Keywords: multi-body mechanism design, nonlinear finite element analysis, adjoint sensitivity analysis, Gaussian layer connectivity parameterization

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Title: Energy-Momentum Consistent Schemes for General Problems of Discrete Mechanical System Subject to Holonomic Constraints

Author(s): *Alexander Janz, *Karlsruhe Institute of Technology (KIT)*; Peter Betsch, *Karlsruhe Institute of Technology (KIT)*;

Energy-momentum consistent (EMC) schemes constitute a specific class of structure-preserving integrators which have been primarily developed in the framework of non-linear structural dynamics.EMC schemes are known for their superior numerical properties in terms of stability and robustness, see Betsch (Structure-preserving Integrators in Nonlinear Structural Dynamics and Flexible Multibody Dynamics. Volume 565 of CISM Courses and Lectures. Springer-Verlag, 2016) for more details concerning these integrators. EMC schemes typically rely on the notion of a discrete derivative which is applied to the stored energy function of the underlying continuum theory (e.g. nonlinear elastodynamics, geometrically exact beams and shells). In the presence of holonomic constraints the discrete derivative is also applied to the corresponding constraint functions to yield EMC schemes for constrained mechanical systems (such as multibody systems).In its original form the discrete derivative concept is confined to functions that can be written in terms of invariants that are at most quadratic in the state variables, see Gonzalez (J. Nonlinear Sci., 6: 449-467, 1996). The invariants are related to specific symmetries of the underlying mechanical system implying the conservation of associated momentum maps. However, there exist specific problems in non-linear dynamics (e.g. contact problems), in which the relevant invariants are cubic functions of the state variables. We present an extension of the previous approach to the design of EMC schemes to cope with the general problem of discrete mechanical systems with symmetry. Our new developments are illustrated within the model problem of a Cosserat point.

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Title: Coupling Porous Media and Free Flow Simulation Using the Multi-Purpose Coupling Library preCICE

Author(s): *Alexander Jaust, *University of Stuttgart*; Miriam Mehl, *University of Stuttgart*;

Coupling porous media and free flow is a typical interface problem appearing in many applications such as soil-water evaporation or drying processes of food or clothes. These type of problems commonly describe two regimes of potentially multi-scale, multi-phase and multi-component flows with very different characteristics that are strongly coupled through a common interface. Proper coupling respecting the underlying physics of both regimes is a non-trivial task. Several monolithic multi-physics solvers have been developed for the simulation of these coupled problems. However, due to the irregular structure and ill-conditioning of the system matrices used in the monolithic approach, such solvers are usually powerful in their regime, but rather inflexible and only moderately scalable to high resolutions and parallel computer architectures. Instead of using a monolithic solver, we aim to apply a partitioned approach. This allows the usage of two different solvers tailored for each regime, and couple them using the black-box coupling library preCICE [1]. The partitioned approach has the potential to be easily applicable to a variety of problem settings as no monolithic solver has to be developed for each case. In addition, it improves the overall parallel performance by exploiting scalability of the involved solvers and preCICE's point-to-point communication and parallel iteration schemes. The coupling library preCICE supports a wide variety of coupling strategies. It has been successfully utilized for fluid-structure interaction and conjugate heat transfer problems, but has not been applied to couple porous media and free flow before. However, preCICE is not tailored to a specific application and its powerful (parallel) coupling strategies can be applied to this new setting. This talk will discuss the challenges occurring when coupling porous media and free flow simulations using preCICE. As the coupling of two solvers involves potentially different meshes and numerical methods, we discuss suitable data mapping techniques. We identify optimal coupling strategies for porous media and free flow. References [1] H.-J. Bungartz, F. Lindner, B. Gatzhammer, M. Mehl, K. Scheufele, A. Shukaev, and B. Uekermann. preCICE – A fully parallel library for multi-physics surface coupling. Computers and Fluids, 141:250–258, 2016. Advances in Fluid-Structure Interaction.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Optimizing Imaging and Force Validation for Computational Modeling of Cardiac Valve Function and Intervention

Author(s): *Morten Jensen, *University of Arkansas*; Jonathan Wenk, *University of Kentucky*;

Since Andreas Vesalius first described the mitral valve in 1543, detailed investigations have established an intuitive approach to increase the biomechanical understanding of the valve and provide a rational basis for innovative repair. The mitral valve apparatus is one of the most complex cardiac structures, operating under high pressures. It is still debated if repair should be uniformly favored over replacement in almost all mitral valve pathologies requiring surgical intervention. An advantage of either approach is contingent upon competent procedures and devices, which is of paramount significance to long term success. Increasing repair durability requires diligent restoration and support of the valve, re-establishing the natural biomechanics. Computational modeling of the mitral valve has made great advances during the last two decades. However, these models are lacking true zero-stress-state geometric data of the valve as well as using intra-valvular force measurements as boundary conditions and validation of the computations. This presentation will summarize efforts if enhancing these models with the three most important aspects of successful computational modeling of cardiac valve function and intervention being: correct imaging techniques (1), biomechanical force measurements as boundary conditions (2), and including the left ventricle in the model of the valve (3). Careful consideration of these factors can ultimately improve procedures to enhance mitral valve repair and replacement devices and techniques from a rational standpoint to support the on-going improvement efforts. This will eventually lead to improving the lives of people with mitral valve deficiencies. REFERENCES: 1. Stephens SE, Liachenko S, Ingels NB, Wenk JF, Jensen MO. High resolution imaging of the mitral valve in the natural state with 7 Tesla MRI. PLoS One. 2017;12(8):e0184042. 2. Askov JB, Honge JL, Nygaard H, Hasenkam JM, Nielsen SL, Jensen MO. Papillary Muscle Force Transducer for Measurement In Vivo. Cardiovascular Engineering and Technology. 2011;2(3):196-202. 3. Wenk JF, Zhang Z, Cheng G, Malhotra D, cevedo-Bolton G, Burger M, Suzuki T, Saloner DA, Wallace AW, Guccione JM, Ratcliffe MB. First finite element model of the left ventricle with mitral valve: insights into ischemic mitral regurgitation. AnnThoracSurg. 2010;89(5):1546-53.

15th U.S. National Congress on Computational Mechanics
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Title: Numerical Fracture Experiments Using Nonlinear Nonlocal Models

Author(s): *Prashant Jha, *Louisiana State University*; Robert Lipton, *Louisiana State University*;

We introduce a regularized peridynamic model for dynamic fracture in materials. The model uses Hölder continuous displacements but reduces to a sharp fracture model in the local limit limit of vanishing horizon. The parameters in the model are calibrated from the elastic properties, strength and critical energy release rate of the material undergoing fracture. We present numerical results which highlight key features of the model. We show a linear rate of numerical convergence, with respect to the mesh size, of the finite difference approximation for the crack propagation problem. The model is seen to capture the fracture energy accurately. We show that the fracture zone localizes as the nonlocal length scale is refined. Samples with notch and void show the nucleation of crack under different loading conditions. We conclude by talking briefly about our ongoing work on the coupling of local and nonlocal models.

15th U.S. National Congress on Computational Mechanics
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Title: IGA-based Stress-related Topology Optimization via MMV

Author(s): *Shan Jiang, *Dalian University of Technology*; Weisheng Zhang, *Dalian University of Technology*; Xu Guo, *Dalian University of Technology*; Sung-Kie Youn, *Korea Advanced Institute of Science and Technology*;

Topology optimization considering stress constraints has been a hot topic in the field of scientific research. The study of two-dimensional structure has become mature. However, the stress-constrained topology optimization problem of the shell structure, with more theoretical significance and more engineering applications, still faces many difficulties such as stress singularity for structural geometry. Generally, stress-constrained topology optimization problems are solved with traditional finite element and approaches with implicit description. But this combination would lead to problems such as the risk of low accuracy at the stress concentration, a large number of design variables and disconnection between optimized results and computer-aided design/engineering (CAD/CAE) systems. In this work, the combination of Moving Morphable Void (MMV)-based topology optimization method and Isogeometric analysis (IGA) with trimming technique is proposed. MMV is an explicit structural topology optimization approach. IGA with trimming technique inherits the advantages of traditional IGA. This combination can guarantee enough accuracy and connect optimized results and CAD system seamlessly. Numerical examples provided demonstrate the effectiveness of the proposed approach combination. [1] X. Guo, W.S. Zhang, W.L. Zhong, Doing topology optimization explicitly and geometrically—a new moving morphable components based framework, Trans. ASME J. Appl. Mech. 81 (2014) 081009-1–081009-12. [2] H.J. Kim, Y.D. Seo, S.K. Youn, Isogeometric analysis for trimmed CAD surfaces, Comput. Methods Appl. Mech. Eng. 198(37–40) (2009)2982–2995. [3] W.S. Zhang, D. Li, J.H. Zhou, Z.L. Du, B.J. Li, X. Guo, A Moving Morphable Void (MMV)-based explicit approach for topology optimization considering stress constraints. Comput. Methods Appl. Mech. Engrg. 334 (2018) 381–413

15th U.S. National Congress on Computational Mechanics
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Title: Atomic-level Modeling and Particle-based Multiscale Simulation of Energetic Materials under Extreme Loading Conditions

Author(s): *Shan Jiang, *University of Mississippi*;

Recently, some effort has been made to develop a multi-scale material point method to simulate some mechanical behaviors of engineering materials as well as to formulate the equation of state for certain type of energetic composites. We proposed that molecular dynamics (MD) and dissipative particle dynamics (DPD) might be hierarchically bridged at nanoscale while the DPD can be concurrently handled in a single computational domain within the framework of the original MPM at microscale. Meanwhile, an initial attempt has been made to develop a predictive constitutive model for single-crystal energetic materials under simple loading conditions using a hierarchical multiscale approach based on MD and the generalized interpolation MPM. However, there are still many challenges for multiscale modeling and simulation of energetic materials, due to one of the reasons that many atomic-level phenomena have not been well studied. In this presentation, atomic-level modeling and simulation of energetic materials including solid-liquid interface under shock loading will be discussed. Recent findings and ongoing research will also be discussed.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Moving Morphable Component (MMC)-Based Approach for Profiled Surface Structures Topology Optimization Considering Buckling Constraints

Author(s): *Xudong Jiang, *State Key Laboratory of Structural Analysis for Industrial Equipment Department of Engineering Mechanics, Dalian University of Technology, Dalian, 116023, P.R. China.*; Xu Guo, *State Key Laboratory of Structural Analysis for Industrial Equipment Department of Engineering Mechanics, Dalian University of Technology, Dalian, 116023, P.R. China.*; Weisheng Zhang, *State Key Laboratory of Structural Analysis for Industrial Equipment Department of Engineering Mechanics, Dalian University of Technology, Dalian, 116023, P.R. China.*;

Profiled surface structures, which have the advantages of light weight, strong bearing capacity and material saving, are widely used in engineering field, such as aircraft, vehicles, submarines, etc. So far, the optimization of profiled surface structures have been widely concerned by both engineering and academia. An important failure mode in profiled surface structures is stability (buckling) and many scholars have made great progress in the research of topology optimization of profiled surface structures considering buckling problems. Most of traditional approaches actually do topology optimization of profiled surface structures under buckling constraint in an implicit way. This means that in these approaches the optimal structural topology is identified from a black-and-white pixel image and it is difficult to extract results for post processing. In order to overcome the aforementioned difficulties, this paper uses MMC method, which is a new topology optimization method based on explicit description, to optimize the profiled surface structures considering buckling constraints Surface based on NURBS is applied in topology optimization of profiled surface. By optimizing the components of the surface on the MMC solution framework, the optimal topology design of profiled surface can be obtained. In structural response analysis, shell elements are used to improve calculation efficiency with high accuracy. Moreover, the optimization process can be implemented by ABAQUS software due to the explicit description of the proposed approach. Some representative examples on topology optimization of profiled surface structures under buckling constraint are presented to illustrate the effectiveness of the proposed approach.

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Title: Topology Optimization with Design-dependent Loading: An Adaptive Sensitivity-separation Design Variable Update Scheme

Author(s): *Yang Jiang, *Georgia Institute of Technology*; Adeildo Ramos Jr, *Federal University of Alagoas*; Glaucio Paulino, *Georgia Institute of Technology*;

In this work, we propose a design variable update scheme specifically designed to solve topology optimization problems with design-dependent loading. Compared with topology optimization with fixed loads only, the problem with design-dependent loading provides design that is more realistic. However, this problem also introduces additional difficulty including the non-monotonous objective function and inactive volume constraint. Here we are interested in compliance minimization problems with design-dependent self-weight in both density-based and ground structure settings. In both settings, we have two formulations: the standard formulation with a material upper bound, and the void formulation with a material lower bound. We raise the void formulation because it is effective in design dominated by design-dependent loads, where standard formulation may lead to designs with too little material and the material upper bound is far from being active. To solve topology optimization problems in the aforementioned settings and formulation, we propose a design variable update scheme, where the design variables are iteratively updated by solving sub-problems using the Karush-Kuhn-Tucker conditions. In each iteration, we construct a sub-problem with a non-monotonous approximation of the objective function based on “sensitivity separation”. This sensitivity separation expresses the gradient of objective as the sum of a positive part and a negative part, such that the objective can be approximated by a non-monotonous function, which is the sum a linearly increasing function and an exponentially decreasing function. As the sensitivity separation influences the aggressiveness of update, we design an adaptive strategy for sensitivity separation to obtain convergent results. Numerical examples in both two and three-dimensional space show that the proposed update scheme generates optimized designs efficiently.

15th U.S. National Congress on Computational Mechanics
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Title: Regularized Explicit Finite Element Formulation of Shear Localization with Global Tracking of Embedded Weak Discontinuities

Author(s): *Tao Jin, *Los Alamos National Laboratory*; Hashem M. Mourad, *Los Alamos National Laboratory*; Curt A. Bronkhorst, *Los Alamos National Laboratory*;

Shear localization is a damage mechanism characterized by the concentration of plastic deformation within thin bands of materials, often observed as a precursor to failure in metals. In this talk, we present a three-dimensional explicit finite element formulation with embedded weak discontinuities for the treatment of shear localization under highly dynamic loading conditions. The proposed computational framework can be classified as a sub-grid method, in which the element characteristic length should be larger than the width of the embedded shear band. The finite shear band width, which is obtained from experiments, is treated as a material parameter severing as a length scale to regularize the material post-localization behavior. The onset of localization is detected via a material stability analysis suitable for rate-sensitive materials, and the continuity of propagating shear bands is ensured using a global tracking strategy involving a heat-conduction type boundary value problem, solved for a scalar level set function over the global domain of the problem. In addition, we propose a modified quadrature rule that is used to compute the contribution of an individual element to the global finite element arrays, taking into account the position of the embedded shear band within that element. The mechanical threshold stress (MTS) model, modified to account for dynamic recrystallization, is adopted as the constitutive model for rate- and temperature-sensitive metallic materials, and the constitutive equations are formulated in a co-rotational framework. The algorithmic setup of the integrated finite element framework, including the global tracking strategy, is described in detail. Thorough mesh-sensitivity analyses are conducted in all the numerical examples provided in this talk to examine the influences of mesh size on various numerical results, including global quantities such as the force-displacement relationship and the volume of the propagating shear band, and local quantities such as the evolution of state variables at Gauss points. By comparing with the conventional finite element method, we demonstrate that the proposed numerical approach consistently alleviates the mesh-dependence typically exhibited in localization problems. Moreover, we show that the total volume and the geometry of the fully developed shear band are mesh-independent.

15th U.S. National Congress on Computational Mechanics
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Title: Multifidelity Uncertainty Quantification in the Exascale-Ready Legion Programming System

Author(s): *Lluis Jofre, *Stanford University*; Manolis Papadakis, *Stanford University*; Aleix Aiken, *Stanford University*; Gianluca Iaccarino, *Stanford University*;

The study of complex physical systems is often based on computationally intensive high-fidelity simulations. To build confidence and improve the prediction accuracy of such simulations, the impact of uncertainties on the quantities of interest must be measured. This, however, requires a computational budget that is typically a large multiple of the cost of a single calculation, and thus may become unfeasible for expensive simulation models featuring a large number of uncertain inputs and highly non-linear behavior. In this regard, multi-fidelity methods have become increasingly popular in the last years as acceleration strategies to reduce the computational cost. These methods are based on hierarchies of generalized numerical resolutions or model fidelities, and attempt to leverage the correlation between high- and low-fidelity models to obtain a more accurate statistical estimator without requiring a large number of additional high-fidelity calculations. Exascale computing resources promise to facilitate the use of these approaches on larger scale problems by providing 1-10k times augmented floating-point capacity, but at expenses of requiring more complex data management as memory is expected to become more heterogeneous and distributed. The objective of this work, therefore, is to explore the performance of multi-fidelity strategies in large-scale multiphysics applications using Exascale-ready computational tools based on the Legion parallel programming system.

15th U.S. National Congress on Computational Mechanics
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Title: Parametric Design and Optimization of Structurally Effective Prosthetic Tricuspid Valves

Author(s): *Emily Johnson, *Iowa State University*; Devin Laurence, *The University of Oklahoma*; Chung-Hao Lee, *The University of Oklahoma*; Ming-Chen Hsu, *Iowa State University*;

A procedure for developing parametrically designed patient-specific tricuspid valves is presented. The modeling process implements patient data to determine a structurally effective model that is optimized to fit the fully-closed shape of the patient's valve. This type of simplified parametric design is intended to provide a baseline for prosthetic valves with less intricate structures than native tricuspid valves. Using the developed modeling approach, the structural function of the native valve can be reproduced in a prosthetic valve that has reduced design complexity, providing improved practicality for production and implant procedures.

15th U.S. National Congress on Computational Mechanics
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Title: The Search for Underlying Mechanisms Driving Differences in HFpEF/HFrEF Cardiovascular Function

Author(s): *Edith Jones, *Department of Molecular and Integrative Physiology, University of Michigan, Ann Arbor, MI 48109*; Scott L. Hummel, *Department of Cardiovascular Medicine, University of Michigan, Ann Arbor, MI 48109*; David Cameron, *Department of Cardiovascular Medicine, University of Michigan, Ann Arbor, MI 48109*; Dan A. Beard, *Department of Molecular and Integrative Physiology, University of Michigan, Ann Arbor, MI 48109*; Brian E. Carlson, *Department of Molecular and Integrative Physiology, University of Michigan, Ann Arbor, MI 48109*;

Diagnosis and treatment of heart failure are intimately tied to the analysis of echocardiography (EC) and right heart catheterization (RHC) measures made in the clinic. In the case of heart failure with reduced ejection fraction (HFrEF) the diagnosis is relatively easy to make with these measures alone. In the case of heart failure with preserved ejection fraction (HFpEF) these measures do not pinpoint whether the failure resides in the heart or the cardiovascular system or both. To tease out more information from these measures to uncover the underlying causes of HFpEF and HFrEF, we use a closed loop model of the cardiovascular system to identify key parameters including the stiffness in the aorta, the contractility of the right and left ventricle, the diastolic relaxation and filling of the ventricles using the patient specific EC and RHC measures. Twelve patient records (six HFrEF, six HFpEF) have been obtained from the Cardiovascular Health Improvement Project (CHIP) database at the University of Michigan and the RHC and EC measures from these records were used to tune the cardiovascular systems model to represent each patient. Model simulations were tuned to match systolic and diastolic pressures in the right ventricle, pulmonary artery, and aorta and cardiac output, wedge pressure, and left ventricular volumes to 3.9 ± 1.8 % in each patient. The underlying physiological parameters of these twelve tuned models were then plotted against model-based norms and compared between the HFrEF and HFpEF groups. Our patient-specific modeling demonstrates HFpEF in these groups show an increase in aortic stiffness, left ventricle contractility and a reduced relaxation during diastolic filling while the main parameter driving HFrEF is shown to be reduced contractility. In addition, the range of parameter values observed in HFpEF patients is much larger than in HFrEF. The wide range of parameter values in HFpEF supports the observed clinical heterogeneity and suggests that cardiovascular system modeling with more clinical data may be able to help phenotype and group HFpEF as different subdiagnoses, elucidating patient specific treatment strategies.

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Title: Exploiting IBM's Data Centric Systems to Develop New Approaches for Subsurface Modeling Incorporating AI Method

Author(s): *Kirk Jordan, *IBM Research*;

The volume, variety, velocity and veracity of data is pushing how we think about computer systems. IBM Research's Data Centric Solutions organization has been developing systems that handle large data sets, such as those found in subsurface modeling, shortening time to solution. This group has created a data centric architecture initially delivered to the DoE labs at the end of 2017 and being completed in 2018. As various features to improve data handling now exist in these systems, we need to begin to rethink the algorithms and their implementations to exploit these features. This data centric view is also relevant for Artificial Intelligence (AI) and Machine Learning (ML). We will show how we are using these data centric AI/cognitive computing systems to address some industrial and societal challenges in new ways actually coupling HPC and AI presenting a few case studies. Motivated by earlier work with Dr. Mary Wheeler on ensembles of a reservoir model for history matching, we will mention how we are starting to formulate and apply the above strategy in reservoir modeling.

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Title: Failure Theories in the Context of Non-Classical Solid Mechanics

Author(s): *A. D. Joy, *University of Maine*; K. S. Surana, *University of Kansas*;

This paper presents the effects of non-classical kinematic measures in continuum mechanics on common failure theories. Internal polar and Cosserat continuum theories introduce rotations as kinematic variables, in addition to the classical translations. The inclusion of these additional measures of deformation results in new stress, strain, and strain energy density distributions compared to identically loaded materials in the classical framework. This in turn results in changes in material failure predicted using maximum shear stress and distortion energy theories. By considering these measures and the resulting conjugate moment and non-symmetric Cauchy stress tensors, numerical studies are presented to compare failure in plane stress using classical continuum theories and non-classical theories. The present work considers mechanically reversible small deformation, small strain conditions.

15th U.S. National Congress on Computational Mechanics
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Title: Uncertainty and Sensitivity of Material Properties to Microstructure for Cement Paste

Author(s): *JI-SU KIM, *Yonsei University*; TONG-SEOK HAN, *Yonsei University*;

Cement paste is most widely used for construction and building materials. It has a complex microstructure with multiple phases. In general, the cement paste, a multi-phase material, can be divided into pore and solid phases, and the response of the material is influenced by the pore distribution. Among several characteristics of pore distribution, porosity is significantly related to the material properties (e.g., mechanical properties or thermal conductivity) [1]. The characteristic corresponding to pore continuity is also related to the material responses. To estimate the sensitivity of material properties to microstructures, information on uncertainty of material properties and its relation to microstructure are required. The first-order second moment (FOSM) method is an approximated probabilistic method to evaluate the distribution of output with the change of the input variables. However, the reconstruction process is required when the microstructure characteristics are selected as input variables for the FOSM method. In this study, using both actual and reconstruction specimens, the uncertainty and sensitivity of material responses to microstructures are estimated based on the FOSM method. The objectives of this study are to investigate the effect of microstructures on material properties (i.e., stiffness and thermal conductivity), and to estimate quantitative measures relate to uncertainty and sensitivity. Microstructures are obtained from micro-CT, and a stochastic optimization [2] is used to reconstruct the virtual specimens similar to actual microstructure with certain characteristics. From the FOSM method, the probability distribution of the properties is predicted and its sensitivities to porosity and pore continuity are quantified. The results of this study from the FOSM method is compared with simulation results from all specimens. It is found that the proposed methodology can be used for estimating sensitivity and uncertainty of material properties efficiently. [1] Mindess, S., Young, J. F., and Darwin, D. Concrete, 2nd ed.; Prentice Hall: U.S.A., 2003, pp. 57-80. [2] Chung, S.-Y., Han, T.-S., Kim, S.-Y., and Lee, T.-H. Investigation of the permeability of porous concrete reconstructed using probabilistic description methods. Construction and Building Materials, 2014, 66, pp. 760-770.

15th U.S. National Congress on Computational Mechanics
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Title: Supporting Multiscale Materials Simulations with Data Science and Informatics Tools

Author(s): *Surya Kalidindi, *Georgia Institute of Technology*;

This paper presents and discusses the potential benefits to the multiscale materials simulations from the adoption of the emergent toolsets from the fields of data sciences and informatics. These approaches generally involve the formulation and validation of novel databases that were specifically designed to have very broad windows of applicability for the multiscale materials simulations of interest. This paper presents specific examples of such high value databases in two distinctly different classes of applications: (i) multiscale simulation of metal forming applications utilizing the governing physics and material structure information over a hierarchy of material length scales, and (ii) objective extraction of the values of the model parameters in the physics-based modeling tools from the available (often limited) experimental datasets. Several challenges need to be addressed in accomplishing the goals outlined above. First, we need a versatile framework for the efficient parameterization of the (hierarchical) material structure space. Addressing this challenge requires a foundational formalism for obtaining high-fidelity but low-dimensional representations that capture all of the salient features in the material hierarchical structure influencing the properties of interest in a significant way. Second, one needs to cast the core materials knowledge, most conveniently expressed as process-structure-property relationships, in computationally low-cost reduced-order forms that exhibit high levels of accuracy and reliability. Third, it becomes necessary to measure reliably the elastic-plastic response of the material in very small volumes at multiple spatial resolutions with high throughput. Fourth, one needs a formal framework for closed-loop iterations between multiscale experiments and multiscale simulations in ways that they inform and guide each other objectively in efficient (possibly autonomous) workflows. Progress in all these directions from our ongoing research will be described and illustrated with selected examples in this paper.

15th U.S. National Congress on Computational Mechanics
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Title: Simplified Approach of Topology Optimization Considering Structural Redundancy

Author(s): *Hiroki Kamada, *Tohoku University*; Junji Kato, *Nagoya University*;

The present study deals with topology optimization considering structural redundancy. One of the common and important design problems may be to develop the optimal design method considering nonlinear and complex structural response such as buckling or elastoplastic behavior. The number of research related to this problem is gradually increasing, however, these approaches request the complicated sensitivity analysis and also high computational costs to achieve optimal results. This is the reason why the optimal design methods based on linear structural analysis are still the central among optimization methods. However, optimal layouts based on linear analysis tend to show vulnerable response, for example, loading capacity suddenly drops when design conditions uncertainly changed. From this background, we propose a simplified approach of topology optimization to increase structural redundancy for a severe loading condition with low computational cost. Finally, we demonstrate the accuracy and performance of the proposed method by a series of numerical examples.

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Title: tIGAr: Isogeometric Analysis with FEniCS

Author(s): *David Kamensky, *Brown University*; Yuri Bazilevs, *Brown University*;

This talk discusses recent work on implementing extraction-based isogeometric analysis (IGA) using software from the FEniCS open source finite element (FE) automation project. The implementation, called tIGAr, retains many of the powerful features that make FEniCS an attractive platform for partial differential equation (PDE)-based analysis. Our initial implementation uses a collection of object-oriented abstractions to separate PDE solution from generation of extraction operators. This permits analysis of many different PDEs on a wide variety of existing spline types, and also provides an interface to add support for future spline constructions. We review several example applications, including Kirchhoff–Love shell structure dynamics, nonlocal contact mechanics, divergence-conforming IGA of incompressible flow, and fluid–structure interaction. The library source code and various demos are available online, and we are open to community feedback or contributions: https://github.com/david-kamensky/tIGAr

15th U.S. National Congress on Computational Mechanics
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Title: Reduced-order Model Techniques for RKPM-based Thermal Fatigue Analysis of Solder Joints

Author(s): *Shigeki Kaneko, *The University of Tokyo*; Qizhi He, *University of California, San Diego*; Haoyan Wei, *University of California, San Diego*; J. S. Chen, *University of California, San Diego*; Shinobu Yoshimura, *The University of Tokyo*;

Among different bonding technologies, surface mount technology (SMT) is very important in electronics industry, because of its capability to increase the I/O interconnection density. When solder joints are subject to cyclic thermal loading, however, the mismatch in coefficients of thermal expansion of the bonded layers can lead to low cycle fatigue. It is difficult to perform thermal fatigue experiments, which are time-consuming and require special thermal cycling equipment. Numerical prediction of fatigue life, on the other hand, are feasible with the use of proper fatigue models. Nevertheless, modeling of a long cyclic loading process for complex 3D structures can result in very high computational cost. In this study, reproducing kernel particle method (RKPM) is adopted for coupled thermo-mechanical fatigue life prediction. RKPM is employed due to its flexibility in constructing approximation functions with arbitrary order of consistency and continuity that are entirely decoupled, which is particularly attractive for approximation of temperature and displacement fields. To reduce computational costs for fatigue analysis, a model order reduction technique based on the proper orthogonal decomposition (POD) and the hyper-reduction method is introduced, under the stabilized conforming nodal integration framework. By collecting state and field snapshots from a few cycles of high-fidelity simulation, an effective reduced-order RKPM model for fatigue analysis is constructed. The proposed meshfree approach yields accelerated thermal fatigue analysis for solder joints.

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Title: Anisotropic Perfectly Matched Layers for Transient Simulation of Elastic Waves

Author(s): *Jun Won Kang, *Hongik University*; Boyoung Kim, *Hongik University*;

This paper introduces perfectly matched layers (PMLs) for the simulation of elastic waves in heterogeneous anisotropic media. The PMLs are used as wave-absorbing boundaries to surround a finite computational domain of interest truncated from the originally semi-infinite extent. In the formulation, standard Navier equations governing the wave motion in the regular domain are combined with mixed unsplit field equations which yield the solution of attenuated waves within the PML. The anisotropic wave equations in the PML can be formulated with a constitutive relationship of material anisotropy. The second-order semi-discrete form of the problem is constructed by using mixed spectral elements with Legendre-Gauss-Lobatto quadrature method, which yields a diagonalized mass matrix. Then the second-order semi-discrete form is integrated in time for the solution of displacements and stresses by using an explicit time integration method. Numerical results are presented for elastic waves propagating in transversely isotropic and orthotropic domains truncated by the anisotropic PML. The wave motion in the anisotropic medium is compared with that in an isotropic medium, and the effectiveness of wave attenuation enforced by the developed anisotropic PML is shown by a series of numerical examples. The developed anisotropic PML method can be applied to various elastodynamic problems such as seismic wave simulation, inverse problems, and the wave propagation analysis in composite materials. References 1. A. Pakravan, J.W. Kang, C.M. Newtson, and L.F. Kallivokas (2014), Hybrid perfectly-matched-layers for transient simulation of scalar elastic waves, Structural Engineering and Mechanics, 51(4), 685-705. 2. A. Pakravan, J.W. Kang, and C.M. Newtson (2017), A Gauss–Newton full-waveform inversion in PML-truncated domains using scalar probing waves, Journal of Computational Physics, 350, 824-846.

15th U.S. National Congress on Computational Mechanics
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Title: Storm Surge Simulation with CYGNSS-derived Parametric Wind Fields

Author(s): *Younghun Kang, *Ohio State University*; Ethan Kubatko, *Ohio State University*; Joel Johnson, *Ohio State University*; Mohammad Al-Khaldi, *Ohio State University*;

The ADCIRC (ADvanced CIRCulation) model is a widely used finite element shallow water model for simulating hurricane storm surge. A key requirement to obtaining accurate storm surge estimates is the input of accurate meteorological forcing data. Many operational storm surge models, such as ADCIRC, generate this meteorological forcing data through the use of so-called parametric wind models, which generate wind fields based on only a small number of storm parameters such as storm track, maximum winds, etc. Obviously, the success of this approach requires accurate retrieval of the parameters from available storm data. A new NASA mission, the Cyclone Global Navigation Satellite System (CYGNSS), which was designed to provide extensive coverage of tropical cyclones [1], offers potential opportunities to improve the estimation of key storm parameters and the resulting storm surge calculations. Therefore, in this study, we assess the potential benefits of using storm parameters obtained from CYGNSS data to inform parametric wind models. We provide a brief overview of the retrieval algorithms used to obtain the storm parameters from CYGNSS data and present results obtained using the CYGNSS-based winds compared to storm surge results using other wind field sources. Model results are validated against observations obtained from several agencies, including the National Oceanic and Atmospheric Administration (NOAA) and the Federal Emergency Management Agency (FEMA). References [1] C. S. Ruf, R. Atlas, P. S. Chang, M. P. Clarizia, J. L. Garrison, S. Gleason, S. J. Katzberg, Z. Jelenak, J. T. Johnson, S. J. Majumdar, A. O’brien, D. J. Posselt, A. J. Ridley, R. J. Rose, and V. U. Zavorotny, “New ocean winds satellite mission to probe hurricanes and tropical convection,” Bulletin of the American Meteorological Society, vol. 97, no. 3, pp. 385–395, 2016.

15th U.S. National Congress on Computational Mechanics
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Title: Multi-material Structural Topology Optimization Considering Material Interface Properties

Author(s): *Zhan Kang, *State Key Laboratory of Structural Analysis for Industrial Equipment, Dalian University of Technology, China*; Pai Liu, *State Key Laboratory of Structural Analysis for Industrial Equipment, Dalian University of Technology, China*; Yaguang Wang, *State Key Laboratory of Structural Analysis for Industrial Equipment, Dalian University of Technology, China*;

For multi-material structures, possible occurrence of displacement discontinuity (e.g. interface debonding) associated with material interfaces is an important issue concerning the structural integrity and durability. In most of existing topology optimization studies of multi-material structures, however, the interface of different materials was assumed to be perfectly bonded. In the present study, we focus on topology optimization of multi-material structures considering interface behaviors described by the cohesive model. The multi-material Velocity Field-Level Set (VF-LS) method, in conjunction with the extended finite element method, is employed to represent the distribution of different material phases and to capture the evolution of the material interfaces. This enables modeling of possible separation of material interfaces, and thus provides a more realistic model of multi-material structures. The optimized designs considering interface behaviors exhibit tension/compression asymmetric topologies, in which material interfaces mainly undergo compression. Material interface-related uncertainties induced by inter-diffusion or reactions between different materials may significantly worsen the actual performance of optimized structures. With the aim to develop a rational method to address this issue in the design of multi-material products implemented by some novel fabrication techniques, we also study robust shape and topology optimization method accounting for uncertain graded interface properties. Using the level set function to track the evolving material interfaces during the optimization process, we model the material interface uncertainties by introducing an intermediate zone with graded properties represented by a random field. The uncertain propagation analysis is implemented with the Polynomial Chaos expansion (PCE) to predict the stochastic response. Then the robust shape and topology optimization problem is stated as a multi-criteria optimization problem to minimize the expected value and the standard deviation of the structural mean compliance. Numerical examples demonstrate the effectiveness of the method. References 1. Pai Liu, Zhan Kang. Integrated topology optimization of multi-component structures considering connecting interface behavior. Computer Methods in Applied Mechanics and Engineering. 2018; 341(1) : 851-887. 2. Yaguang Wang, Zhan Kang. Concurrent two-scale topological design of multiple unit cells and structure using combined velocity field level set and density model. Computer Methods in Applied Mechanics and Engineering. 3. Zhan Kang, Chunlei Wu, Yangjun Luo, Ming Li. Robust topology optimization of multi-material structures considering uncertain graded interface. Composite Structures. 2018; 208:395-406.

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Title: Multimaterial Topology Optimization of Shape Memory Alloy Structures with Non-uniform Temperature Distribution

Author(s): *Ziliang Kang, *University of Illinois at Urbana-Champaign*; Kai James, *University of Illinois at Urbana-Champaign*;

Shape-memory alloys (SMAs) are unique materials that exhibit two-way shape memory effects (TWSMEs) and pseudoelasticity. These two properties, triggered by phase transformation, enable shape memory alloys to undergo recoverable deformations under a prescribed temperature cycle or loading cycle, respectively. Computational design techniques which accurately capture the physical properties of the latent heat exchange process of the phase transformation, and take advantage of both TWSMEs and pseudoelasticity, are of great importance in the study of structures containing SMAs. We present a novel framework for the design of shape-memory activated structures via a topology optimization method, which aims at creating structures that are manufacturable (via 3D printing) and that optimally leverage the shape memory effect. In this study, we couple the thermal conductivity problem together with a nonlinear phenomenological model of shape memory alloys, and solve the thermomechanical response of the shape memory structures through inelastic finite element analysis. In this way, we are able to optimize the distribution of several distinct candidate materials plus a void phase to get optimal shape-memory effects or pesudoelasticity of the structure, under a predetermined temperature cycle or loading cycle. In addition, we also propose an analytical solution for adjoint sensitivity analysis of the coupled thermomechanical model. The proposed design framework is demonstrated using a series of two-dimensional benchmark problems. Keywords: shape-memory alloys, topology optimization, pseudoelasticity, multimaterial optimization, multi-physics design, adjoint sensitivity analysis

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Title: Real-time Time-dependent Density Functional Theory Using Higher Order Finite Element Methods

Author(s): *Bikash Kanungo, *University of Michigan, Ann Arbor, MI, USA*; Vikram Gavini, *University of Michigan, Ann Arbor, MI, USA*;

We present a computationally efficient approach to solve the time-dependent Kohn-Sham equations in real-time using higher-order finite-element spatial discretization, applicable to both pseudopotential and all-electron calculations [1]. To this end, we develop an a priori mesh adaption technique, based on the semi-discrete (discrete in space but continuous in time) error estimate on the time-dependent Kohn-Sham orbitals, to construct a close to optimal finite-element discretization. Subsequently, we obtain the full-discrete error estimate to guide our choice of the time-step. We employ spectral finite-elements along with Gauss-Legendre-Lobatto quadrature to render the overlap matrix diagonal, thereby simplifying the inversion of the overlap matrix that features in the evaluation of the discrete time-evolution operator. We use the second-order Magnus operator as the time-evolution operator in all our calculations. The action of the discrete Magnus operator, expressed as exponential of a matrix, on the Kohn-Sham orbitals is obtained efficiently through an adaptive Lanczos iteration. We observe close to optimal rates of convergence of the dipole moment with respect to spatial and temporal discretization, for both pseudopotential and all-electron calculations. We demonstrate a staggering 100-fold reduction in the computational time afforded by higher-order finite-elements over linear finite-elements, for both pseudopotential and all-electron calculations. We present comparative studies, in terms of accuracy and efficiency, of our approach against finite-difference based discretization for pseudopotential calculations, and demonstrate an 3 ? 50-fold computational savings when compared to the finite-difference method. We also demonstrate the competence of higher-order finite-elements for all-electron benchmark systems. Furthermore, we observe good parallel scalability of the proposed method on many hundreds of processors. Time permitting, we will discuss fast algorithms to accelerate the time-evolution of the Kohn-Sham orbitals beyond conventional schemes. [1] Bikash Kanungo and Vikram Gavini. Real-time time-dependent density functional theory using higher order finite element methods. arXiv e-prints. arXiv:1810.13130, 2018.

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Title: Towards a Self-Aware Aircraft: Data-Driven Decisions, Adaptive Reduced Models, and Digital Twins

Author(s): *Michael Kapteyn, *Massachusetts Institute of Technology*; Karen Willcox, *The University of Texas at Austin*; David Knezevic, *Akselos*;

This talk presents a computational framework that combines reduced-order models (ROMs) with online sensor information in order to enable the next generation of self-aware unmanned aerial vehicles (UAVs). A self-aware UAV is one that maintains knowledge of its own internal state and acts accordingly[1]. The internal state we consider is the vehicle's structural health. The vehicle uses sensor data to detect changes in its structural health, and responds intelligently by adapting the way it performs. This allows the vehicle to fly aggressively when it is healthy, while avoiding structural failures by becoming more conservative as it degrades. Such capability has the potential to improve performance over the full vehicle lifecycle, while also reducing structural health monitoring and maintenance costs. We create a Digital Twin of the UAV, using a combination of physics-based and empirical models that represent the key aspects of the vehicle's performance. A core part of this Digital Twin is a component-based ROM of the aircraft structure[2]. This structural model is evolved and adapted over the lifecycle of the vehicle, such that it reflects the vehicle's current structural health after each mission. The component-based ROM paradigm provides flexibility in structural defect modeling, while also permitting efficient recalibration in the face of dynamic data. The Digital Twin is used to construct a library of ROMs that represent possible future structural states. Each entry in the library is mapped offline to a corresponding estimate of vehicle capability. This library is used in flight, as online sensor data is assimilated, to rapidly classify the evolving structural state over time. The near real-time estimation of the vehicle's structural state enables dynamic mission re-planning in response to in-flight events such as damage to the UAV's wing[3]. This talk will focus on computational aspects of this project, which also includes a 12-foot wingspan flight-test vehicle being constructed by the Willcox Research Group and Aurora Flight Sciences. [1] Allaire, D., G. Biros, J. Chambers, O. Ghattas, D. Kordonowy, and K. Willcox. "Dynamic Data Driven Methods for Self-Aware Aerospace Vehicles." Procedia Computer Science 9 (2012): 1206–1210. [2] Ballani, J., Huynh, D. B. P., Knezevic, D. J., Nguyen, L., & Patera, A. T. (2018). A component-based hybrid reduced basis/finite element method for solid mechanics with local nonlinearities. Computer Methods in Applied Mechanics and Engineering, 329, 498-531. [3] Singh, V., & Willcox, K. E. (2017). Methodology for Path Planning with Dynamic Data-Driven Flight Capability Estimation. AIAA Journal, 2727-2738.

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Title: Finite Element Models of Laser Weld Failure Using Computed Tomography Images

Author(s): *Kyle Karlson, *Sandia National Labs*; Alyssa Skulborstad, *Sandia National Labs*; Maher Salloum, *Sandia National Labs*; Jonathan Madison, *Sandia National Labs*; Helena Jin, *Sandia National Labs*;

Research has shown that laser weld behavior depends significantly on laser weld process parameters. For designers and engineers, identification of the root-cause of the variability is of critical importance to inform process and design choices to mitigate adverse effects in components, and to accurately account for induced variability in engineering analyses. Possible sources for the observed variability in laser weld behavior include material variability, material microstructure, process induced residual stresses, and small scale geometric variability consisting of porosity and weld root geometry. Previous work suggests that the weld material properties are similar to the base material. Therefore, in this study we first investigate the hypothesis that small scale geometry (e.g. porosity, weld root geometry) is the primary cause of the observed variability of the laser weld structural response in tension testing. To this end, nonlinear solid mechanics finite element models with geometrically accurate meshes were evaluated against experimental data. The approach for this work consists of three steps. First, an elasto-viscoplastic material model with a damage model for material failure is calibrated to available base material data. Second, high fidelity geometric meshes are generated from computed tomography (CT) scans of individual laser weld test specimens. Third, simulations are run with the same material model where geometry is the only variable changed. Analysis results show that the models accurately predict trends in laser weld tension behavior while only accounting for differences in geometric variability. In order to account for this geometric variability in larger components, a hierarchical multiscale modeling method is investigated. The models constructed directly from CT scan images have millions of degrees of freedom and length scales on the order of microns. Thus, it is generally impractical to account for small scale geometric variability in larger engineering scale components. Instead, to account for the structural effects due to the observed geometric variability in the laser welds, a coarse macro-scale model is developed. The coarse scale model uses results generated from fine scale models including porosity, and is subject to loading conditions of interest. The methodology is validated using a representative test problem that can be simulated using both the fine scale and macro scale models. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Title: Mixed-Order Mesh Generation for Curved Geometries

Author(s): *Steve Karman, *Pointwise, Inc.*;

Linear hybrid unstructured meshes are elevated to mixed-order meshes in response to geometry curvature. The linear meshes are initialized by first elevating elements near curved geometry to quadratic degree. The deviation of the surface mesh is propagated into volume mesh by elevating adjacent elements to quadratic degree. This is repeated until the deviation of additional elements is below a tolerance level. The surface elements are then tested for elevation to cubic degree. This is again propagated into the volume mesh in a similar manner. Finally, the surface elements are tested for elevation to quartic degree and propagated into the volume mesh. Weighted condition number mesh smoothing is used to optimize the mixed-order mesh. Periodically the mesh is tested for additional element elevation to the appropriate degree up to quartic using a deviation criterion. Once the mesh smoothing is complete the mesh can be exported as a mixed order mesh or uniformly elevated to the desired degree. Details of the mesh elevation and smoothing process are described. Several three-dimensional examples are included that demonstrate the effectiveness of the method to produce high quality mixed-order meshes. Initial publications and presentations of this mesh curving method are listed below. 1.) Steve L. Karman, J T. Erwin, Ryan S. Glasby, and Douglas Stefanski. "High-Order Mesh Curving Using WCN Mesh Optimization", 46th AIAA Fluid Dynamics Conference, AIAA AVIATION Forum, (AIAA 2016-3178) https://doi.org/10.2514/6.2016-3178. 2.) Steve L. Karman, “Recent Advances in High-Order Mesh Generation at Pointwise,” International Conference on Spectral and High Order Methods 2018, London, United Kingdom. 3.) Steve L. Karman, “Curving for Viscous Meshes,” 27th International Meshing Roundtable (IMR27), Albuquerque, NM, 2018.

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Title: Tsunami Evacuation System Using Virtual Reality Technology

Author(s): *Kazuo Kashiyama, *Chuo University*;

Tsunami kill many human beings and damages economic activities seriously, such as tsunami caused by the Great East Japan Earthquake in 2011. It is very important to develop a useful educational system for tsunami disaster in order to perform the planning and design for the community development and the prevention of disaster. The visualization using VR technology is very important to understand the power of tsunami and to improve the consciousness of disaster prevention. Recently, the visualization using smart phone is becoming more popular in accordance with the development of smart devise. In this presentation, the modelling, simulation and visualization methods are presented for tsunami waves. The stabilized finite element method is employed for tsunami simulations based on the shallow water equation and Boussinesq equation. We also propose a visualiation system linked to the evacuation simulation based on multi-agent model using virtual reality technology to understand the power of tsunami and the importance of the evacuation. The present modelling, simulation and visualization methods are shown to be useful tools to realize the high quality computing for large scale tsunami simulation.

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Title: Multi-scale Topology Optimization of 3-dimensional Shell Components with a Periodic Lattice Infill

Author(s): *Hesaneh Kazemi, *University of Connecticut*; Ashkan Vaziri, *Northeastern University*; Julián Norato, *University of Connecticut*;

Advances in additive manufacturing (AM) have facilitated the manufacture of components made of a shell and a porous infill. Although AM technologies that support multiple materials are becoming available, the available materials often have very similar properties due to process limitations, and thus using multiple materials does not necessarily provide a structural advantage. On the other hand, employing infills whose members are porous themselves enables the realization of structures with a considerably wider range of effective properties. Topology optimization has been recently employed for the simultaneous design of the component topology (macro) and infill (micro). This has been achieved for 2-dimensional structures in Wu et al. (2017) and Campagna and Diaz (2017). We present a 3-scale method, wherein we concurrently design the part geome- try and the lattice infill in 3D. In order for the designs to be readily manufactured using stock material, we employ the geometry projection method (Norato et al. (2015) and Zhang et al. (2016)), whereby a completely analytic description of struts is smoothly mapped onto a density field over a fixed analysis grid. The as- signment of a size variable to each strut allows them to be removed entirely from the design space, when it attains a zero value. This method has been extended in Kazemi et al. (2018) to design multi-material structures, where each strut can be made of one of the available materials. A variation of the discrete ma- terial optimization (DMO) method (Stegmann and Lund (2005)) is adapted to accommodate the discrete geometric components. The design of multi-material lattice structures using geometry projection method was presented in Watts and Tortorelli (2017). The material interpolation scheme proposed in Kazemi et al. (2018) can simplify the process for any number of materials. In this work, we present a topology optimization method to simultaneously design the shell topology and the periodic lattice infill of a 3-dimensional component. To design the lattice infill, we design the strut layout in the base cell using homogenization. Moreover, the porosity of the struts is designed by optimizing the diameter of a cylindrical hole inside each strut. Furthermore, the lattice orientation inside the component is determined using three Euler angles. We demonstrate the efficacy of the method via numerical examples of minimum compliance design.

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Title: Towards Risk Averse Structural Design Optimization with Uncertain Wind Loading: Two-dimensional Benchmarks

Author(s): *Brendan Keith, *Technische Universität München*; Anoop Kodakkal, *Technische Universität München,*; Marc Nuñez, *CIMNE*; Ricardo Rossi, *CIMNE*; Barbara Wohlmuth, *Technische Universität München*; Roland Wu?chner, *Technische Universität München*;

This talk will explore a longstanding question in civil engineering from a contemporary viewpoint: How best to design a structure under uncertain environmental conditions? Modern buildings must satisfy a number of well-defined, but computationally challenging, serviceability and failure criteria. For instance, tall or irregular structures are subjected to enormous stresses imparted by uncertain wind loading from turbulent atmospheric boundary layer flows and yet they must remain stable and reliable. Moreover, architects and other planners generally have specific design objectives and fixed expenditures for the final project. Each of these interests must be fully addressed long before construction begins. Informed by modern principles in risk-averse engineering design, we will balance both sets of criteria and objectives in order to arrive at a new class of shape-optimization problems with uncertainty. We will then present and analyze a number of two-dimensional benchmark problems class which pave the way to the full three-dimensional setting and an answer to the question posed above. This work was supported by ExaQUte, a European project funded by the European Unions Horizon 2020 research and innovation programme, that aims at constructing a framework to enable Uncertainty Quantification (UQ) and Optimization Under Uncertainties (OUU) in complex engineering problems using computational simulations on Exascale systems. This is a joint work with the Centre Internacional de Mètodes Numèrics en Enginyeria, the Barcelona Supercomputing Centre, Technische Universität München, and École polytechnique fédérale de Lausanne.

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Title: Topology Optimization with Eigenvalue Constraints Using Spectral Aggregates

Author(s): *Graeme Kennedy, *Georgia Tech*;

Natural frequency and linearized buckling constraints are challenging to apply in large-scale topology optimization applications due to the computational expense of eigenvalue solution methods and the greater degree of multimodality exhibited by eigenvalue-constrained problems. In this work, we will address these challenges with eigenvalue solution methods tailored for large-scale topology optimization and through an advantageous reformulation of the frequency and buckling-constrained problems. First, we will demonstrate the equivalence of conventional generalized eigenvalue constraints with our proposed reformulation for eigenvalue-constrained topology optimization problems that impose a lower bound on the natural frequency or critical buckling load. This reformulation, based on nonlinear semi-definite programming, requires only the solution of a simple eigenvalue problem. The simple eigenvalue problem admits the use of different eigenvalue solution methods that are more efficient than generalized eigenvalue techniques required for frequency or buckling analysis. Next, the minimum simple eigenvalue of the reformulated constraint matrix is approximated using a smooth spectral aggregate. This spectral aggregate can be well-approximated by an inexpensive quadratic expansion that captures the directions of highest constraint curvature. Finally, these quadratic approximations are integrated within a large-scale trust-region optimization framework with quadratically-constrained subproblems. The quadratic approximations of the spectral aggregate are concave, resulting in convex optimization subproblems that can be solved efficiently and robustly. These methods will be demonstrated on a series of problems including the L-bracket domain, cantilever domain, and canonical 3D domains.

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Title: A Posteriori Error Estimation and adaptivity for Goal-oriented PGD Model Order Reduction

Author(s): *Kenan Kergrene, *INRIA Paris*; Serge Prudhomme, *Polytechnique Montreal*; Ludovic Chamoin, *LMT, ENS Paris-Saclay*; Marc Laforest, *Polytechnique Montreal*;

The talk will deal with a formulation aiming at adaptively constructing goal-oriented reduced-order models, that is, reduced-order models built and adapted towards the approximation of quantities of interest. The main idea behind the goal-oriented approach is to formulate a constrained minimization problem that includes refined information in the goal functionals so that the resulting model be capable of delivering enhanced predictions of the quantities of interest. Such a paradigm represents a departure from standard goal-oriented approaches where the model is first derived by minimization of the energy, or of the residual functional, and subsequently adapted via a greedy approach by controlling a posteriori error estimates measured in terms of quantities of interest using dual-based error estimates. In the present approach these dual-based error estimates -- or rather the corrections they suggest -- are directly incorporated into the constrained primal problem. Subsequently, the formulation will be applied to the so-called Proper Generalized Decomposition method, an instance of reduced-order modeling methods, with the aim of providing cheap and accurate solution maps for quantities of interest of solutions of parametric boundary value problems. Various sources of errors, namely discretization and truncation errors, will be controlled using specific error indicators, naturally leading to a greedy adaptive strategy to optimize the accuracy of the PGD approximation. Numerical examples will illustrate the performance of the proposed methodology.

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Title: Preconditioning a Coupled Model for Reactive Transport in Porous Media

Author(s): Laila Amir, *University of Marrakech, Morocco*; *Michel Kern, *Inria, France*;

Coupling transport and chemistry in porous media is a challenging task of importance in various applications. Under a local chemical equilibrium assumption, a large non-linear system of advection-diffusion PDEs coupled with algebraic equations is obtained. Each chemical species gives a transport equation, while each grid cell gives a local algebraic system. Two families of methods have been used for solving the coupled system: - Fixed point methods, where one alternates between solving tansport and chemistry, - Global methods, where the coupled system is solved globally. Reference [3] compares the different approaches in the context of a numerically demanding benchmark. In this talk, we present a a coupled formulation that allows a separation of transport and chemistry at the software level, while keeping a tight numerical coupling between both subsystems. The coupled system, written as a fixed point problem, is solved by a Newton-Krylov method, with a block Jacobian computed from the individual sub-systems (see [1], [2] for details). The Krylov solvers can stagnate, and preconditioning is necessary to improve convergence. Because of the matrix free formulation, only block preconditioner respecting the block structure of the coupled problem can be used, with block Jacobi or Gauss-Seidel being the most natural examples. These methods only act at the linear level. An alternative formulation of the coupled problem, based on the elimination of some unknowns, acts as a non linear preconditioner. Its linearization is equivalent to solving the Schur complement of the block Gauss-Sesidel precondtioner. It is observed that both linear and non-linear convergence become independent of the mesh size. The methods are applied to the MoMaS benchmark. References [1] L. Amir and M. Kern. A global method for coupling transport with chemistry in heterogeneous porous media. Computat. Geosci, 14:465–481, 2010. [2] L. Amir, M. Kern, Preconditioning a coupled model for reactive transport in porous media, Int. J. Num. Anal & Modeling, 16 (1), pp. 18-48, 2019 [3] J. Carrayrou, J. Hoffmann, P. Knabner, S. Kr¨autle, C. de Dieuleveult, J. Erhel, J. van der Lee, V. Lagneau, K. U. Mayer, and K. T. B. MacQuarrie. Comparison of numerical methods for simulating strongly nonlinear and heterogeneous reactive transport problems-the MoMaS benchmark case. Computat. Geosci., 14(3):483–502, 2010

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Title: Stress-Based Topology Optimization under Uncertainty via Simulation-Based Gaussian Process

Author(s): *Vahid Keshavarzzadeh, *University of Utah*; Robert Kirby, *University of Utah*; Akil Narayan, *University of Utah*;

Gaussian process (GP) is a well-established machine learning tool which provides a natural platform for tackling high-dimensional random input data in challenging physical simulations. This work introduces a generic framework for integrating Gaussian Processes with risk-based structural optimization. We solve robust and reliability-based design problems in the context of stress-based topology optimization under imperfections in geometry and material properties, and loading variability. We construct independent GPs for primal and adjoint quantities, namely the global p-norm von Mises stress and its sensitivity where we enhance the computational efficiency by leveraging the information from multiresolution finite element simulations. The GP framework naturally lends itself to modeling noise in data. We investigate the effect of numerical modeling error in high fidelity simulations via a noisy GP emulator and provide a pareto curve that shows the robustness of optimal design with respect to the noise level. We provide an a posteriori error estimate that quantifies the discrepancy between the noisy emulator and true simulations and verify it with a numerical study. We demonstrate our approach on a benchmark L-bracket structure which exhibits stress concentration as well as compliant mechanism design and heat sink design.

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Title: Laser Powder Bed Fusion Additive Manufacturing: Feedforward for Keyhole Mitigation and Microstructure Control Using a High-fidelity Powder Scale Model

Author(s): *Saad Khairallah, *Lawrence Livermore National Laboratory*; Rongpei Shi, *LLNL*; Alexander Rubenchik, *LLNL*; Manyalibo Matthews, *LLNL*; Tien Roehling, *LLNL*; Andy Anderson, *LLNL*;

A mesoscopic high-fidelity simulation model is combined with laser ray tracing to calculate absorptivity of SS316L and Ti64 as well as melt pool dimensions as a function of laser power and scan speed. The experimental validation of these results proves that the laser ray tracing enabled model is a predictive tool with little to no controlled approximations. The model is further employed to optimize laser power during turn around to prevent keyholing. It is also coupled with the Cellular Automata method for microstructure grain growth to explore microstructure control by considering the laser beam shape as a process parameter. IM release LLNL-ABS-765458. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE- AC52-07NA27344. Lawrence Livermore National Security, LLC

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Title: Predictive Simulations of the Mitral Valve Repair Surgery Based on Pre-operative Clinical Imaging Data

Author(s): *Amir Khalighi, *The University of Texas at Austin*; Bruno Rego, *The University of Texas at Austin*; Robert Gorman, *University of Pennsylavia*; Joseph Gorman, *University of Pennsylavia*; Michael Sacks, *The University of Texas at Austin*;

Mitral valve (MV) disease is striking the western world with an ever-increasing prevalence rate. Among the most common forms of MV disorders, ischemic mitral regurgitation (IMR), appears within one month of the infarction in patients who have experienced cardiac arrest. While two major treatment options for IMR (repair and replacement) have improved significantly over the past three decades, long-term survival outcomes have demonstrated a sub-optimal rate of success with a high mortality rate. At the same time, it has been shown that a quantitative assessment of MV function pre-operatively can significantly help with further fine-tuning surgical operations according to patient-specific variations. We thus worked on a novel computational framework to develop predictive models of the MV apparatus from the pre-operative clinical imaging data. Three deidentified imaging datasets were randomly selected from the Cardiothoracic Surgical Trials Network database for patients who have undergone annuloplasty repair surgery. For each patient, the fully open and fully closed states of the MV were processed to extract the leaflet geometry and the average location of the papillary muscle heads. Then, the leaflet surface meshes from the open and closed states were registered using a level-set method that we had previously developed [1]. This technique allowed us to morph the open leaflet mesh onto the closed surface geometry and then develop functionally equivalent models of the MV chordae tendineae per each patient [2]. We combined each patient's leaflet mesh and their functionally equivalent chords and calibrated them to ensure the developed models can reproduce the pre-repair (diseased) closing behavior of the valve. Next, by applying the repair boundary conditions to the papillary muscle heads and the annulus, we simulated the post-repair state of the valve. We applied our framework on three patients who had undergone annuloplasty repair surgery and successfully predicted MV closure following the operation based only on the information collected pre-operatively. In addition, we also computed local deformation patterns of the valve for both circumferential and radial directions with high fidelity. Our results show that our framework successfully allows for the quantitative assessment of different surgical scenarios to treat IMR patients just based on the information that is available prior to the operation. References: [1] Rego, BV et al., Int J Numer Method Biomed Engng, 34:e3142. doi: https://doi.org/10.1002/cnm.3142 [2] Khalighi, AH et al., Ann Biomed Eng, 47:60-74, 2019. doi: https://doi.org/10.1007/s10439-018-02122-y

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Title: The Shifted Interface Method for Multiphase Flows Computations

Author(s): *Mehdi Khalloufi, *Duke University*; Kangan Li, *Duke University*; Guglielmo Scovazzi, *Duke University*;

In modern engineering, numerical simulations with complex geometries remain challenging. Numerical techniques such as embedded and immersed boundary methods are gaining popularity since they avoid the burden of conformal mesh generation. However, the proper imposition of the boundary conditions is cumbersome since these methods do not preserve the optimal rate of convergence of the numerical schemes. To circumvent this issue, we propose to use the Shifted Interface Method [Li & Scovazzi, 2019]. The key feature of the proposed approach is to shift the location of the interface to a surrogate interface, for which the interface conditions are appropriately modified and weakly enforced. In this work, the closest point projection on one side of the interface is used to define the surrogate interface, and a Taylor expansion enables to modify in a proper way the interface conditions. This method is shown to be favorable in terms of accuracy, robustness, and computational cost as demonstrated for the imposition of jump interface conditions in the case of moving interfaces problems such as multiphase flows with surface tension, using a front tracking or a front capturing algorithm.

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Title: Unconditionally Energy Stable, Thermodynamically Consistent, Coupled Cahn-Hilliard Navier-Stokes Framework for Two Phase Flows

Author(s): *Makrand Khanwale, *Iowa State University*; Alec Lofquist, *Iowa State University*; James Rossmanith, *Iowa State University*; Hari Sundar, *University of Utah*; Baskar Ganapathysubramanian, *Iowa State University*;

We report on two phase flow simulations with moderately high density contrasts(1:100), particularly for buoyancy driven flows. We use a diffuse interface approach, which utilizes a thermodynamically consistent set of coupled Cahn Hilliard Navier-Stokes equations. We present a second order numerical time integration scheme and prove that it is unconditionally energy stable in the semi-discrete form. Using the Cahn-Hilliard equation for tracking the interface also allows to maintain explicit mass conservation on the continuous form, and this property is seamlessly inherited in the discretised form. We use a residual based variational multi-scale method to discretise the momentum and advective Cahn-Hilliard equations. The length scales which need to be resolved for correct interfacial dynamics (governed by CH) and the associated velocity scales(governed by NS) are disparate, and call for a fast adaptive meshing framework. To solve this problem, we use linear continuous Galerkin finite elements on octree based meshing strategy, which makes the framework massively parallel and fast, potentially providing a leeway into simulating multiple/bubbles droplets. We present several numerical experiments to validate the framework against experimental datasets, and to illustrate the properties of the numerical scheme.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Solving Parabolic Evolution Equations in Large Space-time Blocks: Space-time Stabilization, A Posteriori Space-time Estimates, and Adaptive Space-time Refinement

Author(s): *Biswajit Khara, *Iowa State University*; Saurabh Kumar, *Iowa State University*; Milinda Fernando, *University of Utah*; Robert Dyja, *Czestochowa University of Technology*; James Rossmanith, *Iowa State University*; Hari Sundar, *University of Utah*; Baskar Ganapathysubramanian, *Iowa State University*;

We study solution strategies for solving time-dependent advection-diffusion-reaction equations in a fully coupled space-time way. While solving these kind of equations in the space-time variational setting, the discrete problem may become unstable when the relative effect of the time derivative term becomes dominant. We formulate and implement a Galerkin/Least Squares stabilization and rigorously prove that the modified problem is stable in the chosen discrete norm. We subsequently develop an a posteriori error indicator for the space-time stabilized variational problem. We solve this class of problems on an octree based structured mesh (DENDRO) that allows for local refinement. We illustrate the utility of this approach by solving an increasingly complex sequence of problems (linear, quasi-linear, non-linear diffusion equations). For problems where the solution varies rapidly not just in space but also in time, this method naturally allows for irregular refinement in both space and time as required.

15th U.S. National Congress on Computational Mechanics
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Title: Structural and Biomechanical Changes of Right Ventricular Remodeling -in PAH – Reduces Left Ventricular Rotation During Contraction

Author(s): *Vitaly Kheyfets, *University of Colorado Denver|Anschutz Medical Campus*; Uyen Truong, *Children's Hospital Colorado*; Dunbar Ivy, *Children's Hospital Colorado*; Robin Shandas, *University of Colorado Denver|Anschutz Medical Campus*;

Pulmonary hypertension (PH) is characterized as a progressive increase in pulmonary arterial impedance and ultimately leads to right ventricular (RV) failure. Ongoing research and clinical focus are concentrated on the RV, but largely overlooks the influence of the adjacent left ventricle (LV) in RV remodeling and ultimate dysfunction. This is an oversight, given that isolating the two ventricles in a canine model has shown that the mechanical energy transfer from pacing only the LV generates over 70% of the pressure and flow in the passive RV [1]. Our studies in children with PH have shown a decrease in LV contractile rotation [2], which would suggest that the mechanical energy transfer to the RV is indeed compromised and possibly a contributor to RV dysfunction. The overall objective of this computational study is to evaluate how structural changes in the RV, which are known to occur in response to increased pulmonary arterial impedance [3], impact LV rotational mechanics. This is intended to provide a mechanistic explanation of the aforementioned clinical imaging study and offer a rationale for ongoing animal studies. We reconstructed the heart at end-systole from a short-axis MRI of a single pediatric patient using ScanIP (Simplewear, CA). After a mesh convergence study, a volumetric mesh with 13691 elements was used to perform a series of computational simulations that compare simulated LV rotational mechanics before and after various structural changes in the RV (e.g. increased RV myocardial stiffness, RV fiber re-orientation). Our results indicate that hypertensive conditions in the RV cause elevated concentrations of stress in the septum and the global LV. Furthermore, structural changes in the RV that are common in PH animal models are shown to decrease LV rotational mechanics. This finding supports our imaging study in a pediatric PH patient cohort. References: 1. Damiano, R.J., Jr., et al., Significant left ventricular contribution to right ventricular systolic function. Am J Physiol, 1991. 261(5 Pt 2). 2. Dufva, M., et al., Left ventricular torsion rate and the relation to right ventricular function in pediatric pulmonary arterial hypertension. Pulmonary Circulation, 2018. 8(3). 3. Hill, M.R., et al., Structural and mechanical adaptations of right ventricle free wall myocardium to pressure overload. Ann Biomed Eng, 2014. 42(12).

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: The Effect of a Surge Barrier on the Salinity of a Highly Industrialized Estuary

Author(s): *Amin Kiaghadi, *The Institute for Computational Engineering and Sciences, University of Texas at Austin*; Clint Dawson, *The Institute for Computational Engineering and Sciences, University of Texas at Austin*; Connie Do, *Rice University*; Philip Bedient, *Rice University*; Jennifer Proft, *The Institute for Computational Engineering and Sciences, University of Texas at Austin*; Mark Chung To Sang, *The Institute for Computational Engineering and Sciences, University of Texas at Austin*;

Previous studies in the Galveston Bay (GB) and Houston Ship Channel (HSC) in Texas have proposed a surge barrier, Mid-Bay Strategy (MBS), to mitigate the effect of storm surge. While it is important to assess the hydrodynamic performance of this strategy, it is equally important to evaluate the environmental impacts associated with the presence of the barriers in the HSC-GB system. Major disruptions in salinity can be detrimental to thriving fish and oyster reefs in the affected areas by the MBS. This study focuses on assessing the impacts of MBS on salinity circulation. Salinity transport was performed using 2-D Advanced Circulation (ADCIRC) v.53 with the transport module and tidal spin-up. Significant additions/modifications to the ADCIRC model were made and several supplementary codes were developed to simulate a physics-based salinity model. Freshwater boundary conditions were introduced to the model to represent the exchange between the bay and the surrounding waterbodies. To investigate how the proposed MBS barrier might potentially change the salinity within the system, two sets of ADCIRC meshes were used. The base mesh was used to represent the conditions prior to building the barriers, and the Mid Bay mesh with open gate cuts was applied to represent the MBS scenario. Three flow scenarios, high, moderate and low flow regimes, were defined for each mesh resulting in six scenarios to simulate all possible circumstances that can affect the salinity within the system. The model was run for 30 days after a 10-day spin-up for each scenario. The results showed that the MBS tends to divide the system into two separate sections that are each hydrodynamically independent. The presence of the MBS can change the salinity in both western and eastern part of the barrier. However, the observed changes in short term runs performed in this study are not major. The effect is more severe in the vicinity of the barrier. The changes range between -1.0 to +1.0, -1.0 to +2.0, and -3.0 to +3.0 ppt in the low, moderate, and high flow regime scenarios, respectively. The effect of the MBS barrier is minimal in the low flow scenario. However, the effect of the barrier on salinity becomes more significant at the presence of more freshwater in the system.

15th U.S. National Congress on Computational Mechanics
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Title: A Finite Element Framework for Magneto-Mechanical Simulations Considering Energy-Relaxing Microstructure Evolution

Author(s): *Bjoern Kiefer, *TU Bergakademie Freiberg*; Thorsten Bartel, *TU Dortmund*; Karsten Buckmann, *TU Dortmund*; Andreas Menzel, *TU Dortmund/Lund University*;

Microstructure evolution in magnetic materials can be interpreted as a non-local effect, in the sense that the behavior at a material point depends on the magnetostatic energy stored in the demagnetization field occupying the entire spatial domain. To account for this, we propose a finite element framework in which three global fields are considered: the displacement field, the scalar magnetic potential, and an additional set of state variables parameterizing the magnetic and crystallographic microstructure. Contrary to conventional micromagnetics, however, the microscale is not spatially resolved and exchange energy terms introducing gradients of the magnetization are neglected in this approach. The influence of microstructure evolution is rather incorporated in an effective sense---through appropriate mixture rules and underlying homogenization schemes---, which allows for relatively efficient computations of meso- and macroscale problems. This approach necessitates the development and implementation of novel mixed element formulations. It further requires the enforcement of inequality constraints at the global level. To handle the latter, we employ Fischer-Burmeister complementarity functions and introduce the associated Lagrange multipliers as additional nodal degrees-of-freedom. As a particular application of this general methodology, a recently established energy-relaxation based model for magnetic shape memory behavior is implemented and tested. Special cases---considering ellipsoidal specimen geometries---are used to verify the magnetization and field-induced strain responses obtained from FE-simulations by comparison to calculations based on the demagnetization tensor concept. Following this verification step, we are able to address response simulations with samples of arbitrary geometry---including prismatically-cut single crystals, that are often used in MSMA characterization experiments and actuator/sensor applications. With the presented approach we are able to overcome systematic errors usually introduced by the application of spatially-averaged demagnetization factors to problems exhibiting macroscopically inhomogeneous magnetization fields. References: [1] Buckmann, K., Kiefer, B., Bartel, T., Menzel, A., Simulation of Magnetised Microstructure Evolution Based on a Micromagnetics-Inspired FE-Framework: Application to Magnetic Shape Memory behavior, Archive of Applied Mechanics, 2018. doi:10.1007/s00419-018-1482-7 [2] Kiefer, B., Buckmann, K., Bartel, T., Numerical Energy Relaxation to Model Microstructure Evolution in Functional Magnetic Materials, GAMM-Mitteilungen, 38(1): 171-196, 2015. [3] Bartel, T., Kiefer, B., Buckmann, K., Menzel, A., A Kinematically-Enhanced Relaxation Scheme for the Modeling of Displacive Phase Transformations, Journal of Intelligent Material Systems and Structures, 26(6): 701-717, 2015.

15th U.S. National Congress on Computational Mechanics
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Title: Phase-Field Fracture Problems Solved by a Nonsmooth Multigrid Method

Author(s): *Daniel Kienle, *University of Stuttgart*; Carsten Gräser, *FU Berlin*; Oliver Sander, *TU Dresden*; Marc-André Keip, *University of Stuttgart*;

Modeling fracture is a challenging task in computational mechanics. Several attempts have been made and methods such as XFEM or cohesive zone models have been developed. Compared with these methods the phase-field approach to fracture based on Griffith's theory and the Ambrosio-Tortorelli approximation has some distinct advantages [1, 2]: The discontinuity of the crack does not have to be taken into account for the discretization. Furthermore, complex crack patterns and crack branching can be modeled in a straightforward manner. The formulation of fracture problems with the phase-field approach results in a biconvex minimization problem. Monolithic approaches based on a standard Newton-Raphson scheme do not always converge. Solutions to this problem are mostly based on predictor-corrector schemes or operator-splitting methods. The disadvantages of these methods are their high computational costs. Consideration of thermodynamic consistency by the incorporation of a local irreversibility of the damage phase field leads to a nonsmooth minimization problem [2]. We apply a nonsmooth multigrid method which exploits the biconvexity of the energy functional. This method can solve such problems in about the time of one equivalent linear problem [3]. We will demonstrate that the suggested solution method leads to the same results as classical solution schemes [2]. In addition, the computational speed by means of classical benchmark problems of brittle fracture will be analyzed. Furthermore, we show the possible extension towards h-adaptivity and ductile fracture. [1] G. A. Francfort and J.-J. Marigo. Revisiting brittle fracture as an energy minimization problem, Journal of the Mechanics and Physics of Solids, 46:1319-1342, 1998. [2] C. Miehe, M. Hofacker and F. Welschinger. A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, Computer Methods in Applied Mechanics and Engineering, 199:2765-2778, 2010. [3] C. Gräser and O. Sander. Truncated Nonsmooth Newton Multigrid Methods for Block-Separable Minimization Problems, IMA Journal of Numerical Analysis, doi.org/10.1093/imanum/dry073, 2018.

15th U.S. National Congress on Computational Mechanics
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Title: A Large-Scale Full-Waveform Inversion for Material Profile Reconstruction

Author(s): *Boyoung Kim, *Hongik University*; Jun Won Kang, *Hongik University*;

This study investigates the effect of spatial-scale variation on the result of subsurface imaging by a full-waveform inversion method. The full-waveform inversion method targets the reconstruction of material profiles using the surficial response of the domain to impact loads. To this end, a multi-grid wave simulation approach is used in the full-waveform inversion framework along with a parallel explicit time integration method for large-scale wave simulation. The full-waveform inversion is implemented based on a PDE-constrained optimization approach, which seeks the optimal values of elastic moduli for the domain of investigation while minimizing a Lagrangian functional. The Lagrangian consists of a least-squares objective functional and regularization terms, augmented by the weak imposition of governing wave equations via Lagrange multipliers. Numerical examples of material profile reconstruction using the finite element grid of various scales are presented to show the effect of the spatial-scale variation on the inversion result. The accuracy and efficiency of inversion results, as well as the extension to real-world problems, are discussed. The large-scale full-waveform inversion method can be applied to various engineering problems such as structural health monitoring, geophysical probing, and site characterization. Reference 1. J. W. Kang and L. F. Kallivokas (2011). The inverse medium problem in heterogeneous PML-truncated domains using scalar probing waves. Computer Methods in Applied Mechanics and Engineering, 200(1), 265-283. 2. A. Fathi, L. F. Kallivokas, and B. Poursartip (2015). Full-waveform inversion in three-dimensional PML-truncated elastic media, Computer Methods in Applied Mechanics and Engineering, 296, 39-72.

15th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization Method with NURBS Curves and Moving Morphable Components

Author(s): *Cheol Kim, *Kyungpook National University*; Rongzhen Zheng, *Kyungpook National University*; Kiseok Kwak, *Kyungpook National University*;

A new structural topology optimization method is developed newly in this study based on the NURBS (non-uniform rational B-spline) curves and the moving morphable components (MMCs). The basic MMC optimization is an explicit and geometrical method that uses a set of morphable structural components to create blocks of topology optimization. Optimal structural topologies may be obtained by optimizing the shapes, lengths, thicknesses, orientations and layout of these components. The proposed method adopts a different way of morphable components creation that combines with NURBS curves. The NURBS curve is widely used in the computer-aided-design (CAD) and advantageous on a B-spline curve. All kinds of complicated curved component can be built with NURBS curves or surfaces. NURBS curves are applied for shaping the geometries of structural components and the coordinates of control points system become the design variables. A MATLAB optimization code has been developed and two numerical examples of short cantilever and MBB beams are provided to prove that the geometric way of structural topology optimization coupled with NURBS curves using morphable components can get optimum solution successfully. As results of comparison with others, we can obtain the same topologies for the two structures. The proposed approach can improve the smoothness of the structural boundaries which are similar to shape optimization results during the topology optimization process.

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Title: Analysis of Tensile Force on Mooring Lines for a Submerged Floating Tunnel

Author(s): *Gyu-Jin Kim, *Dept. of Civil and Environmental Engineering, Korea Advanced Institute of Science and Technology, Republic of Korea*; Hyo-Gyoung Kwak, *Dept. of Civil and Environmental Engineering, Korea Advanced Institute of Science and Technology, Republic of Korea*;

A submerged floating tunnel (SFT) is an infrastructure that floats in water supported by an equilibrium of its buoyancy, weight and supporting force. Recently, research about the tunnel has been actively conducted with its economic efficiency of saving undersea tunnelling costs. When a buoyancy force is larger than a weight of tunnel itself, the tensile force is applied on the mooring lines in the opposite direction of the gravity. This estimation of the tensile force is critical, not only for the design of anchoring system and the connecting section of module, but also for the control of entire process of construction. In this study, a simplified model of the SFT is numerically analysed for the calculation of tensile reaction of mooring lines, which connect the tunnel and the earth. For the analysis, a typical section of 23m outer diameter is designed refer to the Funka Bay SFT, in Japan. A longitudinal length of a module is 50m and four modules of tunnel are connected in total and the mooring system is modelled at 50m interval. In addition to the weight of the tunnel, static pressure of seawater acting vertical direction of entire section is considered, so that the buoyancy force can be calculated. Through the analysis, the reaction and displacement of mooring line according to the relative location is performed and verified.

15th U.S. National Congress on Computational Mechanics
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Title: Multiscale Topology Optimization for Integrated Structural-material Systems

Author(s): Lei Li, *University of California, San Diego*; *Hyunsun Kim, *University of California, San Diego*;

Compliant mechanisms, which are able to transmit applied forces or motions from input ports to output ports by elastic deformation of its underlying materials, have been studied over the past decades. As an advanced free-form structural design method, topology optimization can be utilized for compliant mechanism designs to amplify their mechanical advantages. While topology optimization for compliant mechanisms has been performed in numerous studies, simultaneously optimizing the structure and the material, i.e. multiscale topology optimization, is relatively untouched in the literature. In this study, we present a novel multiscale level set topology optimization scheme to design the macroscopic compliant mechanism structurally and the comprising microscopic material(s) at the same time. Computational homogenization is used to bridge the two length-scales. Both coupled and decoupled strategies for macro and microscale volume constraint are implemented to answer the question: can porous architected materials be utilized to improve a compliant mechanism over a solid isotropic material? A series of example problems with varying boundary conditions are numerically investigated to study the question and demonstrate the proposed multiscale optimization formulation.

15th U.S. National Congress on Computational Mechanics
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Title: Reconstruction of Three-dimensional Microstructures of Two-phase Membrane and Phase Property Estimation through Combination of Real and Virtual Experiments

Author(s): *Se-Yun Kim, *Yonsei University*; Ji-Su Kim, *Yonsei University*; Tong-Seok Han, *Yonsei University*;

Properties of multi-phase materials have correlations with their microstructural features so that the microstructure characterization is important for understanding the behavior of materials. In this study, two-phase polymeric membranes for carbon dioxide capture are used to investigate the effect of the microstructures on the material properties. The microstructural features of the two-phase membranes change depending on constituents. Four two-phase polymeric membranes with different degrees of filler wt% are investigated to reconstruct 3D microstructures from 2D transmission electron microscope (TEM) images [1]. The microstructural information from the 2D TEM images are characterized by probabilistic functions, i.e., cooccurrence correlation functions (CCFs). The CCFs are found to be efficient in reconstructing 3D microstructures using microstructural information obtained from 2D images through stochastic optimization [2]. The CCFs obtained from 2D TEM images are used as target characteristics, and virtual 3D microstructures with the same CCFs are reconstructed. The reconstructed virtual 3D samples of the two-phase membranes are used to evaluate the macro-scale properties. The properties for each phase of the virtual samples are estimated by comparison between real experiments and a series of virtual experiments using a finite element method. A number of simulations are performed, and the potential candidates for the phase stiffness are determined. It is expected that the proposed framework can reduce the cost and time consuming real experiments. [1] J. Lee, C. Park, J. Jung, J.-H. Kim, J. Kim, Dual-phase all-polymeric membranes with graft copolymer filler for co2 capture, Chem. Eng. J.334 (2018) 939–947. [2] J. Feng, X. He, L. Qing, Y. Li, Reconstruction of three-dimensional heterogeneous media from a single two-dimensional section via co-occurrence correlation function, Comput. Mater. Sci. 144 (2018) 181–192.

15th U.S. National Congress on Computational Mechanics
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Title: Wave Guiding in Two-dimensional Metamaterials: Phononic Topological Insulator

Author(s): Jaehyung Hong, *UNIST*; Joo Hwan Oh, *UNIST*; *Sung Youb Kim, *UNIST*;

Metamaterials are artificial micro-structured materials which have extraordinary properties not founded in nature. Those properties facilitate wave controlling in low frequency broadband with effective mass quantities. Phononic crystal, one of the method for designing metamaterial based on periodic characteristic of the structure, makes possible to cut off specific frequency range. This selective permeability can be applied in various mechanical fields. In this research, a topological insulator based on a phononic crystal metamaterial will be developed with real-time wave propagation simulation using finite element method. In order to obtain broadband in low frequency range, phononic bandgap opening phenomenon calculated from two-dimensional graphene-like nano-resonator with nonlinearly coupled-geometric parameters. Topological insulator characteristic will be obtained by configuring artificial interface, so called, edge states of the metamaterials that realize not only selective wave control also role of wave guide.

15th U.S. National Congress on Computational Mechanics
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Title: Enforcing Positivity with Bernstein Polynomials

Author(s): *Robert Kirby, *Baylor University*; Larry Allen, *Baylor University*;

Bernstein polynomials are a geometrically decomposed, nonnegative, partition of unity polynomial basis. In addition to long-standing work in computational geometry, recent work in the finite element literature has led to fast algorithms for many critical tasks [1,2]. These algorithms freqently have complexity comparable to sum-factored algorithms on hexahedra. Besides such fast algorithms, the highly geometric flavor of Bernstein polynomials makes it possible to enforce positivity or bounds constraints [3]. Rather than numerical PDE, this talk considers simpler approximation-theoretic problems, but subject to bounds constraints. Beyond first degree polynomials, positivity of the Bernstein coefficients is sufficient but not necessary for pointwise positivity, and even determining whether a polynomial is positive can be quite difficult. This talk addresses questions related to approximation under bounds constraints, as well as under well one can approximate functions subject to computable bounds constraints such as positive Bernstein coefficients. We also show how Bernstein polynomials can be used to produce approximations that are monotone or convex. [1] Ainsworth, Mark, Gaelle Andriamaro, and Oleg Davydov. "Bernstein–Bézier finite elements of arbitrary order and optimal assembly procedures." SIAM Journal on Scientific Computing 33(6): 3087-3109 (2011). [2] R. C. Kirby, “Fast simplicial finite element algorithms using Bernstein polynomials,” Numerische Mathematik 117(4): 631 — 652 (2011). [3] C. Lohmann, D. Kuzmin, J. Shadid, S. Mabuza, "Flux-corrected transport algorithms for continuous Galerkin methods based on high order Bernstein finite elements,", JCP 344: 151-186 (2017)

15th U.S. National Congress on Computational Mechanics
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Title: The Influence of Binder Mobility to the Viral Entry Driven by the Receptor Diffusion

Author(s): *Sandra Klinge, *Institute of Mechanics, TU Dortmund University, Germany*; Tillmann Wiegold, *Institute of Mechanics, TU Dortmund University, Germany*; Robert P. Gilbert, *University of Delaware, Newark, USA*; Gerhard A. Holzapfel, *Graz University of Technology, Austria*;

The current presentation deals with the simulation of the viral entry into a cell. There are two dominant mechanisms typical of this process: the endocytosis und the fusion with the cellular membrane. However, we only focus on the first scenario. To this end, we consider a virus as a substrate with a constant concentration of receptors on the surface. Differently, the concentration of receptors of the host cell varies and these receptors are free to move over the membrane. When the contact with the cell surface has been achieved, the receptors start to diffuse to the contact (adhesion) zone. The membrane in this zone inflects and forms an envelope around the surface of the virus. This is the way the newly formed vesicle imports its cargo into the cell. In order to simulate the process described, we assume that the differential equation typical of the heat transport is suitable to simulate the diffusion of receptors. Additionally, we formulate two boundary conditions: First, we consider the balance of fluxes on the front of the adhesion zone. Here, it is supposed that the velocity is proportional to the gradient of the chemical potential. The second subsidiary condition is the energy balance equation depending on four different contributions: the energy of binding receptors, the free energy of the membrane, the energy due to the curvature of the membrane and the kinetic energy due to the motion of the front. The differential equation itself along with two boundary conditions forms a well-posed problem which can be solved by applying a direct method, for example the finite difference method. The talk also includes numerical examples showing the distribution of receptors over the membrane as well as the motion of the front of the adhesion surface. In particular, the influence of the mobility of receptors has been studied.

15th U.S. National Congress on Computational Mechanics
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Title: Multi GPU Implementation of Isogeometric Finite Element Solver for Tumor Simulations

Author(s): *Adrian Klusek, *AGH University of Science and Technology*; Marcin Los, *AGH University of Science and Technology*; Witold Dzwinel, *AGH University of Science and Technology*; Maciej Paszynski, *AGH University of Science and Technology*;

We present the efficient multi-GPU/CUDA realization of the isogeometric L2 projection numerical FEM [1,2] solver in the context of simulation of tumor evolution in 3D. We present the model implemented with the spatio-temporal vascular remodeling. In order to make the modeling and simulation of tumor dynamics a useful tool in planning anticancer therapy, its computational complexity has to be considerably reduced. We suppose that our solver implemented in multi-GPU environment will meet this requirement. The IGA-FEM numerical solver has been successfully applied for computer simulation of non-linear systems e.g. wind turbine aerodynamics or the blood flow simulations. In our simulations, we use the explicit method of the IGA-FEM. In the consecutive time steps we perform forward and backward substitutions and we simulate graph of network representing vessels in stochastic way. Unfortunately, this updating consist of many nested loops results in not acceptable execution time for both the serial and parallel C++ versions of the solver. For example in the 3D heat equation problem, one iteration of the solver needs 152 seconds for 120^3 mesh size for one thread. Our multithreaded C++ implementation scale up well with increasing number of threads for the Intel Xeon E5-2680v3 processor but the solver required servers because only serwers has many processors. To resolve this problem, we have implemented the same solver in CUDA. On the same tests, as those previously mentioned, we can perform the same task in 600 milliseconds on one Nvidia Tesla K40 XL and in 300 miliseconds for two GPUs. For 2 Nvidia Tesla K40 XL we have achieved execution time demonstrating more than 500 speed-up comparing to its classical multithread parallel version. We have noticed that this speed-up can considerably improve with the higher resolutions of the computational mesh. Acknowledgement: This research is supported by the Polish National Science Centre, Poland grant no. 2016/ 21/B/ST6/01539. References: [1] ?o?, M., K?usek, A., Hassaan, M. A., Pingali, K., Dzwinel, W., & Paszy?ski, M. (2019). Parallel fast isogeometric L2 projection solver with GALOIS system for 3D tumor growth simulations. Computer Methods in Applied Mechanics and Engineering, 343, 1-22. [2] Hughes, T. J., Cottrell, J. A., & Bazilevs, Y. (2005). Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. Computer methods in applied mechanics and engineering, 194(39-41), 4135-4195.

15th U.S. National Congress on Computational Mechanics
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Title: The Conforming Reproducing Kernel Method: Recent Developments and Applications

Author(s): *Jacob Koester, *Sandia National Laboratories*; Michael Tupek, *Sandia National Laboratories*; J.S. Chen, *University of California, San Diego*;

Efficient model development for complex systems remains a challenge. Generating a mesh of sufficient quality for the Finite Element Method (FEM) can take months [1]. Research in agile design-to-simulation processes seeks to alleviate this bottleneck by taking on the difficult task of pairing automatic discretization techniques with numerical methods that are capable of producing satisfactory results. To address this challenge, we have been developing the Conforming Reproducing Kernel (CRK) method [2]. CRK is designed to address the boundary related challenges common to many meshfree methods, allowing accurate simulations of nonconvex geometries and material interfaces while also simplifying imposition of essential boundary conditions. This presentation will discuss recent developments for simulating large deformation and failure of complex geometries. Volumetric locking is handled with a new approach based on the stabilized conforming nodal integration method [3]. Ideas from peridynamics and phase-field are used to predict material separation. Also presented is an approach for improving solution accuracy in the presence of the low quality discretizations that are common products when automatically meshing complex geometries. Examples utilizing the conforming kernels are shown and results are compared to predictions using FEM and RKPM. [1] M. Hardwick, R. Clay, P. Boggs, E. Walsh, A. Larzelere and A. Altshuler, DART system analysis, SAND2005-4647, Sandia National Laboratories, Albuquerque, NM, 2005. [2] J. J. Koester and J.S. Chen. Conforming window functions for meshfree methods. Computer Methods in Applied Mechanics and Engineering, 347:588 – 621, 2019. [3] J.S. Chen, C.T. Wu, S. Yoon, and Y. You. A stabilized conforming nodal integration for Galerkin mesh-free methods. International Journal for Numerical Methods in Engineering, 50(2):435–466, 2001. *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

15th U.S. National Congress on Computational Mechanics
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Title: Immersed Interface Methods for Biomedical Fluid-Structure Interaction

Author(s): *Ebrahim M. Kolahdouz, *University of North Carolina at Chapel Hill*; Brent A. Craven, *US Food and Drug Administration*; Boyce E. Griffith, *University of North Carolina at Chapel Hill*;

Numerous systems involving fluid-structure interaction (FSI) in which flexible bodies with complex geometries are immersed in a fluid are found in medicine and biology. An FSI coupling strategy is presented within the framework of the immersed interface method that allows fluid and solid subproblems to be solved in a partitioned manner and coupled through interface conditions. The formulation uses an Eulerian description of the fluid and a Lagrangian description of the solid, and independent, nonconforming discretizations are used for the fluid and solid regions. In the coupling of the fluid to the solid, the interfacial fluid stresses drive the solid motion, and a penalty method is used to ensure that the fluid satisfies the no-slip condition along the fluid-solid interface. Interfacial coupling between the fluid and solid subdomains is implemented using an immersed interface method for faceted surfaces that allows for general complex geometries while retaining sharp resolution of stresses at the fluid-solid interface. This approach enables the use of unstructured finite element discretizations of the solid domain while allowing for the use of structured-grid solvers for the incompressible Navier-Stokes equations. This numerical approach to FSI is tested against multiple numerical and experimental benchmark problems. Applications of this method to biomedical applications, including the dynamics of mechanical heart valves as well as deformable blood clots in the inferior vena cava will also be presented.

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Title: Nonlinear Multilevel Method for Phase-field Models of Fracture

Author(s): *Alena Kopanicakova, *Università della Svizzera italiana*; Rolf Krause, *Università della Svizzera italiana*;

The numerical simulation of failure mechanism in solids is computationally challenging, as crack-paths with a possibly complex topology have to be resolved. Phase-field models for fracture ease and eventually overcome these difficulties by regularizing the sharp crack interfaces by means of a diffusive damage model. This is computationally challenging due to huge number of unknowns and the ill conditioning caused by local changes in the damage variable. As a consequence, the design of efficient solution method becomes an important task. In order to obtain an overall optimal solution strategy, we employ a recursive multilevel trust region method (RMTR). The RMTR method combines the global convergence property of the trust region method and the optimality of the multilevel method. The solution process is accelerated by employing level dependent objective functions, minimization of which can yield good coarse level corrections for the fine level problem. In the context of the phase-field fracture approach, it is challenging to design efficient level dependent objective functions as the underlying mathematical model relies on the mesh dependent parameters. We introduce solution dependent objective functions that combine fine level description of the crack path with the coarse level discretization. The presented numerical examples will demonstrate the overall performance and scaling behavior of the RMTR method.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Variational Multi-Scale Modeling for Cavitating Flows on Moving Domains

Author(s): *Artem Korobenko, *University of Calgary*; Ahmed Bayram, *University of Calgary*;

In this talk we present the numerical framework for turbulent cavitating flows on moving domains with applications to hydrokinetic turbines (HKT) and ship propellers. The Arbitrary Lagrangian-Eulerian Variational Multi-scale (ALE-VMS) formulation is used to govern the highly turbulent flow including wake-structure interaction. The homogeneous mixture-model is used to model the cavitation. In addition, the sliding interface formulation is adopted to handle the components in a relative motion, i.e. rotor-tower interaction. Weak enforcement of essential boundary conditions is used for the solid structure surfaces. This relax the requirements on a boundary layer resolution while still providing a good accuracy. The equations are discretized in space using standard finite elements. The framework is applied to model multiple vertical-axis HKT. A detailed validation with open-filed experiment conducted by our industrial partner and mesh convergence study is presented. The results assure the robustness of the ALE-VMS formulation and how it can be used in marine/offshore engineering applications.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Multigrid Method for Unfitted Finite Element Method

Author(s): *Hardik Kothari, *Università della Svizzera italiana*; Rolf Krause, *Università della Svizzera italiana*;

Interface problems occur in many applications in physics. For these problems, it is important to capture discontinuous behavior in order to obtain a good approximation of the mathematical model. In this work, we use a Lagrange multiplier approach to enforce the interface conditions and present a multigrid method for solving the constrained optimization problems. The unfitted finite element methods allow to use relatively uncomplicated meshes for discretization and use the modified finite element spaces to incorporate the geometrical details. Nitsche's method is widely used in unfitted finite element paradigm to enforce the interface conditions or the boundary conditions. Even though this method retains the accuracy and robustness of the standard finite element methods, it is well-known that small cuts in the elements can give rise to ill-condition problems. The Lagrange multiplier is a better choice for enforcing the interface conditions weakly, as the method does not depend on any additional stabilization parameters and provides the same accuracy of the fitted methods. The downside of this method is that we need to solve a constrained optimization problem. A multigrid method comprises of two essential components, a smoother and transfer operator for passing the information from a fine level to a coarse level. We employ a modified projected Gauss-Seidel method as a smoother, which can enforce the constrains effectively while minimizing the energy functional. For the transfer operator, we use a pseudo-L2 projection based prolongation and restriction operators to transfer the information between the mesh hierarchies. We will show the essential modifications for the smoother and the projection operator for the unfitted finite element framework. Lastly, the robustness and the efficiency of the proposed multigrid method will be demonstrated and a comparison with the other saddle point solvers will be made. References: (1) R. Krause. A Nonsmooth Multiscale Method for Solving Frictional Two-Body Contact Problems in 2D and 3D with Multigrid Efficiency, SIAM Journal on Scientific Computing, 31(2) 1399-1423 (2009) (2) T. Dickopf and R. Krause. Evaluating local approximations of the L2 orthogonal projections between non-nested finite element spaces, Numerical Mathematics, 7(03), 288-316 (2014) (3) E. Burman and P. Hansbo. Deriving Robust Unfitted Finite Element Methods from Augmented Lagrangian Formulations Geometrically Unfitted Finite Element Methods and Applications, Springer International Publishing, 1-24 (2017)

15th U.S. National Congress on Computational Mechanics
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Title: A Multi-scale, Multi-physics Modeling Framework to Predict Spatial Variation in Additive-manufactured Metals

Author(s): Carl Herriott, *University of Utah*; Xuxiao Li, *University of Utah*; *Nadia Kouraytem, *University of Utah*; Vahid Tari, *Carnegie Mellon University*; Wenda Tan, *University of Utah*; Benjamin Anglin, *Carnegie Mellon University*; Anthony Rollett, *Carnegie Mellon University*; Ashley Spear, *University of Utah*;

The microstructure of additively manufactured (AM) metals has been shown to be quite heterogeneous and exotic when compared to conventionally manufactured metals. Consequently, the effective mechanical properties of AM metal parts are expected to vary both within and among different builds due to the laser interaction with the melt pool and solidification characteristics. This work presents a multiphysics modeling framework for simulating the process, microstructure, and properties of AM metal volumes. The framework is entirely automated, from the generation of the microstructure to the resulting spatial-property maps. The framework uses a 3D solidification and nucleation model to simulate a grain-resolved build domain created by a multi-pass, multi-layer, Directed Laser Deposition (DLD) process. The entire build domain is automatically divided into discrete sub-volumes to interrogate site-specific effective mechanical properties. Each sub-volume is first passed into DREAM.3D, where microstructural statistics are recorded, and an input file is written out to simulate mechanical testing on the sub-volume using a parallelized elasto-viscoplastic fast Fourier Transform (EVP-FFT) model. The effective stress-strain response of each sub-volume is analyzed automatically to extract the effective mechanical properties. The Young's modulus is found by applying a Hough transform to the stress-strain response to identify the elastic region. Based on the Young's modulus, a 0.2% yield offset is applied to approximate the yield strength of each sub-volume. Once these effective mechanical properties are found, they are then used to generate heat maps showing how these properties vary spatially throughout the simulated-build domain. As a demonstration, the framework is applied to DLD SS316L volumes with microstructures ranging from fully columnar to fully equiaxed. In this demonstration, we investigate three orthogonal planes (and multiple locations of each plane) throughout each build volume. The first plane, the transverse-direction-- build-direction plane, highlights the impact of successive build layers on resulting mechanical properties. The next plane, the transverse-direction--laser-scanning direction plane, highlights variability of the mechanical properties across the build plane at three specific build layers: just above the substrate, mid-build height, and the top of the build volume. Finally, the scanning-direction--build-direction plane, sampled on the center of the track and between two successive tracks, looks at the variability between successive laser tracks. Site-specific property maps are generated for each case to compare the range of properties both within and among each of the build domains. The multiphysics framework and property maps could provide a path toward design and qualification of AM metal parts.

15th U.S. National Congress on Computational Mechanics
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Title: Multifidelity Estimation of Risk Measures in Robust Design

Author(s): *Boris Kramer, *MIT*; Matthias Heinkenschloss, *Rice University*; Timur Takhtaganov, *Lawrence Berkeley National Lab*; Karen Willcox, *University of Texas at Austin*;

We present two reduced-order model based approaches for the efficient and accurate evaluation of the Conditional-Value-at-Risk (CVaR) of quantities of interest (QoI) in engineering systems with uncertain parameters. CVaR is used to model objective or constraint functions in risk-averse engineering design and optimization applications under uncertainty. Estimating the CVaR of the QoI is expensive. While the distribution of the uncertain system parameters is known, the resulting QoI is a random variable that is implicitly determined via the state of the system. Evaluating the CVaR of the QoI requires sampling in the tail of the QoI distribution and typically requires many solutions of an expensive full-order model of the engineering system. Our reduced-order model approaches substantially reduce this computational expense.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Fictitious Domain Method for Fluid Structure Interaction with Contact

Author(s): Maria Giuseppina Chiara Nestola, *Institute of Computational Science, Università della Svizzera italiana, Lugano (Switzerland)*; Patrick Zulian, *Institute of Computational Science, Università della Svizzera italiana, Lugano (Switzerland)*; Lisa Gaedke-Merzhäuser, *Institut für Mathematik, Freie Universität Berlin, Berlin (Germany)*; *Rolf Krause, *Institute of Computational Science, Università della Svizzera italiana, Lugano (Switzerland)*;

We present an embedded approach for the numerical solution of contact problems between multiple elastic structures immersed in a fluid flow. The solid bodies in pur FSI problem are modelled as hyper-elastic anisotropic materials, whereas the fluid is regarded as an incompressible and viscous flow in a transitional regime. The mathematical modelling of such material properties and the contact mechanics give rise to a large-scale coupled nonlinear problem which is challenging to discretize. Therefore, it is necessary to design flexible and parallel approaches, which ensure efficiency, stability, and convergence. For both structure and fluid, our approach relies on the finite element method, and it is inspired by the Fictitious Domain Method for their interaction. We employ a localized version of the L2-projections for handling the fluid-structure volumetric coupling and a variant of the mortar method for coupling the surfaces of the structures in contact. All the non-linear subproblems are accurately solved independently in a staggered manner with fully parallel techniques. Both the methodology and the implementation are validated with several benchmarks and comparisons with analytical solutions. The proposed strategy is finally employed to model the full dynamics of a bio-prosthetic heart valve placed in the aortic root. We model the blood-valve interaction, the blood-aortic wall interaction, and the contact among leaflets during the valve closure.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Multi-Phase Field Topology Optimization Considering Crystal Orientation

Author(s): *Hirofumi Kudo, *Tohoku University*; Junji Kato, *Nagoya University*;

Crystalline materials, such as metals and ceramics, are important materials necessary for various fields. Most of the actual crystalline materials are not composed of only a single material and have anisotropy that the physical characteristics are different depending on the direction (crystal orientation) in which atoms and molecules are aligned within the microstructure. In this research, we propose a new material design method for the crystalline materials in consideration of the anisotropy in the microstructure. In this framework, the multi-phase field method is introduced into topology optimization of microstructures and combined with a decoupling multi-scale analysis based on the homogenization method.

15th U.S. National Congress on Computational Mechanics
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Title: Coupling of Peridynamics and Finite Element Method Using Arlequin Framework

Author(s): *Shank Kulkarni, *University of North Carolina at Charlotte*; Xiaonan Wang, *ANSYS Inc*; Alireza Tabarraei, *University of North Carolina at Charlotte*;

Simulating a crack propagation is always a challenging task because of the presence of discontinuity in the displacement field near the crack tip. Traditional numerical methods such as finite element methods (FEM) are not capable of handling such discontinuities. Therefore a new method called ‘Peridynamics’ was introduced in order to remove deficiencies associated with traditional methods. Peridynamics (PD) is able to model crack propagation naturally due to its nonlocal integral formulation. However, PD is computationally expensive and has some of its own disadvantages. The best way to avoid all disadvantages is to couple PD with the finite element. In this method, PD is used only in critical areas such as the vicinity of crack tip and FEM is used everywhere else. The main issue associated with such coupling is the spurious wave reflections occurring at the interface of PD and finite elements. This issue is studied analytically and the solution is proposed to avoid spurious reflections. The proposed method follows the Arlequin framework and addition of viscous damping. References- 1. Shank S. Kulkarni, Alireza Tabarraei. "An analytical study of wave propagation in a peridynamic bar with nonuniform discretization." Engineering Fracture Mechanics, Vol: 190, pp: 347-366, 2018. 2. Xiaonan Wang, Shank Kulkarni, Alireza Tabarraei. ”Concurrent coupling of peridynamics and classical elasticity for elastodynamic problems.” Computer Methods in Applied Mechanics and Engineering, Vol:344, pp: 251-275, 2019. 3. Shank S. Kulkarni, Xiaonan Wang, Alireza Tabarraei. “Study of Spurious wave reflection at the interface of Peridynamics and Finite element region.” ASME 2018 International Mechanical Engineering Congress and Exposition, Pittsburgh PA, USA, Nov-2018 (In press).

15th U.S. National Congress on Computational Mechanics
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Title: The Poker-chip Experiment Explained

Author(s): *Aditya Kumar, *University of Illinois at Urbana-Champaign*; Oscar Lopez-Pamies, *University of Illinois at Urbana-Champaign*;

The internal nucleation of cavities/cracks in elastomers, a phenomenon commonly referred to as cavitation in the literature, was first reported by Busse (1938) and Yerzley (1939) and later made more prominent by the work of Gent and Lindley (1959). All of them conducted tension tests on thin disks of rubber ("poker-chips") bonded to plane metal end-pieces and observed the sudden appearance of cavities/cracks in the mid-plane of the rubber disks. Gent and Lindley, in their landmark study, attributed this phenomenon to the unstable elastic growth of pre-existing defects in elastomers. This popularized the notion of cavitation as an elastic phenomenon. However recent experiments by Poulain et al. (2017), analogous to the classical experiments by Gent and collaborators but carried out at higher spatio-temporal resolution (of 1 micron in space and 60 ms in time), along with the analysis of Lefevre et al. (2015) made it clear that elasticity alone is insufficient to explain the cavitation event and that cavitation is fundamentally a by-product of fracture. In this talk, I will examine the poker-chip experiments in the light of a recently developed macroscopic field theory (Kumar et al., 2018) that has the capability to explain, describe and predict the nucleation and propagation of fracture and occasional healing in elastomers in a unified manner. This theory, which is a generalization of the variational theory of brittle fracture (Francfort and Marigo, 1998), rests on two central ideas. The first one is to view elastomers as solids capable to undergo finite elastic deformations and capable also to phase transition to another solid of vanishingly small stiffness: the forward phase transition serves to model the nucleation and propagation of fracture while the reverse phase transition models the possible healing. The second central idea is to take the phase transition to be driven by the competition between a combination of strain energy and hydrostatic stress concentration in the bulk and surface energy on the created/healed new surfaces in the elastomer. After outlining the numerical implementation of the theory, comprehensive 3D comparisons between the theory and the poker-chip experiments will be presented to definitively explain these classical experiments and establish cavitation as primarily a fracture phenomenon. References [1] Gent, A.N., Lindley, P.B., Proc. R. Soc. Lond. A 1959:249, 195–205. [2] Poulain, X., Lefèvre, V., Lopez-Pamies, O., Ravi-Chandar, K., Int. J. Fract. 2017:205, 1-21 [3] Kumar, A., Francfort, G., Lopez-Pamies, O., J. Mech. Phys. Solid 2018:112, 523-551

15th U.S. National Congress on Computational Mechanics
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Title: Clustered Multiscale Topology Optimization

Author(s): *Tej Kumar, *University of Wisconsin-Madison*; Krishnan Suresh, *University of Wisconsin-Madison*;

There has been a recent interest in High-resolution Topology Optimization (HTO)1,2, enabling unprecedented details in the design. However, the computational cost in HTO can be massive. An alternate approach is to rely on Multiscale Topology Optimization (MTO) where microstructures are optimized at a smaller scale, while simultaneously optimizing the structure at the macroscale. The two scales are linked through homogenization theory. In MTO, microstructures are typically clustered to reduce the computational cost. Various clustering schemes have been proposed; here, we propose a density-and-strain based clustering. This scheme entails rotating microstructures along the principal directions to reduce the variability in the design and to enhance desired microstructure characterization. It is known that the use of multiple microstructures in the design domain leads to incompatibility at the microstructure boundaries. The problem is further exacerbated due to the application of microstructure rotation, i.e., even the adjacent identical microstructures become disconnected due to the applied rotation. This issue is solved by using an auxiliary coordinate system to map the microstructures into the design domain with rotation. A naïve mapping approach may lead to designs requiring clean-up. Therefore, the mapping is carefully performed to minimize the clean-up process. Numerical experiments are performed for both 2D and 3D design domains to show the merit of the proposed clustering scheme and understand the effect of different clustering sizes. Various advantages of the proposed method along with existing challenges and future research will be discussed. 1. Aage, N., Andreassen, E., Lazarov, B. S. & Sigmund, O. Giga-voxel computational morphogenesis for structural design. Nature 550, 84–86 (2017). 2. Liu, H., Zhu, B., Matusik, W., Hu, Y. & Sifakis, E. Narrow-Band Topology Optimization on a Sparsely Populated Grid. ACM Trans. Graph 37, 14 (2018).

15th U.S. National Congress on Computational Mechanics
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Title: Micromechanical Modelling of Ductile and Brittle Fracture of Metals

Author(s): *Meinhard Kuna, *TU Bergakademie Freiberg, Germany*; Geralf Huetter, *TU Bergakademie Freiberg, Germany*; Ngoc-Anh Giang, *TU Bergakademie Freiberg, Germany*;

The paper gives a survey about micromechanical modelling tech-niques to simulate the actual fracture and damage processes occurring at a crack tip in metallic materials. The aim of such simulations is to establish a relationship between microstructural properties of the ma-terial and its macroscopic fracture toughness. For this purpose, the crack growth behavior is calculated by means of the finite element method (FEM). A small scale yielding boundary layer concept is used, i.e. an increasing K-factor field is imposed as external load. The three-dimensional microstructural details of the fracture process zone are discretized in the model. Arrays of spherical voids or rigid inclusions are arranged around the crack tip to simulate ductile failure. In the ligaments between the forming voids and along the interface to the inclusions, cohesive elements are placed, which al-low to capture cleavage. The deformation behavior of the material in-side the process zone is treated by J2-plasticity, whereas far away damage is included by the Gurson-Tvergaard-Needleman model. This modelling strategy is applied to nodular cast iron (NCI) [1] and ferritic steel [2] in the brittle, ductile and brittle-ductile transition re-gion. The microstructure of NCI is characterized by spherical graphite particles of about 10 vol%, which can be simulated as voids. In steel, carbides are represented by initial inclusions. When simulating ductile behavior, the plastic collapse between intervoid ligaments in front of the crack was identified as the dominating mechanism. Other remote void arrays in the plastic zone caused a shielding effect for the crack. With decreasing temperature, ferritic materials show a transition to brittle fracture. This is modelled by increasing the yield stress, where-as the cohesive strength is assumed to be temperature independent. With increasing ratio between yield stress and cohesive strength, the brittle failure of the cohesive elements becomes the dominating effect. Thus, a smooth transition from dimple fracture to cleavage can be ad-justed in the simulations. The simulation results are compared with experimental crack growth resistance curves from literature. Both for NCI and ferritic steel a good quantitative agreement of the J-Da curves in the whole temperature range could be obtained with a minimum number of constitutive parameters. Moreover, the influence of microstructural parameters could be well predicted. [1] G. Hütter, L. Zybell, M. Kuna, Eng. Frac. Mech. 144 (2015) 118-141. [2] N. A. Giang, M. Kuna, G. Hütter, Theor. Appl. Fract. Mech. 92 (2017) 89-98.

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Title: Multiphase Flow for Pressurized Thermal Decomposition of Polymer Foams

Author(s): *Matthew Kury, *Sandia National Laboratories*; Sarah Scott, *Sandia National Laboratories*; Victor Brunini, *Sandia National Laboratories*; Ryan Keedy, *Sandia National Laboratories*;

Polymer foam encapsulants provide mechanical, electrical, and thermal isolation in engineered systems. In adverse thermal environments (e.g. fuel fires), polymers will decompose and produce gases. This alters heat transfer behavior and pressurizes the sealed system. Pressurization leads to the potential to damage other components through violent breaching of the system. Modeling encapsulating polymer foams in adverse thermal environments is critical for systems safety analysis, but it is challenging due to the coupled multi-physics within the system. The heat transfer within encapsulating foam systems exhibits a strong orientation dependence due to the different advection patterns that develop in the buoyancy-driven flow.[1] Previous models have coupled energy and mass transfer with chemical kinetics and phase equilibrium equations. Most recently, the porous media vapor-liquid equilibrium (PMVLE) model can capture the decomposition evolution of the polymer foams and the relocation of energy and mass as the gaseous species transport them away from the heat source (via Darcy flow). While the PMVLE model captures much of the orientation-dependent heat transfer patterns, no advection of the condensed phase occurs. In cases where heating occurs from the bottom, condensed phases can flow back to the heat source and be evaporated. The evaporation of the condensed phase will cause more pressurization and impact the heat flow patterns within the container. To introduce the flow of a condensed phase, models for the mechanics of partially molten rock were adapted to the encapsulated foam problem.[2] Using theory of mixtures, mass, momentum, and energy equations were derived for the motion of a condensed phase within a porous matrix that coexists with a gaseous phase. Using these equations and applying creeping assumptions to the gaseous flow, one recovers the transport equations from the PMVLE model and gains a set of evolution equations for the condensed phases, coupled together through porosity, gas pressure and relative drag forces. The new mixture equations were added to the PMVLE model, permitting the flow of condensed phases. This work will discuss the physics of the foam decomposition problem and how the flow of condensed and gas phases were introduced to increase the fidelity of thermal safety analysis. [1] S. Scott, et al. Validation of PMDI-based polyurethane foam model for fire safety applications. Proceedings of the Combustion Institute, 2018. [2] D. Mckenzie. The generation and compaction of partially molten rock. Journal of Petrology, 25(3):713–765, 1984.

15th U.S. National Congress on Computational Mechanics
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Title: On the Computational Design for High Energy Density Superconducting Magnets

Author(s): *Sergey Kuznetsov, *Commonwealth Fusion Systems, PSFC/MIT*; Alexey Radovinsky, *PSFC/MIT*; Dan Brunner, *Commonwealth Fusion Systems, PSFC/MIT*; James Guest, *Johns Hopkins University*;

Recent advances in the High Temperature Superconducting tape technology create new possibilities in the development high-field magnets requiring minimization of superconducting materials for the field generation. We present methodologies to find optimal magnetic source distributions providing required magnetic field profiles for Nuclear Fusion, Superconducting Magnetic Energy Storage and Magnetic Levitation applications. We show that these techniques identify non-trivial current distributions and shapes of the magnets. We take into account structural considerations becoming critical at high magnetic fields and current densities.

15th U.S. National Congress on Computational Mechanics
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Title: Isogeometric Boundary Element Methods (IGABEM) for Acoustic Scattering

Author(s): *Trond Kvamsdal, *Norwegian University of Science and Technology*; Jon Vegard Venas, *NTNU*;

Acoustic scattering is the physical phenomena of how sound interacts with objects and medium fluctuations. The acoustic scattering problem is often modelled by the Helmholtz equation. Combining isogeometric methods and the boundary element method (IGABEM) [1] and the infinite element method (IGAIEM) [2] has shown superior results on benchmark problems. The workshop Benchmark Target Strength Simulation (BeTSSi) has been a forum for acoustic scattering of submarines, where several benchmark objects has been analysed using different numerical methods. The complexity of these objects varies all the way up to a full submarine including torpedo tubes. Common for all objects is that no analytic solutions are found. Comparisons using several methods have been presented in the BeTSSi conference, with deviating results. We will herein present results for our developed IGABEM code, which builds upon the work done in [2]. First, we will show convergence plots obtained for a classical benchmark problem with analytical solution. Both Galerkin and collocation is considered in combinations with the conventional, hyper-singular and the Burton-Miller formulation. One of the main findings in this work is the deviation from the best approximation using BEM as opposed to classical FEM. Finally, we show results for BeTSSi submarine model, which in addition to its complexity include trimming curves and non-Lipschitz domains. Emphasis has been made to create an analysis suitable benchmark model (which for future benchmarking is given in many different file formats), see [3] for more details. REFERENCES [1] R. N. Simpson, M. A. Scott, M. Taus, D.C. Thomas, H. Lian, Acoustic isogeometric boundary element analysis, Computer Methods in Applied Mechanics and Engineering, 269:265-290. [2] J. V. Venås, T. Kvamsdal and T. Jenserud, Isogeometric analysis of acoustic scattering using infinite elements, Computer Methods in Applied Mechanics and Engineering, 335:152-193. [3] J. V. Venås and T. Kvamsdal, Isogeometric boundary element method, Computer Methods in Applied Mechanics and Engineering, To be submitted April 2019.

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Title: Blast Analysis of RC Beams and Columns Based on the Hysteretic Moment-curvature Relation

Author(s): *Hyo-Gyoung Kwak, *Korea Advanced Institute of Science and Technology*; MinJoo Lee, *Korea Advanced Institute of Science and Technology*; Gang-Kyu Park, *Korea Advanced Institute of Science and Technology*;

A numerical method to describe the nonlinear behavior of reinforced concrete beams and columns is introduced on the basis of the hysteretic moment-curvature relation. Based on the monotonic moment-curvature relation, the unloading and reloading curves of the moment-curvature relation can be inferred from the cyclic curves of the reinforcing steel because a structural behavior after the yielding is largely dependent on the behavior of the reinforcing steel. A DIF equation which is a function of the curvature rates, instead of the strain rates, is designed for the direct application to the moment-curvature relation of an RC section. In order to describe the large deformation beyond the yielding of the reinforcing steel, the moment-curvature relation should be modified to consider the bond-slip effect between the steel and the surrounding concrete, which is generally occurred within the critical regions. Then, the validity of the introduced model is performed by comparing with the experimental results which show the flexural behavior. In addition, direct shear behavior is implemented in the numerical model, and the influence of the direct shear behavior, which generally occurs within a very short time, on the flexural structural behavior is examined. Acknowledgment: This work is supported by the Korea Agency for Infrastructure Technology Advancement(KAIA) grant funded by the Ministry of Land, Infrastructure and Transport (Grant 13IFIP-C113546-01). References 1. Menegotto M, Pinto PE. Method of Analysis for Cyclically Loaded R. C. Plane Frames Including Changes in Geometry and Non-Elastic Behavior of Elements under Combined Normal Force and Bending. Proc IABSE Symp Resist Ultim Deform Struct Acted by Well Defin Loads 1973:15–22. 2. Krauthammer T, Astarlioglu S. Direct shear resistance models for simulating buried RC roof slabs under airblast-induced ground shock. Eng Struct 2017;140:308–16.

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Title: Modeling of Twinning Using an Implicit Time Integration Scheme in Finite Element Methods

Author(s): *Soondo Kweon, *Southern Illinois University Edwardsville*; Daniel Raja, *Southern Illinois University Edwardsville*;

Modeling twinning in computation has been a difficult task in the mechanics community for many decades. The materials that deform by twinning show highly nonlinear and abruptly changing mechanical responses. These highly nonlinear complex mechanical responses are caused by the interaction hardening among many different kinds of slip and twin modes and give rise to computational difficulties such as issues of convergence and stability. Due to these difficulties, computation of twinning materials runs with small time steps, which makes the simulation time lengthy. To take into account these complex interaction hardening responses and to efficiently deal with the above computational difficulties, a sophisticated numerical scheme based upon the implicit time integration algorithm is proposed in this study. Although many computational researchers have worked on twinning using crystal plasticity frameworks, most of the former computational works have not provided the detailed implementation steps that they used to make their results. Therefore, this work describes in detail procedures in which the proposed implicit computational scheme is implemented into a large deformation finite element code providing to the mechanics community a computational platform for twinning materials. The mechanics community has been using only the pyramidal II slip ({11-22} ?-1-123?) as the pyramidal ?a + c? slip for the deformation of magnesium. However, recent experimental and computational (molecular dynamic simulation) works revealed that the main pyramidal ?a + c? slip mode in magnesium is the pyramidal I slip, not the pyramidal II slip ({11-22} ? -1-123?). This work takes into account this new finding in the simulation of magnesium. The most number of slip and twin modes including the pyramidal I slip are employed in this work in order to reproduce the channel-die compression test data of both single crystal and polycrystal magnesium shown in (Kelley and Hosford, 1967, 1968). References Kelley, E. W., Hosford, W. F., 1967. The plastic deformation of magnesium. Technical report. Kelley, E. W., Hosford, W. F., 1968. Plane-strain compression of magnesium and magnesium alloy crystals. Transactions of the Metallurgical Society of AIME 242, 5–13.

15th U.S. National Congress on Computational Mechanics
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Title: Peridynamic Modelling of Metal Materials under High-Speed Velocity Impact

Author(s): *Xin Lai, *Wuhan University of Technology*; Sai Li, *Wuhan University of Technology*; Lisheng Liu, *Wuhan University of Technology*; Jiale Yan, *Harbin Engineering University*;

High-speed velocity and hypervelocity impact have drawn so much attentions of the researchers in the past decades. The problem often emerges from fields of industry and aerospace, such as impact molding and the defense of space debris. It is cumbersome to repeat the phenomena in the lab and capture the dynamic progress during the impact using the experiment manner. Thus it is quite practical for numerical methods to make prediction and representations for understanding the fundamentals of the mechanical behaviors of the materials, which then serves as a guidance for structure and material design. In this work, the Peridynamic framework is adopted to model the metal material with rate-dependent effect. State-based Peridynamic framework has been used to model the mechanical properties of the material under high strain-rate. Benchmark tests and validations are carried out, and discussions are made against the experimental results.

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Title: Constitutive Modeling of Shape Memory Alloys and Simulation of Structural Response

Author(s): *Chad Landis, *University of Texas at Austin*; Stelios Kyriakides, *University of Texas at Austin*; Dongjie Jiang, *Shanghai Jiao Tong University*; Karlos Kazinakis, *University of Texas at Austin*;

Recent work on the modeling of the structural response of shape memory alloy tubes, bars, and beams is presented. We have developed a new constitutive model that captures pseudoelastic transformation induced recoverable deformation in SMAs including the strong asymmetries in the tensile and compressive responses. The model is based on a J2-type nonlinear kinematic hardening framework with the back stress represented through a weighted mix of two potential functions that are calibrated to the tensile and compressive stress-strain responses of the material. The constitutive model has been used to simulate numerically the interaction of these complex material behaviors with structural nonlinear behavior observed in experiments. Problems analyzed include the buckling and recovery of NiTi tubes under axial compression, the propagation of a well defined deformation front in uniaxial tension, and the reversible propagation of curvature localization as well as buckling in NiTi tubes under bending. The numerical simulations reproduce the structural behavior both qualitatively and quantitatively demonstrating the fidelity of the constitutive modeling framework developed.

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Title: Modeling the Nonlinear Bilateral Thermo-electro--mechanical Coupling in Polycrystalline Ferroelectrics

Author(s): *Stephan Lange, *University of Kassel*; Andreas Warkentin, *University of Kassel*; Marius Wingen, *University of Kassel*; Andreas Ricoeur, *University of Kassel*;

Ferroelectric materials, such as lead zirconate titanate (PZT) or barium titanate (BT) are technically attrac- tive ceramics because of their special properties. They are often used for actuators or sensors in the precision range. The materials are mostly subjected to high frequencies and large electrical loads, which is why insufficient heat dissipation can lead to undesirable temperature developments, so-called self heating. The letter is due to irreversible domain wall motion and leads to changes in the material properties and sometimes even to phase transformations, whereupon the devices finally are inoperative. In case of insufficient heat dissipation, struc- tural problems due to phase transformations and thermal stresses occur. In low Curie temperature materials, such as barium titanate, even depolarization is possible. Besides the aforementioned nonlinear self–heating, the reversible elasto- and electrocaloric effects demonstrated in experiments have become increasingly important in recent years with regard to the design of smart cooling devices. In conventional ferroelectric materials, however, large reversible effects occur at high temperatures and are thus often negatively influenced by phase transformation. In [2] a FE model and related simulations are presented with nonlinear ferroelectric materials, forcing into account domain switching induced heating. Although complex thermomechanical boundary value problems can be solved with the FEM, the calculations are very time-consuming. The aim of this work is to extend the so-called condensed method (CM) according to [1] to realize a time-saving and discretization-free possibility to predict the temperature evolution in ferroelectric materials on the basis of a single polycrystalline material point. For this purpose, the CM is extended by the nonlinear bilateral thermo– electro–mechanical couplings. In addition, a comparison of the results by this work and those of the FEM according to [2] is presented. For verification, the theoretical results from the CM and FEM are compared to the experimental results. References [1] S. Lange and A. Ricoeur. “A condensed microelectromechanical approach for modeling tetragonal ferro- electrics”. Int. J. Solids Struct. 54 (2015), pp. 100–110. [2] M. Wingen and A. Ricoeur. “Caloric aspects of nonlinear ferroelectric constitutive behavior: modeling and simulation”. Continuum Mechanics and Thermodynamics (2018). DOI: 10.1007/s00161-018-0711-1

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Computational Parametric Modeling of Residual Velocities and Depth of Penetration from Impact Experiments on PAM-35 Concrete

Author(s): *William Lawrimore, *U.S. Army Engineer Research and Development Center*; Robert Browning, *U.S. Army Engineer Research and Development Center*; Andrew Barnes, *U.S. Army Engineer Research and Development Center*; Jared Brown, *U.S. Army Engineer Research and Development Center*; James O'Daniel, *U.S. Army Engineer Research and Development Center*;

Even though research has been ongoing into high strength concretes for many years, most installations are still being built with conventional concrete. This is primarily due to the cost and the validity of the existing design criteria which do not include high strength concretes. In order to push the use of high strength concrete, current standards need to be extended to include performance metrics for high strength concrete. Toward that goal, a series of impact experiments were conducted on PAM-35 cylindrical targets measuring residual velocity and depth of penetration. While PAM-35 is a conventional strength concrete, it was chosen to provide a baseline from which to test the validity of design criteria as well as the fidelity of the modeling methods. A variety of target diameters and thicknesses were struck by 0.5 in. diameter ball bearings traveling at a variety of impact velocities. Finite element meshes for the targets and the projectiles were built using TrueGrid and Cubit and were then imported into ParaDyn for finite element analysis. A parametric analysis was conducted to compare the relative influence of two parameters, i.e., concrete target thickness and concrete material strength. Results from the simulations were compared to those from the experiments in order to determine the predictive capacity of the simulation methodology. Permission to publish was granted by Director, Geotechnical & Structures Laboratory.

15th U.S. National Congress on Computational Mechanics
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Title: Modeling Organic Material Decomposition Kinetics Using Bayesian Inversion

Author(s): *Ellen Le, *Sandia National Laboratories*; Sarah Scott, *Sandia National Laboratories*; Ari Frankel, *Sandia National Laboratories*; Ryan Keedy, *Sandia National Laboratories*; Victor Brunini, *Sandia National Laboratories*; Brent Houchens, *Sandia National Laboratories*; Terry Johnson, *Sandia National Laboratories*;

Organic materials (such as polymers and fiber reinforced polymers) are increasingly used in systems where a lightweight material is needed, such as aircraft and vehicles. Unlike traditional engineering materials, such as metals, these materials decompose at relatively low temperatures (250C). In order to understand the fire safety implications of using such materials, comprehensive decomposition models for organic materials are being used in computationally-intensive macroscale system modeling and uncertainty quantification. Thus, both accurate and efficient modeling of organic material decomposition are critical for evaluating fire safety. This work investigates the thermal decomposition of a range of organic materials using the framework of Bayesian inversion. A cycle for the development, calibration, and validation of a decomposition kinetics model for an organic material of interest is demonstrated. In the calibration stage, kinetic parameters are fitted to data from transient thermogravimetric analysis (TGA) experiments using Bayesian calibration. This method is more informative than the point estimates sought in traditional deterministic calibration via inverse modeling, as it seeks a joint probability distribution of the kinetic parameters (the solution to the Bayesian inverse problem), thus uncertainty in the input parameters is also quantified. The calibration is performed via an adaptive Markov Chain Monte Carlo (MCMC) sampling method in DAKOTA. First a Laplace approximation for the MCMC proposal distribution is computed using gradient-based optimization of the negative log-posterior. The log-posterior is an augmented form of the objective function commonly used in fire science engineering that has both a residual mass component and a mass loss rate component. However, the likelihood covariance used in the literature does not account for the correlation between the two data components. To help account for data correlation, a method for constructing a block-form for the likelihood covariance is presented. Additionally, known coupling between kinetic parameters is added via a joint regularization (negative log-prior). The new posterior covariance leads to faster MCMC convergence. Improvement in model agreement, especially in sharply peaked regions of data where deterministic calibration can have difficulties, is shown. Model uncertainty quantification and validation results are presented using out-of-sample data. The method is compared to current inverse modeling methods in the fire safety literature and recommendations are made. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. SAND2019-0270 A

15th U.S. National Congress on Computational Mechanics
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Title: Fluid-Structure Interaction Simulation of Light-Weighted Structures with Thin-Walled Bodies

Author(s): *Trung Le, *North Dakota State University*;

In many engineering problems, dynamics of thin-walled structures interacting with fluid media needs to be analyzed. Fluid-Structure Interaction simulations have been shown as an effective tool to study such a problem. In this work, we proposed new coupling strategies for fluid and solid solvers using the sharp interface immersed boundary method. The fluid solver is based on the Curvilinear Immersed Boundary method which uses the hybrid staggered/non-staggered approach to solve the governing equations in generalized curvilinear grids. The Navier-Stokes equations are discretized via a hybrid staggered/non-staggered approach using three-point central differencing for all spatial derivatives and integrated in time via a second-order accurate fractional step method. The fluid equations are solved using projection methods, which requires solving the momentum and Poisson equations. The momentum equations are solved with a Jacobian-free solver while Flexible Generalized Minimal Residual method with multigrid pre-conditioner is used to solve the Poisson equation to satisfy the discrete continuity equation to the machine-zero precision. Complex immersed boundaries are handled using a sharp-interface immersed boundary method with velocity reconstruction along the local normal to the body. The continuity conditions for the velocity field (Dirichlet boundary) and the traction (Neumman boundary condition) are enforced across the fluid-structure interface. This requirement leads to the natural Dirichlet-Neumann partitioning technique that seeks the displacement field of the solid body under a fixed-point iteration. In the current work, fixed point iteration with relaxation (Aitken's acceleration) is used to accelerate the convergence of the coupling strategy. Several examples are discussed including: a) aortic tri-leaflet valve; b) thin-walled blades to demonstrate the capability of the method.

15th U.S. National Congress on Computational Mechanics
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Title: An Overlay Grid Driven Geometric Model Extraction

Author(s): *Nicolas Le Goff, *The French Alternative Energies and Atomic Energy Commission*; Franck Ledoux, *The French Alternative Energies and Atomic Energy Commission*; Jean-Christophe Janodet, *Université d'Évry-Val-d'Essonne / Paris-Saclay*;

Some overlay grid methods [1] take a Cartesian grid or an adaptively refined grid carrying materials volume fraction data as an input and produce an unstructured mesh with pure cells as an output. Such algorithms generate full hexahedral unstructured meshes but with low quality elements along the geometric model boundary. As a consequence, obtained hexahedral meshes do not fit the requirement of all numerical simulation codes that need hexahedral elements. But, such algorithms have a great interest when the geometry is not explicitly known, or in an intercode context where two simulation codes are executed one after the other, the first one providing the data needed to build the input of the second one. While the output of those methods is already a full-hex unstructured mesh with pure cells, we propose to use an overlay-grid algorithm to build a geometric model only. This model can be deduced from the cells assigned to each materials and the knowledge of the underlying hexahedral mesh gives us much information and more degrees of freedom to modify and clean up the geometric model. In practice, users expect some topological relations between the geometric model entities (surfaces, curves, points) and the ability to remove small features, preserve some sharp features or ensure the manifoldness property. Driven by such constraints, our approach consists in extracting a geometric model from the output of an overlay-grid algorithm. The approach that we will present iterates between the mesh and the generated geometric model so as to ensure the expected properties on the geometric model. During the iterative process, the overlay-grid algorithm can be launched with a locally-refined input depending on the local properties to ensure. Modifying the geometry or the topology of the mesh will require the use of techniques such as those seen in [2]. The results of our implementation based on our generic meshing data and services [3] will be presented both in 2D and 3D. [1] S. J. Owen, M. L. Staten and M. C. Sorensen. Parallel hex meshing from volume fractions, Engineering with Computers 30 (2014). [2] A. M. Herring, O. Certik, C. R. Ferenbaugh, R. V. Garimella, B. A. Jean, C. M. Malone and C. M. Sewell. (u) introduction to portage (2017). [3] F. Ledoux, J.-C. Weill and Y. Bertrand. GMDS: a Generic Mesh Data Structure. 17th International Meshing Roundtable (2008).

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Surface Quad Blocking Using Frame Fields and Mesh Adaptation

Author(s): Ana-Maria Vintescu, *CEA*; *Franck Ledoux, *CEA*;

To discretize 3d surfaces, quadrilateral meshes have been widely used for many years in Computer-Aided Design and numerical simulation where they overcome triangular meshes for some types of applications and numerical algorithms. But depending on the numerical algorithm to be implemented and the type of simulations (structure, fluid, hydrodynamics, etc.), quadrilateral meshes must ensure some properties. More specifically, we focus on block-structured quadrilateral meshes, which means a coarse structure of patches where each patch is subdivided into refined regular grids. We call this coarse structure a meta-mesh and the final mesh a quadrilateral block-structured mesh. Such quadrilateral block-structured meshes are in practice difficult to be automatically generated for any type of surfaces. As a consequence, many meshing tools rely on semi-automatic approaches where users interactively build or modify the meta-mesh. Such a practice is shared with computer animation, where designers draw the patch structure onto the surface model. In order to reduce the time spent to generate such meshes, many research works have been led to generate quadrilateral block-structured meshes using the formalism of cross fields. A cross fields gives a piece of informations about how to locally align final quadrilateral cells into the geometric domain. For 3D smooth manifold surfaces, such cross fields are naturally connected to the principal curvature directions. The presented work is based on cross fields with the aim of obtaining a robust software component for generating the expected meta-mesh for any 3D manifold surfaces. The proposed solution is based on a three main stages : (1) Cross field generation; (2) Mesh adaptation; (3) Meta-mesh generation and simplification. Cross field generation can be done using any existing techniques where crosses are computed at the vertices or cell centers of a triangular mesh. The computation is done by minimizing an objective function, which corresponds to a simple diffusion problem. But all of the approaches to generate cross fields have a common drawback: they are very sensitive to the discretization of the triangular mesh. That’s why we propose to enrich the cross field generation with an adaptive loop where the triangular mesh is refined in some areas of interest. Eventually, we suggest to build the meta-mesh in an indirect manner: we first generate the dual of the meta-mesh and then we deduce the primal mesh. It gives us a much more robust algorithm that is much numerically stable than trying to directly generate the primal mesh.

15th U.S. National Congress on Computational Mechanics
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Title: A Generalized Polynomial Chaos Expansion for Stochastic Design Optimization under Dependent Random Variables

Author(s): *Dongjin Lee, *The University of Iowa*; Sharif Rahman, *The University of Iowa*;

This paper presents a novel Polynomial Chaos Expansion (PCE) method for stochastic design optimization of high-dimensional complex systems subject to dependent random variables with an arbitrary, non-product-type probability measure. The method is premised on (1) a generalized version of PCE entailing measure-consistent multivariate orthogonal polynomials in dependent variables; (2) an innovative coupling between the generalized PCE and score functions for estimating the first-order design sensitivities of the statistical moments and failure probability; and (3) standard gradient-based optimization algorithms. The statistical moments or failure probabilities and their design sensitivities are both determined concurrently from a single stochastic analysis or simulation. Numerical results from a mathematical problem indicate that the new method developed is theoretically convergent and provides computationally efficient design solutions. Finally, shape optimization for an industrial-scale computer-aided design model was performed, demonstrating the power of the new method in solving practical engineering problems.

15th U.S. National Congress on Computational Mechanics
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Title: Towards In Vitro Experimental Validation of Fluid-Structure Interaction Models of Bioprosthetic Heart Valves Using Commercial Pulse Duplicator

Author(s): *Jae Lee, *University of North Carolina at Chapel Hill*; Robert Hunt, *University of North Carolina at Chapel Hill*; Boyce Griffith, *University of North Carolina at Chapel Hill*;

Every year, nearly 70,000 aortic valve replacement procedures are performed in the U.S. to treat severe aortic valve stenosis [1]. Because of expanded patient access to surgery, heart valve replacement procedures continue to increase. Although current commercially available replacement valves are considered safe and effective, there are still problems related to durability and clotting. One of the two main classes of surgical prosthetic heart valves is bioprosthetic heart valves (BHVs). BHVs are becoming increasingly popular for their hemodynamic flow patterns that are close to those with normal human aortic valves and do not require chronic anticoagulation therapy. However, BHVs have finite durability and experience tissue degradation, which is still challenging to resolve. Computer modeling and simulation is a powerful tool that may be utilized in the design and analysis phase to optimize device design. Credible simulation data may also be used in regulatory applications to the U.S. Food and Drug Administration (FDA) for device safety and effectiveness. However, these simulation results must be shown to be credible by performing rigorous verification and validation (V&V), as emphasized by the recently published ASME V&V 40 standard [2]. We present our work towards in vitro experimental validation focusing on the fluid-structure interaction (FSI) models of surgical BHVs using the hyperelastic immersed boundary (IB) method [3]. The validation study is conducted by comparing the numerical results to the experimental data from a ViVitro pulse duplicator, which is used by industry and regulatory agencies to assess the performance of prosthetic heart valves. We will compare the detailed flow patterns from our simulations to those from particle image velocimetry (PIV) as well as leaflet kinematics using high speed videographic method. As we assess the leaflet kinematics, we will also investigate the role of valve size on leaflet kinematics. This work will be a foundational work towards in vitro experimental validation of a numerical method that may lead to a high-fidelity platform for evaluating the efficacy of BHVs. Reference [1] M. A. Clark, et al., Clinical and economic outcomes after surgical aortic valve replacement in Medicare patients, Risk Manag Healthc Policy 5 (2012) 117–126. [2] ASME V&V 40-2018, Assessing credibility of computational modeling through verification and validation: Application to medical devices (2018). [3] B. E. Griffith, X. Y. Luo, Hybrid finite difference/finite element immersed boundary method, Int J Numer Meth Biomed Engng 33 (11) (2017) e2888.

15th U.S. National Congress on Computational Mechanics
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Title: Applications of Root-Finding Absorbing Boundary Conditions to Anisotropic Scalar and Elliptically Anisotropic Elastic Waves

Author(s): *Jin Ho Lee, *Pukyong National University*; Jeong-Tae Kim, *Pukyong National University*;

Wave propagation plays main roles in many areas of acoustics, elasticity, and electromagnetics. Therefore, relevant theories have been developed in order to resolve problems in the fields. It should be noted that many wave-propagation problems must be solved in infinite media. Because analytical solutions for these problems can be obtained only under very restricted conditions, numerical approaches are desirable for many of the problems. In the case, the infinite domains are truncated at some distances and certain numerical models are combined on the boundaries with those for the interior regions in order to represent the effects of the exterior regions. Recently, new absorbing boundary conditions, root-finding absorbing boundary conditions (RFABCs), were developed for scalar- and elastic-wave propagation problems [1, 2]. Their accuracy and stability at continuous level were proven. In order to combine the RFABCs with finite elements for the truncated interior regions, their discretized versions were formulated and shown to be stable at discrete level. It was demonstrated that various wave-propagation problems can be solved accurately and efficiently using the developed boundary conditions. In this study, an RFABC for scalar waves in anisotropic media will be developed. Without loss of generality, antiplane shear problems in transversely isotropic elastic media will be considered. A relation between traction and displacement on the truncated boundary will be derived following the approach of RFABCs. It will be shown that the boundary conditions can consider waves that propagate or decay in the outward direction of the truncated boundary. The accuracy and stability of the developed boundary condition will be proven. Then, its finite-element formulation will be derived and applied to antiplane shear wave propagation in an anisotropic waveguide. It will be demonstrated that the calculated wave fields are accurate when compared with reference solutions from extended mesh. Then, the developed RFABC will be applied to wave-propagation problems in elliptically anisotropic elastic media because dynamic motions in the media can be decomposed into two components of anisotropic scalar waves. References 1. J.H. Lee and J.L. Tassoulas, Absorbing boundary condition for scalar-wave propagation problems in infinite media based on a root-finding algorithm, Computer Methods in Applied Mechanics and Engineering, 330 (2018), 207-219. 2. J.H. Lee and J.L. Tassoulas, Root-finding absorbing boundary conditions for scalar and elastic waves in infinite media, Computer Methods in Applied Mechanics and Engineering 346 (2019), 592-611.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Enriched Galerkin Methods for Flow and Transport in Porous Media

Author(s): *Sanghyun Lee, *Florida State University*; Mary Wheeler, *The University of Texas at Austin*;

We present and analyze enriched Galerkin ?nite element methods (EG) to solve coupled ?ow and transport system in porous media such as viscosity and density-driven flows. The EG is formulated by enriching the conforming continuous Galerkin ?nite element method (CG) with piecewise constant functions. This approach is shown to be locally and globally conservative while keeping fewer degrees of freedom in comparison with discontinuous Galerkin ?nite element methods (DG). Linear solvers and dynamic mesh adaptivity techniques using entropy residual and hanging nodes will be discussed. Some numerical tests in two and three dimensions are presented to con?rm our theoretical results as well as to demonstrate the advantages of the EG.

15th U.S. National Congress on Computational Mechanics
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Title: Design and Analysis of Computer Experiments for Aluminum Powders to Maximize Pressure Under Reverse Taylor Impact

Author(s): *Sangmin Lee, *University of Notre Dame, Notre Dame, Indiana 46556, USA*; Karel Matous, *University of Notre Dame, Notre Dame, Indiana 46556, USA*;

An aluminum powder is studied using co-designed numerical simulations and experiments in the paradigm of predictive science. An aluminum powder pellet is impacted by a high-speed projectile and experiences high-strain rates induced by the mechanical deformations during the impact. To accomplish this co-design, we develop a novel poro-visco-plastic model and implement it into the highly parallel finite element solver, PGFem3D. PGFem3D is a highly optimized, transient, multiphysics and multiscale solver with a rich selection of numerical schemes and constitutive models. In order to identify conditions under which the internal pressure is maximized, we perform Design and Analysis of Computer Experiments (DACE). First, we evaluate the experimental pre-shots to limit the complex parameter space due to the large number of optimization conditions, complex material response, and difficulties of sample recovery and postmortem testing. Next, we perform careful material calibration. The co-designed study includes computationally expensive parameter sensitivity analysis including Uncertainty Quantification (UQ). UQ analysis provides a platform for model selection and propagation of uncertainties through the computational framework by means of stochastic and physically-based statistical techniques. Predictions of Quantities of Interest (QoIs) by numerical simulations are compared with the experimental results with confidence intervals.

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Title: Ultrasound Imaging-based Machine Learning Approach to Identify Altered Characteristics of Burned Tissue

Author(s): *Sangrock Lee, *Rensselaer Polytechnic Institute*; FNU Rahul, *Rensselaer Polytechnic Institute*; Hanglin Ye, *Rensselaer Polytechnic Institute*; Deepak Chittajallu, *Kitware, Inc*; Uwe Kruger, *Rensselaer Polytechnic Institute*; Tatiana Boyko, *University at Buffalo*; James Lukan, *University at Buffalo*; Andinet Enquobahrie, *Kitware, Inc*; Suvranu De, *Rensselaer Polytechnic Institute*;

Ultrasound imaging modality has emerged as a viable technique for the non-invasive assessment of altered soft tissue characteristics that are proven to be useful for diagnostic purposes. As an example, ultrasound elastography is routinely used to assess changes in the elasticity of soft tissue in pathologies, such as liver fibrosis and breast cancer. Elastography alone, however, may be unable to discern the tissues with altered characteristics, when their elastic properties are not contrast to the surrounding tissues. For example, ultrasound shear-wave elastography is known to be unreliable in differentiating malignant from benign prostate tissue [1]. In our previous work, we have shown that the ultrasound elastography can reliably differentiate between unburned and burned tissues, however, it fails to identify burn severity with acceptable accuracy [2]. We propose an ultrasound imaging-based machine learning approach to identify altered tissue characteristics with specific application to classification of thermally injured ex vivo porcine skin tissue. The model is based on the statistical measures of the image texture extracted from a grey-level co-occurrence matrix (GLCM) [3], which is drawn from the ultrasound B-mode images of tissues. These texture features are variables that allow pairwise separation based on a support vector machine (SVM) classifier. Utilizing leave-one-out cross-validation (LOOCV) ensures an independent assessment of SVM classifier. The model is tested for pairwise binary classification of four burn conditions: (i) 200 ºF for 10s, (ii) 200 ºF for 30s, (iii) 450 ºF for 10s, and (iv) 450 ºF for 30s, resulting in four different burn severities ranging from partial thickness to full-thickness burns. Independent assessment analysis confirms an average accuracy of 99% in correctly classifying the four different burn severities with just over 30 samples in each burn groups. The ultrasound imaging based classification approach, in conjunction with the GLCM texture features, is shown to be instrumental in accurately assessing altered tissue characteristics, even with a small sample size, which is to be expected for most experimental and clinical dataset. The proposed method is shown to have the potential for assisting clinical assessment of burn degrees. REFERENCES [1] Porsch, M., Görner, C., Wendler, J.J., Liehr, U.B., Lux, A., Siedentopf, S., Schostak, M., Pech, M. (2016). Journal of Ultrasonography, 16, 348. [2] Ye, H., Rahul, Dargar, S., Kruger, U., De, S. (2018). Burns, 44, 1521. [3] Haralick, R.M., Shanmugam, K. (1973). IEEE Transactions on Systems, Man, and Cybernetics, SMC-3, 610.

15th U.S. National Congress on Computational Mechanics
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Title: Recent Development of Numerical Methods for Practical Reservoir Simulation

Author(s): *Seong Lee, *Chevron ETC*;

This paper discusses modeling and mathematical challenges in developing efficient, accurate numerical methods to solve multi-phase flow in heterogeneous porous media. The major mathematical difficulties originate from the uncertainties in governing equations and boundary geometries and scale-dependent complexity in physical parameters and measurements. For instance, the permeability of natural formations displays high variability levels and complex structures of spatial heterogeneity which spans a wide range of length scales. Relative permeabilities for multi-phase flow are measured in a laboratory by a core sample of 1-2 inches, and they are directly applied in a reservoir simulation grid of 10-100 feet that may include large and different heterogeneity. This paper reviews recent development of numerical methods for non-linear transport equations in practical reservoir simulation: (1) hierarchical approach to naturally fractured reservoir with multiple length scales, (2) multi-scale finite volume method, (3) hybrid upwinding schemes, and (4) sequential fully implicit method for compositional simulation. The paper also reviews issues and challenges in practical simulation of field scale models.

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Title: Predicting the Effect of Aging and Flap Design on the Mechanical Stress Profiles of Skin Through Gaussian Process Surrogates

Author(s): *Taeksang Lee, *Purdue University*; Arun Gosain, *Northwestern University*; Ilias Bilionis, *Purdue University*; Adrian Tepole, *Purdue University*;

Mechanical cues guide the healing response following reconstructive surgery, with excessive stress linked to complications such as hypertrophic scarring. Deterministic, high-fidelity finite element (FE) models of reconstructive surgery have led to treatment recommendations in idealized cases and patient-specific geometries. However, the inherent variability of skin mechanical behavior with age, sex, anatomical location, and across patients, has been ignored. Similarly, the influence of different flap designs and skin lesion size on the resulting stress contours remains poorly understood. A major challenge in the development and adoption of predictive models for surgery planning stems from the fact that high-fidelity simulations are computationally demanding, require expert input and specialized software. To circumvent this challenge, here we build computationally inexpensive surrogates of the FE models that allow us to evaluate the stress for arbitrary material properties and a range of lesion sizes for the three most common reconstructive procedures: advancement, rotation, and transposition flaps [1]. To build the surrogate models we first create a training dataset that uniformly samples the input space, defined by the lesion size and the material parameters of a structurally-motivated strain energy function. We bound the parameter space based on experimentally-determined skin properties from the literature. After running the FE simulations corresponding to the training set, we do principal component (PC) analysis of the stress contours to reduce the dimensionality of the training data. This step reduces the dimension from thousands -the nodes in the FE mesh- to less than ten -the PC scores that capture more than 99% of variance in the data. We then build surrogate models through Gaussian process (GP) regression of the relevant PC scores. The GP surrogates predict stress contours with relative errors that are on average 2% in the L2-norm compared to the high-fidelity models. Evaluation of the GP surrogates is inexpensive and allows propagation of realistic joint probability distributions of the input parameters to obtain the corresponding probability of the stress fields. We apply our GP surrogates to study the effect of propagating probability distributions of the parameters associated with two different age groups. In conclusion, our approach is a significant step in the field of predictive computational tools for reconstructive surgery planning by replacing high-fidelity FE models with inexpensive GP surrogates that are accurate for arbitrary material parameters, a range of defect sizes, and different flap strategies. [1] Lee, Gosain, Bilionis, Tepole. Journal of the Mechanics and Physics of Solids, Accepted, 2019.

15th U.S. National Congress on Computational Mechanics
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Title: Nonlinear Model Order Reduction for Eulerian Fluid-Structure Interaction Problems

Author(s): *Lei Lei, *Stanford University*; Charbel Farhat, *Stanford University*;

Recently, a projection-based approach was developed in [1] for reducing the dimensionality of generic, nonlinear, embedded boundary models of Fluid-Structure Interaction (FSI) problems formulated in the Eulerian setting. This approach was successfully demonstrated for two-dimensional FSI problems whose underlying high-dimensional CFD models were constructed on Cartesian grids. In this work, this nonlinear model order reduction approach is extended to the FIVER (Finite Volume method with Exact two-phase Riemann problems) framework [2] for multi-material flow problems, which operates on Cartesian, structured, and unstructured grids. In particular, two challenging issues are identified and addressed. The first one is the reduction of the formulation and solution of a status change problem, when a grid point in the occluded region of the computational fluid domain is uncovered at a given time-step — and therefore its status changes from “ghost” (or inactive) to “real” (or active). This issue is addressed here by incorporating status changes in the construction offline of the Reduced-Order Basis (ROB). The second challenge is associated with the construction of a ROB that addresses the issues arising from the presence of occluded regions in the embedding computational fluid domain. Singular Value Decomposition (SVD) generates a hierarchy of nested ROBs, but fails to account for the presence of occluded regions. On the other hand, the Alternating Least-Square (ALS) method proposed in [1] for constructing a hierarchy of ROBs accounts for the occluded regions but not for the nesting property that is typically desired in any approximation procedure. For these reasons, an alternative approach is presented here for constructing a hierarchy of ROBs for embedded boundary models of FSI problems that accounts for occluded regions and satisfies the desired nesting property. The corresponding nonlinear model order reduction method is illustrated, and its performance is assessed, for several vortex-dominated FSI problems. References [1] M. Balajewicz, C. Farhat, Reduction of Nonlinear Embedded Boundary Models for Problems with Evolving Interfaces, Journal of Computational Physics, vol. 274, pp. 489-504, 2014. [2] C. Farhat, J.F. Gerbeau, Arthur Rallu, FIVER: A Finite Volume Method Based on Exact Two-Phase Riemann Problems and Sparse Grids for Multi-Material Flows with Large Density Jumps, Journal of Computational Physics, vol. 231, no. 19, pp. 6360-6379, 2012.

15th U.S. National Congress on Computational Mechanics
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Title: Three-dimensional Computational Modeling of Valve Interstitial Cells

Author(s): *Emma Lejeune, *University of Texas at Austin*; Alex Khang, *University of Texas at Austin*; Michael Sacks, *University of Texas at Austin*;

To date, most progress in mechanical modeling of heart valve tissue has focused on understanding the extracellular matrix (ECM) across scales. While much can be learned from understanding the ECM, robust multiscale computational modeling of heart valves must incorporate the influence of valve interstitial cells (VICs) on both physiological and abnormal tissue function. Here we describe the beginnings of a fully three-dimensional computational model of VICs that we are developing in conjunction with experiments conducted on cells cultured in three-dimensional hydrogels. To integrate experimental data into the computational model, we use tools from spatial statistics to interpret experimental data on the geometric and mechanical properties of VICs in vitro. Unlike traditional statistical theory, spatial statistics does not assume that observations are independent. By computing these statistics, such as spatial autocorrelation of stiffness from Atomic Force Microscopy experiments, we are better able to interpret experimental results and translate representative information into the computational setting. Then, in the computational setting, we include discrete sub-cellular components of VICs, and run simulations on suites of representative cells with heterogeneous geometries. From these simulations and the associated analysis, we are better able to understand the influence of cell behavior across scales. Ultimately, this multiscale computational framework will allow us to understand the connection between the behavior of cells cultured in vitro, and the behavior of cells in the demanding in vivo environment.

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Title: Super-convergence of Reproducing Kernel Approximation

Author(s): *Yu Leng, *The University of Texas at Austin*; Xiaochuan Tian, *The University of Texas at Austin*; John Foster, *The University of Texas at Austin*;

Reproducing kernel (RK) approximations are meshfree methods that construct shape functions from sets of scattered data. Reproducing kernel particle method (RKPM) is based on RK approximations and super-convergence is often observed in RKPM. We provide a theoretical analysis of super-convergence in Sobolev norms for even order basis reproducing kernel (RK) approximations. We prove first, that even order continuous RK approximations are always super-convergent. For discrete RK approximation, we show super-convergence behaviour only with uniform discretization and selected RK kernel functions (B-spline functions) and support sizes. In addition, we introduce, for arbitrary RK support size, a concept called pseudo-super-convergence, which states super-convergence is a numerical artifact rather than a mathematical property. Our analysis is general for multi-dimensional RK approximations.

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Title: Biomechanical Modeling of Lung Deflation for the Prediction of Target Localization During Minimally Invasive Surgery

Author(s): *Anne Cecile Lesage, *The University of Texas MD Anderson Cancer Center*; Kristy Brock, *The University of Texas MD Anderson Cancer Center*; Alda Tam, *The University of Texas MD Anderson Cancer Center*; Bastien Rigaud, *The University of Texas MD Anderson Cancer Center*; David Rice, *The University of Texas MD Anderson Cancer Center*; Guillaume Cazoulat, *The University of Texas MD Anderson Cancer Center*;

Video-assisted thoracoscopic surgery (VATS) for lung tumor resection significantly decreases postoperative pain, morbidity and hospitalization length compared to traditional open thoracotomy. However, localization of the resection target during VATS usually relies only on visual inspection, limiting the eligibility for this technique to patients with tumors located close to the lung surface. Localization of nodules deeper in the lungs becomes uncertain as the lung is deflated to make room in the chest cavity. The goal of this work is to develop a biomechanical model of the lung deflation solely based on the pre-operative CT scan in order to predict the localization of these nodules during surgery, thus potentially allowing to expand the VATS eligibility criteria. For preliminary experiments, CT scans from 3 patients whose pneumothorax occurred during lung biopsy were retrospectively analyzed. For each patient, a CT scan showing the deflated lung and a CT scan showing the re-inflated lung after chest tube insertion were collected. The following workflow developed for the lung deflation prediction will be presented: First, the contours of the inflated lungs and patient body were segmented and used to define a first order tetrahedral mesh with elastic properties for the lung parenchyma (Young's modulus of 4kPa and Poisson's ratio of 0.3) and with sliding boundaries of the lung relative to the pleura surface. Simulations of the lung deflation under gravity and constant pressure loading of the lung surface (800 Pa) was performed with the Altair RADIOSS FEM solver. The predicted deflation state presenting a lung volume close to the volume measured on the CT of the deflated lung was selected for comparison. For the 3 patients, a promising good agreement was found between the shape of the predicted lung surface and the ground truth shape. Ongoing work includes the identification of corresponding anatomical landmarks inside the lungs to quantitatively evaluate the accuracy of our model to predict the localization of deep tumors. The inclusion of the vessel trees as a stiffer structure in the model or the use of different mesh options (2nd order tetrahedral, hexahedral) or mechanical models (image-based inhomogeneous elastic model, visco-hyperelastic model) are being investigated.

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Title: Image-Based Modeling of Ceramic Additive Manufacturing

Author(s): *Brian Lester, *Sandia National Laboratories*; Adam Cook, *Sandia National Laboratories*; Harlan Brown-Shaklee, *Sandia National Laboratories*; Laura Swiler, *Sandia National Laboratories*; Joseph Bishop, *Sandia National Laboratories*;

In ceramic manufacturing, sintering is an essential step. Such a process involves taking a mechanically pressed body of powders (green-bodies) and thermally inducing densification to remove porosity. Importantly, the initial configuration of the powder particles in the green-body plays an essential role in the microstructure evolution and thus final configuration. In new additive manufacturing techniques, more complex green-body configurations can result necessitating further understanding of the role of microstructure. To this end, image-based modeling represents an enabling capability to establish such linkages between processing and structure. Here, such a possibility is explored for the direct write process. Specifically, a representative ceramic specimen is “written” and the resultant green-body characterized via x-ray microtomography. Key microstructural features arising from the direct write process are clearly observed. A finite element model is then constructed for the green body. First, a fully-implicit form of the Skorohod-Olevsky Viscous Sintering (SOVS) continuum, constitutive model is implemented in a finite element code. Second, the tomography images are segmented and used to inform an initial relative density distribution of a finite element mesh. The constructed finite element model directly incorporating microstructure is then used to simulate a sintering profile. Results of both local field (e.g. relative density, stress) and macroscale quantities (e.g. shrinkage) are considered and compared. The impact of different microstructure features is considered and their impact on sintering performance explored. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Title: Nonlinear Nonlocal Multicontinua Upscaling Method

Author(s): *Wing Tat Leung, *University of Texas at Austin*; Eric T. Chung, *Chinese University of Hong Kong*; Yalchin Efendiev, *Texas A&M University*; Mary F. Wheeler, *University of Texas at Austin*;

We are going to present a non-local upscaling methods for non-linear multiscale problems. This method is an extension of the recently developed non-local multicontinuum (NLMC) method. The main idea of this approach is to use calculate some upscaling parameters or multiscale basis functions by solving a constrainted local problem in an oversampled regions for constructing macroscopic equations. There are two approaches to handle the nonlinearity of the problem. The first approach is constructing the multiscale basis functions by solving a constrainted non-linear problem. Then the solution is approximated a linear span of these basis functions. This approach is easy to implement but it lacks the nonlinear interpolation. For the second approach, we will develop a nonlinear coarse scale model by calculating the upscaling parameter by solving a constrainted non-linear problem. We present some numerical result for both of the approaches to demonstrate the performance of the method.

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Title: Reaction Diffusion System Prediction Based on Convolutional Neural Network

Author(s): *Angran Li, *Carnegie Mellon University*; Yongjie Jessica Zhang, *Carnegie Mellon University*; Ruijia Chen, *Carnegie Mellon University*; Amir Barati, *Carnegie Mellon University*;

The reaction-diffusion system is naturally used in chemistry to represent substances reacting and diffusing over the spatial domain. Its solution not only illustrates the underlying process of a chemical reaction but also displays diverse spatial patterns of the substances due to the instability of the chemical equilibrium. These features inspire its application in the biological pattern morphogenesis, spatial ecology study, etc. Numerical methods like finite element method (FEM) are widely used to derive the approximate solution for the reaction-diffusion system. However, these methods require long computation time and huge computation resources when the system becomes complex. In our work, we studied the physics of a two-dimensional one-component reaction diffusion system by using machine learning. An encoder-decoder based convolutional neural network (CNN) was designed and trained to directly predict the concentration distribution, bypassing the FEM calculation process. Different simulation parameter and geometry configurations were considered as the input features of the proposed learning model. The trained CNN model is capable of providing concentration prediction with high test accuracy (mean relative error < 0.9%) and 300 times faster than the traditional FEM. From our model, we found the effect of the domain geometry and the ratio between reaction and diffusion on the reaction-diffusion distribution. Together, our CNN-based learning model provides a rapid and accurate tool for predicting the concentration distribution of the reaction-diffusion system. Reference: [1] Li, A., Chen, R., Farimani, A. B, & Zhang, Y. (2019). Reaction diffusion system prediction based on convolutional neural network. In preparation.

15th U.S. National Congress on Computational Mechanics
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Title: Meshfree Simulations of Additive Manufacturing of Metals at Powder-scale

Author(s): *Bo Li, *Case Western Reserve University*; Zongyue Fan, *Case Western Reserve University*; Hao Wang, *Case Western Reserve University*;

We present a powder-scale meshfree direct numerical simulation (DNS) capability for the powder bed fusion (PBF) based additive manufacturing (AM) processes using the Hot Optimal Transportation Meshfree (HOTM) method. The HOTM method is an incremental Lagrangian meshfree computational framework for materials behaviors under extreme thermomechanical loading conditions. It combines the Optimal Transportation Meshfree (OTM) method and the variational thermomechanical constitutive updates for general dissipative systems. The realistic multi-layer powder bed geometry is modeled explicitly in the HOTM simulations based on experimental data. The governing equations including the linear momentum and energy conservation equations are solved for the multiphase flow simultaneously to predict the deformation, temperature and local state of the powder bed. A phase-aware constitutive model is developed to predict the dynamic response of metal particles involving melting/vaporization/solidification and multiphase mixing during the PBF AM processes automatically. The powder-scale DNS is employed to study the melt pool thermodynamics and quantify the AM process-microstructure-property-performance relations.

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Title: A New Robust 3D Constitutive Model for the Passive Properties of Left Ventricular Myocardium

Author(s): *David Li, *The University of Texas at Austin*; Reza Avazmohammadi, *The University of Texas at Austin*; Samer Merchant, *University of Utah*; Tomonori Kawamura, *University of Pennsylvania*; Edward Hsu, *University of Utah*; Joseph Gorman, *University of Pennsylvania*; Robert Gorman, *University of Pennsylvania*; Michael Sacks, *The University of Texas at Austin*;

Myocardium exhibits complex behavior that demands a comprehensive 3D constitutive formulation in order for its mechanical properties to be captured in a computational model. Current modeling efforts remain limited in that they are not based on full 3D deformation datasets, do not use optimal loading paths, and have not been able to define the optimal form of the strain energy function and determine its associated material parameters. To this end, we employed a novel numerical-experimental methodology to determine the optimal form of the strain energy function for passive ventricular myocardium. Full 3D structural-mechanical measurements of ovine myocardium specimens were obtained from cuboidal sections cut out from the left ventricles of adult Dorset sheep. Each specimen was subjected to a comprehensive set of 3D loading paths, and the internal fiber structure of each specimen was quantified using diffusion tensor imaging. We then modeled the myocardium as an orthotropic material with material directions f (myofiber), s (sheet or cross-fiber), and n (normal to the fiber-sheet plane), using an initial form by Holzapfel and Ogden [1]. The model was used to fit both a set of six simple shear loading paths, akin to the experiments performed by Dokos et al. [2], and a set of optimally selected paths consisting of simple and pure shear [3], and we determined model parameters using inverse finite element simulations and nonlinear least-squares regression. While the model fit the simple shear paths well, it was unable to fully capture the mechanical anisotropy in the optimal paths. Hypothesizing that the myocardium exhibits further modes of coupling, we determined that additional coupling terms were required by the model in order to fit the optimal paths. Further examination of the model revealed that the optimal paths cause both relative stretching and shearing of fiber, sheet, and normal families in the myocardium, which could be explained by interactions between myofibers and the surrounding collagen matrix. Specifically, the substantial relative shearing drove the need for the extended terms. This extended constitutive model has particular relevance in the simulation of myocardium in non-physiological states like myocardial infarction. Ultimately, development of more robust models in this manner will make them better suited for clinical evaluation and simulating treatment of cardiac diseases. [1] Holzapfel et al., Philos Trans Royal Soc A, 367:3445-3475, 2009. [2] Dokos et al., Am J Physiol Heart Circ Physiol, 283:H2650-9, 2002. [3] Avazmohammadi et al., Biomech Model Mechanobiol, 17:31-53, 2018.

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Title: Explicit Structural Topology Optimization Based on Isogeometric Analysis with Trimming Technique

Author(s): *Dingding Li, *Dalian University of Technology*; Weisheng Zhang, *Dalian University of Technology*; Xu Guo, *Dalian University of Technology*; Sung-Kie Youn, *Korea Advanced Institute of Science and Technology*;

Abstract: Traditionally, structural topology optimization problems are often solved by adopting implicit geometry representation model and finite element method (FEM) on fixed mesh. This may lead to the inherent inconsistency among the geometric model, analysis model and CAD model. In order to resolve the aforementioned issues straightforwardly, in the present work, we propose an explicit structural topology optimization approach integrating the Moving Morphable Void (MMV)-based topology optimization method and Isogeometric analysis (IGA) with trimming technique. By means of the proposed approach, it inherits the advantages of IGA and the explicit structural topology description can be link with CAD systems seamless, leading to closer integration of topology design and analysis. Numerical examples provided demonstrate the effectiveness of the proposed approach. References: [1] X. Guo, W.S. Zhang, W.L. Zhong, Doing Topology Optimization Explicitly and Geometrically—A New Moving Morphable Components Based Framework, J. Appl. Mech. 81 (8) (2014) 081009. [2] H.-J. Kim, Y.-D. Seo, S.-K. Youn, Isogeometric analysis for trimmed CAD surfaces, Comput. Methods Appl. Mech. Eng. 198 (37–40) (2009) 2982–2995. [3] W.S. Zhang, J. Yuan, J. Zhang, X. Guo, A new topology optimization approach based on Moving Morphable Components (MMC) and the ersatz material model, Struct. Multidiscip. Optim. 53 (6) (2016) 1243–1260.

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Title: Non-Intrusive Coupling of Abaqus and a 3-D Scale-Bridging Generalized Finite Element Method

Author(s): *Haoyang Li, *University of Illinois at Urbana-Champaign*; Patrick O'Hara, *AFRL/RQHF Structural Sciences Center*; Travis Fillmore, *The U.S. Army Corps of Engineers ERDC-CHL*; C. Armando Duarte, *University of Illinois at Urbana-Champaign*;

In many engineering applications, it is necessary to account for interactions among multiple spatial scales through numerical simulations. Resolving fine-scale features such as cracks and localized nonlinearities with high fidelity is critical for the accurate prediction of service life or failure of structures. Three-dimensional models with detailed meshes and advanced modeling techniques are usually required to capture accurate fine-scale responses. However, adopting such models on the structural/global-scale is computationally inefficient and sometimes unfeasible for problems involving a large number of local features. A coarse mesh is often sufficient for predicting the global behavior of a structure. In this talk, we present a multi-scale computational framework that couples Abaqus models and 3-D Generalized FEM discretizations based on numerically-defined enrichment functions – the GFEMgl. The structural-scale problem is modeled in Abaqus using a coarse mesh of 3D or shell elements suitable for capturing the macro-scale response of the structure. Fine-scale problems solved in parallel provide enrichment functions for the GFEMgl. These functions enable the GFEMgl to accurately approximate localized phenomena using coarse meshes. The interactions between structural (Abaqus) and GFEMgl models are captured using the Iterative Global-Local method (IGL). In this method, global-scale displacements are passed to GFEMgl models as boundary conditions while residual forces along the interface between the two models are applied to the structural model. The proposed multiscale framework is non-intrusive in the sense that only standard output quantities from the finite element simulations are exchanged during the coupling process. The interaction between Abaqus and the GFEMgl solver requires no knowledge of the discretization technique adopted in the other solver. Furthermore, the GFEMgl models can be nonlinear while the Abaqus model remains linear. Numerical examples of a hat-stiffened panel with a large number of spot welds and a T-joint structure subjected to fatigue crack propagation are presented to demonstrate the accuracy and applicability of the proposed framework.

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Title: Clustering Discretization Methods for Generation of Material Performance Databases in Machine Learning and Design Optimization

Author(s): Wing Kam Liu, *Northwestern University*; *Hengyang Li, *Northwestern University*; Cheng Yu, *Northwestern University*; Orion Kafka, *Northwestern University*;

This talk introduces the recently developed Self-Consistent Clustering Analysis (SCA), a reduce order method, to compute the mechanical performance of materials based on representative volume elements (RVEs) accounting for microstructure [1-5]. This belongs to a class of data-driven clustering discretization methods, designed to provide vast speedup compared to equivalent Finite element methods (FEM) or Fast Fourier Transform (FFT) solutions, especially in cases where multiple load cases of the same microstructure are to be conducted. SCA consists of two steps: offline and online. In the offline stage, a three-step process involving data collection, domain decomposition, and computation of the interaction tensors is employed. In the online stage, SCA solves a generalized Lippmann-Schwinger equation over the domain by iteratively computing the discrete integral equation to predict mechanical behavior under arbitrary loading cases. If developed carefully, such a database would be suitable for training neural networks; a trained neural network could provide even faster prediction of the overall response of an RVE than the data-driven clustering methods. I will explain the concept behind this, and outline the benefits and applications of two different neural networks that could be trained on data from these reduced order models. These would be able to solve large design problems relatively quickly, or may be fast enough for use as part of controls schemes. Applications to advanced and additive manufacturing will be presented. References: 1. Zeliang Liu, M.A. Bessa, Wing Kam Liu, “Self-consistent clustering analysis: An efficient multi-scale scheme for inelastic heterogeneous materials,” Comput. Methods Appl. Mech. Engrg. 306 (2016) 319–341. 2. W. Yan, OL. Kafka, J. Yan, S. Wolff, E. Agbor, M. Mozaffar, K. Ehmann, Jian Cao, GJ. Wagner, WK. Liu, “Data-driven multi-scale multi-physics models to derive process–structure–property relationships for additive manufacturing’” Computational Mechanics, 61(5), 521-541, 2018. 3. M.A. Bessa, R. Bostanabad, Z. Liu, A. Hu, Daniel W. Apley, C. Brinson, W. Chen, Wing Kam Liu, “A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality,” Comput. Methods Appl. Mech. Engrg. 320 (2017) 633–667. 4. M. Shakoor, O.L. Kafka, C. Yu, and W.K. Liu, “Data science for finite strain mechanical science of ductile materials,” Computational Mechanics, 2018. 5. Bostanabad, R., Zhang, Y., Li, X., Kearney, T., Brinson, CL., Apley, D.W., Liu, W.K., Chen, W., Computational Microstructure Characterization and Reconstruction: Review of the State-of-the-art Techniques, Progress in Materials Science, 95, 1–41 (2018).

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Title: Superconvergence Analysis of High-order Edge Elements with Applications to Maxwell's Equations

Author(s): *Jichun Li, *University of Nevada Las Vegas*; Yunqing Huang, *Xiangtan University*;

Since early 1970s, the superconvergence study of finite element methods has been a very active research topic due to its applications in leading to more efficient numerical methods for solving various differential equations. Many excellent superconvergence results have been obtained for elliptic equations, parabolic equations and linear hyperbolic equations. For Maxwell's equations, the first superconvergence result was derived in 1994. Since then, some results have been obtained. But there are many unsolved problems. In this talk, I'll present our recent breakthrough result obtained for both the second and third order edge elements. Theoretical analysis and numerical results will be presented. I will conclude the talk with some open issues. Main references: 1. J. Li and Y. Huang, “Time-Domain Finite Element Methods for Maxwell's Equations in Metamaterials”, Springer Series in Computational Mathematics, vol.43, Springer, 2013. 2. M. Sun, J. Li, P. Wang and Z. Zhang, Superconvergence analysis of high-order rectangular edge elements for time-harmonic Maxwell's equations, Journal of Scientific Computing 75(1) (2018) 510-535. 3. Y. Huang, J. Li and C. Wu, Superconvergence analysis of second and third order rectangular edge elements with applications to Maxwell's equations, Computer Methods in Applied Mechanics and Engineering 329 (2018) 195-218. 4. Y. Huang, J. Li and Q. Lin, Superconvergence analysis for time-dependent Maxwell’s equations in metamaterials, Numerical Methods for Partial Differential Equations 28 (2012) 1794-1816. 5. Y. Huang, J. Li, W. Yang and S. Sun, Superconvergence of mixed finite element approximations to 3-D Maxwell's equations in metamaterials, Journal of Computational Physics 230 (2011) 8275–8289.

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Title: Quantum Couple Stress and Quantum Flexoelectricity

Author(s): *Jun Li, *Wuhan University of Technology*; Lisheng Liu, *Wuhan University of Technology*; Shaofan Li, *University of California-Berkeley*;

In this work, we have developed a novel quantum couple stress theory and derived its quantum mechanical formulations in the framework of density functional theory. Formal expressions of quantum couple stresses are derived in relation to total quantum energy and curvatures. Lattice curvature may cause a redistribution of charge density, inducing net dipole moments and hence flexoelectricity coupling, which may be regarded as quantum flexoelectricity. This theory provides physical insights on higher order stress state of nanostructures under nonuniform strain distributions, and it can then be used to explore the related physical mechanisms, such as flexoelectricity. We have applied the theory of quantum couple stress to study a nanoscale dielectric beam to demonstrate the effect of quantum flexoelectricity, and we calculated the flexoelectric coefficients for a variety of dielectric materials, including piezoelectric materials. The flexoelectric coefficients is critical for both application of flexoelectricity as well as developing novel flexoelectric materials. We expect that the quantum couple stress theory developed here can provide a systematic analytical tool to explore the origin of high order stress state for nanostructures and to determine the flexoelectric coefficients for different materials, especially for piezoelectric materials, so that it then can be used to design and make novel functional electromechanical nanodevices.

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Title: Modeling Fracture of 3D Printed Polymers for Enhanced Performance

Author(s): *Jun Li, *University of Massachusetts Dartmouth*;

Additive manufacturing (or 3D printing) is being increasingly used in a wide range of areas including aerospace, mechanical, civil and biomedical engineering where it offers significant advantages for model prototyping. However, the reduced fracture performance often observed in 3D printed materials limits its application to end-user load-bearing components. A combination of computational and experimental investigation is performed to study 3D printed materials with various build orientations for enhanced fracture properties, including single edge notched tension (SENT) and bending (SENB) specimens made of acrylonitrile-butadiene-styrene (ABS) polymers by fused filament fabrication. The measured fracture properties were found to highly depend on layer/filament orientations and crack kinking was observed to often follow the weak planes along those directions. The extended finite element method (XFEM) using cohesive zone approach with anisotropic damage initiation and evolution criteria has been developed to capture the results measured in experiments. Numerical parametric studies further show that the inter-layer and inter-filament bonding strength could be tuned to create alternate crack paths for maximum fracture energy. Finally, toughening mechanisms using 3D printed topological patterns on the surface to deflect crack paths are explored. This study sheds light on predicting fracture of 3D printed materials for enhanced performance.

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Title: The Shifted Interface Method: A Flexible Approach to Embedded Interface Computations

Author(s): *Kangan Li, *Duke University*; Nabil Atallah, *Duke University*; Alex Main, *Duke University*; Guglielmo Scovazzi, *Duke University*;

We propose a new finite element method for embedded interface computations, which falls in the category of surrogate/approximate interface algorithms. The key idea of this method is shifting the location where interface jump conditions are applied from the true interface to a surrogate interface. In order to preserve optimal convergence rates of the numerical solution, the jump conditions will be appropriately modified on the surrogate interface. This method is simple, robust, and e■cient, as it avoids the presence of cut cells in computations. We apply this new concept to the Poisson operator in mixed form, that is the Darcy flow operator, and we demonstrate its qualities with an extensive set of numerical tests.

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Title: Design of Architected Materials Using Multiscale Level Set Topology Optimization

Author(s): *Lei Li, *University of California, San Diego*; Zongliang Du, *University of California, San Diego*; Hyunsun Kim, *University of California, San Diego*;

The rapidly developing additive manufacturing (AM) techniques enable the fabrication of topologically optimized porous architected materials with an unprecedented geometrical complexity, which in turn, attracts an increasing attention to the design of periodic microstructural patterns using topology optimization. Currently, most of the relevant studies have been focusing on the designs of architected material tailored to the extremum or target effective properties, e.g. maximum constitutive stiffness, negative Poisson's ratio, negative thermal expansion, and many others. However, it is not always known a priori, what property would offer the optimum performance when designed into a structure. Studies have shown that the extremum properties may not induce the optimum structural performance for the given design environment. The optimum structural performance can be achieved via a combination of multiple architected materials and their optimum properties are dependent on the overall structural design. This study investigates such material design problems with multiscale topology optimization with the level set method. Several numerical investigations and the corresponding optimum material designs will be discussed. It will also show that the proposed method is able to design arbitrary number of unit cells within the macroscopic design domain by optimizing only one objective function on the macroscale, thus tailoring the designed material for different design regions.

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Title: Recent Developments in Isogeometric Analysis with Solid Elements in LS-DYNA

Author(s): *Liping Li, *LSTC (Livermore Software Technology Corp.)*; David Benson, *LSTC (Livermore Software Technology Corp.)*; Attila Nagy, *LSTC (Livermore Software Technology Corp.)*; Marco Pigazzini, *LSTC (Livermore Software Technology Corp.)*; Stefan Hartmann, *Dynamore*;

Isogeometric analysis (IGA) has advanced rapidly with the increasing effort by computational scientists from both academia and industry particularly in the past decade. One of the basic functions needed in IGA is the modeling of 3D solid elements. However, the representations of solid structures in modern computer-aided design (CAD) are the collections of surfaces, and thus constructing the splines for solids is not straightforward. This talk is focused on the recent development of IGA solid analysis in LS-DYNA, using the input format of Non-Uniform Rational B-Spline (NURBS) and Bezier extraction. NURBS input for IGA in LS-DYNA was developed first due to its simplicity for computational analysis of surfaces, and has since been extended to solids. To accommodate more complicated industrial models, a Bezier extraction input format has also been added to LS-DYNA. Examples of analyzing complex structures demonstrate the potential of IGA in realistic applications.

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Title: Modeling and Simulation of Rotation of a Crawling Cell

Author(s): *Shaofan Li, *University of California-Berkeley*; Xin Lai, *University of California-Berkeley*;

Quantitative modeling of cell motility is a challenge. In particular, it is difficult to simulate rotation of a crawling cell. Spatially controlled polymerization of actin is at the origin of cell motility and is responsible for the formation of cellular protrusions like lamellipodia. In the talk, we shall present a recent developed soft matter mechanics model of eukryotic cells, or an aggregate of actin filament, which can model the actin-based cell motility. In particular, we shall use this model to simulate to simulate the substrate-based cell rotation and protrusive crawling.

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Title: Isogeometric Analysis Based on Hybrid Non-uniform Recursive Subdivision

Author(s): *Xin Li, *USTC*; Xiaodong Wei, *EPFL*; Yongjie Zhang, *CMU*;

This talk introduces a new non-uniform subdivision surface representation, called hybrid non-uniform subdivision surface (for short, HNUSS). The subdivision scheme is constructed through two steps. The rst step inserts a set of edges and converts a valence-n extraordinary point into a valence-n face. The second step combines both primal and dual subdivision schemes to de fine the subdivision rules. The developed subdivision scheme generalizes bi-cubic NURBS to arbitrary topology and is proved to be G1-continuous for any valence extraordinary points and any non-negative knot intervals. The HNUSS limit surface has comparable shape quality as non-uniform subdivision via eigen-polyhedron [1] and has better shape quality than all the other subdivision schemes. In addition, HNUSS based isogeometric analysis yields improved convergence rates compared to any existing non-uniform subdivision schemes.

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Title: Investigation of Dispersion Relation of the 1D Coupling of the Nonlocal and Local Mechanics

Author(s): *Xingjie Helen Li, *University of North Carolina Charlotte*; Pablo Seleson, *Oak Ridge National Lab*; Kelsey Wells, *University of Nebraska-Lincoln*; Hayden Pecoraro, *University of North Carolina Charlotte*;

In this talk, we explore the dispersion relations of two consistent nonlocal-to-local coupling methods in 1D: (1) the quasi-nonlocal coupling and (2) the force-based coupling. We propose a finite difference numerical method for the spatial and temporal discretizations, and study the dispersion relation on both continuous and discrete settings. Both coupling methods are rigorously proved that the imaginary parts of their dispersion relations on the transitional region are of first order of horizon size, whereas most other existing coupling methods are at most of order of one over horizon size. In addition, we numerically showed that the imaginary part of dispersion relation of the force-based coupling is smaller than that of the quasi-nonlocal coupling, which suggests that wave amplitude are preserved better in the force-based coupling. Several numerical tests are performed to confirm the theoretical findings.

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Title: Coarse-graining of Overdamped Langevin Dynamics via the Mori-Zwanzig Formalism

Author(s): Thomas Hudson, *University of Warwick, UK*; *Xingjie Helen Li, *University of North Carolina, Charlotte*;

The Mori-Zwanzig formalism is applied to derive an equation for the evolution of linear observables of the overdamped Langevin equation. To illustrate the resulting equation and its use in deriving approximate models, a particular benchmark example is studied both numerically and via a formal asymptotic expansion. The example considered demonstrates the importance of memory effects in determining the correct temporal behavior of such systems.

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Title: Membrane Wrapping Efficiency of Elastic Nanoparticles during Endocytosis: Size and Shape Matter

Author(s): *Ying Li, *University of Connecticut*;

Using coarse-grained molecular dynamics simulations, we systematically investigate the receptor-mediated endocytosis of elastic nanoparticles (NPs) with different sizes, ranging from 25 to 100 nm, and shapes, including sphere-like, oblate-like, and prolate-like. Simulation results provide clear evidence that the membrane wrapping efficiency of NPs during endocytosis is a result of competition between receptor diffusion kinetics and thermodynamic driving force. The receptor diffusion kinetics refer to the kinetics of receptor recruitment that are affected by the contact edge length between the NP and membrane. The thermodynamic driving force represents the amount of required free energy to drive NPs into a cell. Under the volume constraint of elastic NPs, the soft spherical NPs are found to have similar contact edge lengths to rigid ones and to less efficiently be fully wrapped due to their elastic deformation. Moreover, the difference in wrapping efficiency between soft and rigid spherical NPs increases with their sizes, due to the increment of their elastic energy change. Furthermore, because of its prominent large contact edge length, the oblate ellipsoid is found to be the least sensitive geometry to the variation in NP's elasticity among the spherical, prolate, and oblate shapes during the membrane wrapping. In addition, simulation results indicate that conflicting experimental observations on the efficiency of cellular uptake of elastic NPs could be caused by their different mechanical properties. Our simulations provide a detailed mechanistic understanding about the influence of NPs' size, shape, and elasticity on their membrane wrapping efficiency, which serves as a rational guidance for the design of NP-based drug carriers.

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Title: Vehicular Impact Analysis and Safety Evaluation of Clustered Mailboxes

Author(s): *Zheng Li, *The University of North Carolina at Charlotte*; Emre Palta, *The University of North Carolina at Charlotte*; Joshua Fatoki, *The University of North Carolina at Charlotte*; Howie Fang, *The University of North Carolina at Charlotte*;

Roadside utilities structures such as clustered mailboxes and bus shelters are increasingly used with the rapid development and urbanization of large cities. Vehicular impacts into these utilities structures could results in severe injuries to the occupants and adjacent pedestrians in addition to damages to the striking vehicles and economic loss. In this study, vehicular impacts on clustered mailboxes are conducted using finite element (FE) modeling and simulation. The test vehicles used in this study, i.e., a small passenger car and a pickup truck, are in compliance with the Manual for Assessing Safety Hardware (MASH). Different impact speeds and impact angles are considered for both test vehicles. A Hybrid III crash test dummy is also used in the FE models to directly obtain occupant responses. The results of this research could provide insights into vehicular responses and potential occupant risk in the impacts of clustered mailboxes. The results could also shed light on transportation safety enhancement and future guideline developments regarding the design or installation of roadside utilities structures.

15th U.S. National Congress on Computational Mechanics
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Title: Simulations of Turbulent Flows over Periodic Hill with Multiple-Relaxation-Time Lattice Boltzmann Method on Multi-GPU Cluster

Author(s): Xiao-Ying Huang, *National Tsing Hua University*; Chi-Wei Su, *National Tsing Hua University*; Wei-Jie Lin, *National Tsing Hua University*; *Chao-An Lin, *National Tsing Hua University*;

Turbulent channel flows over periodic hill were simulated with multiple-relaxation-time lattice Boltzmann method at a wide range of Reynolds numbers. The simulation was conducted on multi-GPU cluster with two-dimensional domain decomposition using message passing interface (MPI). The pressure-driven flow was simulated by adding an external force to the flow field in the streamwise direction and the curved boundary was mimicked by a modified bounce back formulation. The results were compared with simulations from Breuer et al. [1]. [1] Breuer, M., Peller, N., Rapp, C. & Manhart, M. Flow over periodic hills-numerical and experimental study in a wide range of Reynolds numbers. Computers & Fluids, 2009, 38, 433-457

15th U.S. National Congress on Computational Mechanics
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Title: Micromechanics Modeling of Multiferroic Particulate Composites

Author(s): You-shu Zhan, *National Cheung Kung University*; *Chien-hong Lin, *National Cheung Kung University*;

Multiferroic composites are used in many technological application such as actuators, energy harvesters, and so on. Previous studies have generally considered the linear effective response exhibited by such composites under small electric driving fields. However, under practical application, multiferroic particle-reinforced composites are often subjected to large electric driving fields, which induces nonlinear behavior rather than linear response. Thus, this study proposes a simplified unit-cell model to predict the nonlinear behavior of multiferroic composites. In order to obtain the overall nonlinear response, the linearized micromechanical relations are introduced for providing trial solution following an iterative scheme to minimize the error resulted from linearization. In addition, the result from Mori-Tanaka approximation and experimental data from available literatures are both provided for the purpose of comparison. Parametric study is also conducted in order to examine the effect of the different constituent and loading condition on the overall responses of the multiferroic composites. The results show significantly different responses between linear and nonlinear effective responses. In conclusion, it is necessary to study the nonlinear effects of smart materials prior to designing those active devices which consists of multiferroic composites.

15th U.S. National Congress on Computational Mechanics
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Title: Study on the Morphological Features of the Melt Track of the Mesoscopic Simulation for Electron Beam Powder Bed Fusion

Author(s): *Feng Lin, *Tsinghua University*; Ya Qian, *Tsinghua University*; Wentao Yan, *National University of Singapore*;

In the electron beam powder bed fusion process, the quality of each deposited melt track is significant to the properties of manufactured parts. However, the formation of melt tracks influenced by various physical phenomena and process parameters, among which the correlation is complicated and difficult to be established via experiments. Currently, mesoscopic modeling technique has been introduced to simulate the EB melting process efficiently and reveal detail of the melt track formation, but the results are not able to link the process parameters to the feature of melt track quantitatively. This presentation will present the resent study on the morphological features of the melt track from mesoscopic simulation results. Some key descriptive indexes are introduced, like melt track width and height, to assess the deposition quality numerically. Furthermore, the effects of various processing parameters are investigated through mesoscopic simulations in combination with the introduced indexes quantitatively. In this way, the correlation between processing conditions and melt track feature is derived. Finally, a simulation-driven optimization framework consisting of mesoscopic modeling and data mining is proposed, and its potentials and limitations are discussed.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Naturally Stabilized Nodal Integration for Meshfree Methods in Thermoelasticity

Author(s): *Kuan-Chung Lin, *The Pennsylvania State University*; Michael Hillman, *The Pennsylvania State University*;

In simulation of natural materials such as metals, the mechanical response is often assumed to be uncoupled from its temperature response due to the fact that the ratio of parameters controlling thermomechanical coupling is sufficiently small [1]. However, when the ratio is large, such as in many man-made materials, the temperature variation caused by mechanical deformation could have significant influence on the solution, and a fully coupled system should be considered. In this work, a meshfree approach for solving the governing equations for the fully coupled theory of thermoelasticity is developed. In order to obtain an effective meshfree solution, accurate, low order quadrature is desired, such as a stabilized and corrected nodal integration. To this end, a naturally stabilized nodal integration [2] is proposed for thermoelasticity to provide a stable nodal integration technique for this problem. Several benchmark problems solved to demonstrate the effectiveness of the proposed method for fully coupled thermoelasticity problems. References [1] Boley, B.A., Weiner, J.H., 1960. Theory of Thermal Stresses. Wiley, New York. [2] Hillman, Michael, Chen, J. S., 2016. An accelerated, convergent, and stable nodal integration in Galerkin meshfree methods for linear and nonlinear mechanics. International Journal for Numerical Methods in Engineering, 107(7), 603-630.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Strain Induced Crystallization and Fracture of Rubber-like Materials

Author(s): *Christian Linder, *Stanford University*; Prajwal Arunachala, *Stanford University*; Reza Rastak, *Stanford University*;

A multi-scale polymer network model is proposed for strain-induced crystallization phenomena in rubber-like materials \cite{rr+cl} and extended to account for phase field fracture. At the microscopic scale, the thermodynamic behavior of a polymer chain inside a stretching polymer network and its crystallization is studied and a new polymer chain model is presented. The chain model accounts for the thermodynamics of crystallization and presents a rate-dependent evolution law for crystallization based on the gradient of the free energy with respect to the crystallinity variable to ensure the dissipation is always non-negative. The multiscale framework allows anisotropic crystallization of rubber which has been observed experimentally. Two different approaches for formulating the orientational distribution of crystallinity are studied. For the discrete distribution, crystallization is tracked at a finite number of orientations. On the other hand, the continuous distribution captures the anisotropic behavior with only a few distribution parameters. To connect the deformation of the micro with the macro scale, the recently developed maximal advance path constraint is combined with the principle of minimum free energy, resulting in a non-affine deformation model for polymer chains. The model is then combined with a phase field approach to fracture. Various aspects of the proposed model are validated by existing experimental results, including the stress response, crystallinity evolution, crystallinity distribution, the rotation of the principle crystallization direction, and the effect on the fracture behavior of rubber-like materials.

15th U.S. National Congress on Computational Mechanics
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Title: Bridging Elements for Properties of Low Alloy Steels

Author(s): *Lars-Erik Lindgren, *Luleå University of Technology*;

Simulation of coupled thermo-mechanical processes like additive manufacturing requires at least constitutive models accounting for the temperature dependency. Further complications arise in the presence of microstructural changes. Low alloy steels are a typical case where phases and micro-constituents like ferrite, austenite, pearlite, bainite and martensite exist. The talk will describe models for thermal and mechanical properties of low alloy steels that accounts for chemistry, microstructure and temperature. Transport properties, like heat conduction and plasticity, are more sensitive to details in the material structure than storage properties like heat capacity and elasticity. The models account for the physics on the small scales and the used variables are physical variables, i.e. variables that can be measured. The models can be considered as bridging elements coupling material chemistry and structure to properties. These models are one step towards the vision of ICME. The models are based on internal state variables where each point in the numerical model is a representative volume with microstructure. Therefore, it is not necessary to resolve the microstructure spatially by the FE mesh. Some simple example illustrating the models will also be presented.

15th U.S. National Congress on Computational Mechanics
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Title: Comparison of Stratum Corneum Failure Mechanics at the Macro- and Micro-scale

Author(s): *Zachary Lipsky, *Binghamton University*; Guy German, *Binghamton University*;

Biological tissues are heterogenous mosaics at cellular and sub-cellular length scales. Some tissues, like the outermost layer of human skin, or stratum corneum (SC), also exhibits a rich topography at larger length scales[1], which further contributes to the heterogeneity. While this is well recognized, contemporary studies continue to characterize the global mechanical properties of biological tissues by assuming they are a homogenous material. We anticipate that local topographical features play an important role in defining the global mechanical response of the SC. This is a familiar concept from basic mechanics—where it is well known that the global failure of a material can be determined by the concentration of stress around defects, which for example, can nucleate cracks. To interpret the influence that heterogeneities have on the global failure mechanics of tissue, the microscale energy cost of creating new crack interfaces are compared with the macroscale work of fracture. This is accomplished using traction force microscopy (TFM)[2]. Circular samples of isolated SC tissue are adhered to a thin PDMS membrane upon which fluorescent beads are chemically bonded. Substrates are radially strained to induce fracture. Bead displacements surrounding propagating crack tips are then tracked using fluorescent high-speed macrophotography. Tracked bead profiles from sequential images are used to establish the total strain energy released due to the incremental crack propagation, and the surface energy of the newly created crack interface[3]. This energy cost per unit length is then compared with the macroscale work of tissue fracture scaled by the total crack length, established from conventional uniaxial tensometry. These comparisons aim to evaluate the validity of the prevailing paradigm that macroscopic testing techniques can provide meaningful information about the energy cost of fracture in soft tissues. [1] Schellander, F. A. & Headington, J. T. The stratum corneum—some structural and functional correlates. Br. J. Dermatol. 91, 507–515 (1974). [2] Style, R. W. et al. Traction force microscopy in physics and biology. Soft Matter 10, (2014). [3] Irwin, G. R. Analysis of stresses and strains near the end of a crack traversing a plate. J. appl. Mech. (1957).

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Free Fracture Propagation Using State Based Peridynamics

Author(s): Prashant Jha, *Lousiana State University*; *Robert Lipton, *Louisiana State University*;

We introduce a state based peridynamic model for free fracture propagation. Here the peridynamic force includes both tensile and hydrostatic components. The resulting evolution is shown to be physically well posed. The discretization error is found to decrease linearly with the size of time step and mesh size. Here the fracture set is the location in which the nonlocal strain has exceeded critical value for tensile strain. We show that energy balance holds for this evolution and that the fracture set localizes to a surface in the limit of vanishing nonlocality. For displacements away from the fracture set we show that the nonlocal model converges to the linear elastic model. Several numerical examples are presented and analyzed that apply this model to free dynamic fracture evolution for notched and pre-cracked specimens.

15th U.S. National Congress on Computational Mechanics
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Title: A Multi-component Multi-reaction Model for Aluminized Explosives

Author(s): *Shannon Lisenbee, *University of Alabama at Birmingham*; David Littlefield, *University of Alabama at Birmingham*;

Traditional reactionary models for energetic materials generally fell into one of two camps: a single reaction model used for the decomposition of the energetic material or a separate code that computed all of the chemical reactions present in the decomposition process. More recently, a multi-component multi-reaction model that focused on the two main reactions was developed (Asay, et al, 2014): one for the explosive and one for the oxidation of aluminum. Such a model achieved higher accuracy than single reaction models and more computational efficiency than using a separate chemical code. Currently the model uses the excess oxidizers from the explosive to fuel the oxidation reaction of the aluminum but ignores any input from the outside air. This paper demonstrates the implementation of the described model in our own 2D axisymmetric hydrocode and adds in mixing along the explosive product boundary to incorporate contributions from the outside air and measure its effects on the oxidation rate of the aluminum. Asay, et al. (2014). A Multi-component Detonation Reaction Zone Model for Blast Explosives. 15th International Detonation Symposium.

15th U.S. National Congress on Computational Mechanics
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Title: A Contact Model for Multi-material Eulerian Hydrocodes: Extensions for Self-contact

Author(s): *David Littlefield, *The University of Alabama at Birmingham*;

Realistic and accurate modeling of contact for problems involving large deformations and severe distortions presents a host of computational challenges. Due to their natural description of surfaces, Lagrangian finite element methods are traditionally used for problems involving sliding contact. However, problems such as those involving ballistic penetrations, blast-structure interactions, and vehicular crash dynamics, can result in elements developing large aspect ratios, twisting, or even inverting. For this reason, Eulerian methods have become popular. However, additional complexities arise when these methods permit multiple materials to occupy a single finite element. Multi-material Eulerian formulations in computational structural mechanics are traditionally approached using mixed-element thermodynamic and constitutive models. These traditional approaches treat discontinuous pressure and stress fields that exist in elements with material interfaces by using a single approximated pressure and stress field. However, this approximation often has little basis in the physics taking place at the contact boundary and can easily lead to unphysical behavior. In previous work we have presented an approach that is a significant departure from traditional Eulerian contact models by solving the conservation equations separately for each material and then imposing the inequality constraints associated with contact to these solutions. One limitation of the original model was that it could not be applied to ‘self-contact’ scenarios. This occurs, for example, when a thin body folds over and contacts itself. We have generalized our approach in this work, so that it is now applicable to self-contact. Computational examples are shown to demonstrate the veracity of this new development.

15th U.S. National Congress on Computational Mechanics
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Title: Computational Solid Mechanics and Contact on Next-Generation Computing Hardware

Author(s): *David Littlewood, *Sandia National Laboratories*; K. Noel Belcourt, *Sandia National Laboratories*; San Le, *Sandia National Laboratories*; Brian Lester, *Sandia National Laboratories*; Lynn Munday, *Sandia National Laboratories*; J. Antonio Perez, *Sandia National Laboratories*; Patrick Xavier, *Sandia National Laboratories*;

The future of large-scale scientific computation is strongly tied to hardware architectures characterized by hierarchical parallelism. Effective utilization of on-node accelerators, in particular GPUs, requires performance portability across disparate hardware and the ability to manage data over multiple memory spaces. In this presentation, we review an ongoing effort to develop the NimbleSM solid mechanics finite-element code for massively parallel simulations on next-generation supercomputers. Key elements of this work are the adaption of constitutive models within the Library of Advanced Materials for Engineering (LAME) [Littlewood and Tupek, 2017] and the development of contact algorithms capable of utilizing GPU hardware for both search and enforcement. Increased parallelism is achieved using the Kokkos software package [Edwards, Trott, and Sunderland, 2014], which provides a parallel-for mechanism and corresponding data structures that are configured at compile time for optimal performance on the target architecture. An additional concern is future-proofing against the evolving nature of next-generation hardware. This is addressed by encapsulating hardware-specific source code such that it can be altered at a later date without the need for invasive changes to the physics models themselves. Our implementation strategy will be discussed, followed by performance analysis of constitutive models and contact algorithms in the context of explicit transient dynamics. The ability to utilize increased on-node parallelism is shown to be a vital component of next-generation engineering analysis codes, with the potential to enable simulations that have been considered computationally intractable to date. [1] D.J. Littlewood and M.R. Tupek. Adapting material models for improved performance on next-generation hardware. Memorandum SAND2017-11100 O, Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2017. [2] H.C. Edwards, C.R. Trott, and D. Sunderland. Kokkos: Enabling manycore performance portability through polymorphic memory access patterns. Journal of Parallel and Distributed Computing, 74(12), 2014.

15th U.S. National Congress on Computational Mechanics
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Title: Theory, Formulation and Properties Of High Order Smoothed Finite Element Methods

Author(s): *Guirong Liu, *Department of Aerospace Engineering and Engineering Mechanics, University of Cincinnati, USA*;

This talk discusses theory, formulation and properties of high order smoothed finite element methods (high-order S-FEM). In a high-order S-FEM approach, smoothed strains in a smoothing domain are expressed in polynomial functions with linear and high-order terms. In particular, a high order node-based smoothed finite element method (high-order NS-FEM) using triangular elements that can be automatically generated is presented for static, free and forced vibration analyses of solids. We provide first proofs on convergence. Then, versions of high-order NS-FEM and CS-FEM are presented. Numerical results will also be presented to demonstrate the performance and unique properties of these high order modes, including (1) close-to-exact stiffness which is softer than the “over-stiff” FEM and stiffer than the “over-soft” standard NS-FEM using constant smoothed strains; (2) insensitive to mesh distortion; (3) ultra-accuracy in term of displacements; (4) no spurious non-zero energy modes, hence temporally stable and working well for dynamic problems. Keywords: high-order NS-FEM, strain field reconstruction, strain smoothing, close-to-exact, temporally stability. Reference [1] G.R. Liu and S.S. Quek. The finite element method: a practical course. Butterworth Heinemann, Oxford, 2003. [2] J.S. Chen, C.T. Wu, S. Yoon and Y. You. A stabilized conforming nodal integration for Galerkin meshfree method. IJNME. 50:435-466. 2000. [3] G.R. Liu. A generalized gradient smoothing technique and the smoothed bilinear form for Galerkin formulation of a wide class of computational methods. IJCM. 5(2): 199-236. 2008. [4] G.R. Liu, G.Y. Zhang, K.Y. Dai, Y.Y. Wang, Z.H. Zhong, G.Y. Li and X. Han. A linearly conforming point interpolation method (LC-PIM) for 2D mechanics problems. IJCM. 2(4): 645-665. 2005. [5] G.R. Liu and G.Y Zhang. Upper bound solution to elasticity problems: A unique property of the linearly conforming point interpolation method (LC-PIM). IJNME. 74: 1128-1161. 2008. [6] G.R. Liu and N.T. Trung. Smoothed finite element methods. CRC press, 2016. [7] G.R. Liu, T. Nguyen-Thoi and K.Y. Lam. An edge-based smoothed finite element method (ES-FEM) for static, free and forced vibration analyses of solids. JSV. 320:1100-1130. 2009. [8] G.R. Liu and G.Y. Zhang. Smoothed Point Integration Methods: G Space theory and Weakened Weak Forms; WorldScientific, Singapore. [9] G.R. Liu. Meshfree Methods: Moving Beyond the Finite Element Method, 2nd Edition. CRC Press, Boca Raton, 2009. [10] G.R. Liu. A Novel Pick-Out Theory and Technique for Constructing the Smoothed Derivatives of Functions for Numerical Methods, IJCM,15(3). 2018.

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Title: Optimization of Resin Pellet Shape for High Performance LAN Cable Manufacturing in the IoT Era

Author(s): *Jihong Liu, *Daikin Industries, Ltd.*;

The demand for LAN cables is greatly increasing with the rapid progress of IT. LAN cable is made up of electrical wires which are coated with resin. The resin is usually manufactured into pellets of about several millimeters for easy processing. It is sometimes seen that the coating layer on the electrical wires is not uniform. One of the reasons for this is presumed to be that outflow rate of the resin pellets from a hopper of an extruder is not constant and the resin pellets are not stably supplied to the wires during coating process. Although it is empirically known that the shape of resin pellet affects the outflow behavior of the resin pellets from a hopper, theoretical research has not been done. There are two reasons for this. One is that the governing equations of the pellets motion are not yet established theoretically due to the fact that pellets are discrete and interactions between pellets are complicated. Another is that it is difficult to simulate actual phenomenon due to limitations on the scale of analysis model and calculation time. At present, the shape of pellet is determined based on experience and intuition. In order to improve the stability of the coating layer of the electrical wires, it is desired to elucidate influence of pellet shape on its flowability. In this paper, we proposed a simulation approach based on the dynamic explicit finite element method to evaluate the flowability of pellets, which fill into a hopper by free-fall and then flow out from the hopper by gravity. Specifically, first, we verified the simulation results in a small scale analysis model by statistical method to ensure randomness of pellet filling and established a simulation method of pellet flow. Next, we confirmed that we can deduce simulation results in a large scale analysis model from those in a small scale analysis model. Then, using the proposed simulation method, we clarified that the shape of pellet had a large influence on its flowability and found an optimal oblate and prolate spheroid pellet shape respectively that can improve the flowability of pellets in hopper. Finally, we confirmed that the optimal pellet shapes are in dependent of the amount of pellets, kind of material and angle of hopper. It is an interesting phenomenon that optimal oblate and prolate spheroid have a reciprocal relationship between ratios of equatorial diameter and polar diameter respectively.

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Title: A Computational Framework for Vascular Growth and Remodeling

Author(s): *Ju Liu, *Stanford University*; Alison Marsden, *Stanford University*;

The constrained mixture theory has been demonstrated to be a unique tool for describing and predicting diverse vascular conditions. However, most previous investigations are limited to axisymmetric motions and membrane assumptions. To deliver a truly three-dimensional theory, the constrained mixture framework has been generalized with the goal of incorporating multilayered structure and melding with hemodynamics. Parallel to the theoretical development, a suite of algorithms have been developed to handle the challenges of numerical simulations. A novel theoretical foundation based on the Gibbs free energy has been laid to handle the incompressibility constraint and ease the coupling with fluid dynamics [1]. A preconditioning technique based on the nested block factorization has been developed to address the saddle-point nature of the governing equations [2]. A higher-order method based on the isogeometric analysis concept is proposed to provide higher-order accuracy with improved robustness [3]. Since the evolving natural configuration assumption inevitably requires storing a significant amount of historical variables, the proposed higher-order method is demonstrated to be critical for the success of simulating vascular growth and remodeling in three dimensions. Numerical examples will be provided to justify the effectiveness of the proposed methodology. [1] J. Liu and A.L. Marsden. A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction. Computer Methods in Applied Mechanics and Engineering, 337:549--597, 2018. [2] J. Liu and A.L. Marsden. A robust and efficient iterative method for hyper-elastodynamics with nested block preconditioning. Journal of Computational Physics, 2019. [3] J. Liu, A.L. Marsden, and Z. Tao. An energy-stable mixed formulation for isogeometric analysis of incompressible hyper-elastodynamics. International Journal for Numerical Methods in Engineering, In Review.

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Title: A Combined Physical-phenomenological Modeling Methodology for Shape Memory Polymer

Author(s): *Jun Liu, *Institute of High Performance Computing, A*STAR, Singapore*; Choon Chiang Foo, *Institute of High Performance Computing, A*STAR, Singapore*; Tianfu Guo, *Institute of High Performance Computing, A*STAR, Singapore*;

Shape memory polymers (SMP) have attracted many research interests in recent decades. They are polymeric smart materials that can change back to their original morphology through an external actuation, such as temperature or light. Compared with their alloy counterpart such as shape memory alloys, they generally exhibit large deformation capability, lightweight property, and require small amount of actuation energy. These properties make them a good candidate in a wide range of applications, such as biomedical device, flexible electronics, and aerospace applications. However, the small actuation force and strength restricts the application as a structural component. In order to best utilize this material in real industry applications, a simulation model is always demanded to better understand, optimize, and predict the mechanical behavior of this material. However, because of its intrinsic highly non-linear property, developing a suitable and useful constitutive model is not trivial. Many simulation tools have been developed by researchers these years and good correlations with experiments have been observed. However, these models are either too simple to be useful in a real 3D large deformation application, or very complex that makes parameter calibration onerous. In this work, we developed a combined physical-phenomenological constitutive model to solve this difficulty. The physical part of this model can best fit the physical nature of the SMP material, such that it obeys basic thermodynamics laws and material microstructure evolution, while the phenomenological part is adopted to eliminate overly-detailed mechanisms and greatly reduce the number of fitting material parameters. The model should minimize the number of material parameters required for calibration, while capturing the material behavior at finite strain condition in a wide range of operating temperatures. A comprehensive application of this model in a finite element software is also illustrated.

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Title: The Multiscale Coupling Model between Lithium Ion Diffusion and Stress in Polycrystalline Electrodes

Author(s): *Lisheng Liu, *Wuhan University of Technology*; Li Chen, *Wuhan University of Technology*; Jun Li, *Wuhan University of Technology*; Qiwen Liu, *Wuhan University of Technology*;

Lithium-ion batteries have attracted much attention due to their high energy density and light weight, as a rechargeable battery, it works with diffusion of lithium ions between the positive and negative electrodes. The resulting stress can cause cracking and failure of the material, which threatens the safety of the battery and also causes loss of its capacity. Under this background, an atomistic-based multiscale interphase finite element model is proposed to simulate the diffusion--mechanics coupling behavior in electrode of Polycrystalline lithium batteries, in which a finite deformation stress-dependent chemical potential and simplified boundary conditions are considered for the derivation of diffusion equation and the Cauchy-born rule is used to bridge the mechanical behavior between atomic scale to mesoscale, so that the calculations for deformation and diffusion are coupled by combining the chemical energy with the strain energy. In this work, the concentration and stress evolution caused by lithium ion intercalation in the electrode film material are calculated, the precrack and grain boundary are also considered. the Voronoi tessellations is used to generate randomly shaped polycrystalline grain and the multiscale interphase model is used to simulate the diffusion in grain and the cohesive zone element to simulate the grain boundary. With the atomistic information, the mesoscale constitutive relations and physical properties of materials are enriched by CB rule. So the damage and fracture process when electrode is woking can be better captured, as well as the stress and lithium concentration variation in this process. With the newly coupled approach, a realistic expansion process of electrode in lithium-ion battery is simulated. Key words: Lithium-ion battery ; Diffusion-mechanics coupling; Multiscale interphase finite element; Polycrystalline; Cauchy born rule [1] Liu L, Li S. A Finite Temperature Multiscale Interphase Zone Model and Simulations of Fracture[J]. Journal of Engineering Materials & Technology, 2012, 134(3): 031014. [2] Qian J, Li S. Application of Multiscale Cohesive Zone Model to Simulate Fracture in Polycrystalline Solids[J]. Journal of Engineering Materials & Technology, 2011, 133(1): 839-858. [3] Cui Z, Gao F, Qu J. A finite deformation stress-dependent chemical potential and its applications to lithium ion batteries[J]. Journal of the Mechanics & Physics of Solids, 2012, 60(7): 1280-1295. [4] Zuo P, Zhao Y P. A phase field model coupling lithium diffusion and stress evolution with crack propagation and application in lithium ion batteries[J]. Physical Chemistry Chemical Physics Pccp, 2014, 17(1): 287-297.

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Title: Coupling Analysis of Ablation and Temperature Field of C/C Composite Based on Peridynamics Theory

Author(s): *Qiwen Liu, *Wuhan University of Technology*; Mingwei Chen, *Wuhan University of Technology*; Yang Tan, *Wuhan University of Technology*;

Carbon/carbon composite is a new composite of carbon fiber reinforced with carbon matrix. The aerospace use it as ablative material widely. Under thermo-chemical ablation, carbon/carbon composite reacts chemically with the atmosphere, which causes a loss of mass, takes away a large amount of heat, thus prevents high temperature from damaging internal structural components. Thermo-chemical ablation of carbon/carbon composite is a typically nonlinear and discontinuous problem. Different from the singularity of traditional partial differential equations on discontinuous boundaries, the peridynamics avoids this problem by using integral-differential equations, which can be used to describe the movement problem of the ablation interface without introducing other complicated decision conditions. The ablation performance of C/C composites under the coupling of thermo-chemical ablation and temperature field is analyzed by peridynamics simulation of the loss of C/C composite mass and the boundary movement process of the structure with the thermo-chemical ablation.

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Title: A Non-Ordinary State-Based Peridynamic Method to Model Elastic-Plastic Behavior of Ice

Author(s): *Renwei Liu, *Harbin Engineering University*; Yanzhuo Xue, *Harbin Engineering University*; Shaofan Li, *University of California, Berkeley*;

An elastic-plastic constitutive model for ice is investigated with non-ordinary state-based peridynamics. The deformation gradient is decomposed into two components, i.e. elastic deformation gradient and plastic deformation gradient using multiplicative decomposition. In the proposed constitutive model the elastic response of ice is based on a hyperelastic model assuming a nonlinear elastic response of ice. In order to incorporate this strain rate effect in the present model, the equations of damage criterion and damage evolution laws were improved by introducing dynamic factor and delay effect in the model, which can also indicate that there is dependency of yield stress on the strain rate applied and the strain hardening in the plastic region. Numerical simulations about uniaxial tension and compression, as well as biaxial loading, and un-notched and notched three-point bend tests are conducted to validate the performance of the work. In order to study the rate effect on the stress–strain response, the uniaxial compressive and tensile loading are repeated for a range of strain rate values.

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Title: Simulation of Fracture Propagation in Soft Rocks Using Broken Elements

Author(s): *Ruijie Liu, *UTSA*;

Modeling of fluid-driven fracture propagation in brittle permeable porous media has gained a significant progress by adopting cohesive zone elements (CZM) or cohesive zone-based XFEM methods. However, it is time consuming to construct CZM elements in practical applications. On the other hand, few successful stories about CZM-based methods have been reported in modeling fracture propagation in soft rocks where plastic deformation occurs. This talk focuses on applying discontinuous Galerkin (DG) elements to model crack initiation and propagation in soft rocks with plastic deformation. From the computer implementation point of view, construction of DG elements for fracturing is much easier than creation of cohesive zone elements. More importantly, the instability issue from CZM-based methods due to crack opening in plastic media is much avoided in the proposed DG method. A numerical example will be presented to demonstrate the performance and the capability of DG elements in modeling fracture in soft rocks.

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Title: Machine Learning Data-driven Discretization Theories, Modeling and Applications

Author(s): *Wing Kam Liu, *Northwestern University*;

Direct representation of material microstructure in a macroscale simulation is prohibitively expensive, if even possible, with current methods. However, the information contained in such a representation is highly desirable for tasks such as topology optimization, material/alloy design, and manufacturing process control. Thus, our goal is a method that can capture all the material scales relevant to predict mechanical response and enable the systematic development of new materials. To do this, a mechanistic machine learning framework for the mechanical science of materials is developed for fast multiscale analysis of material response and structure performance. The new capabilities provided by the proposed framework stem from three major factors: (1) the use of an unsupervised learning-based discretization method to achieve significant order reduction at both macroscale and microscale, resulting in material points that each represent a carefully constructed region within the domain; (2) the generation of a database of interaction tensors among these material regions; (3) concurrent macroscale and microscale response prediction based on a supervised learning algorithm to solve the mechanistic equations. These three factors allow for an orders-of-magnitude decrease in the computational expense involved in predictions that capture all scales of interest to mechanical response when compared to direct numerical simulation or schemes such as FE^2. This method provides sufficiently high fidelity and speed to reasonably conduct inverse modeling for, e.g., material design and manufacturing process control.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Molecular and Dislocation Dynamics Simulations of Dislocation Motions in Graphene Reinforced Aluminum Composites

Author(s): *Xia Liu, *Beijing University of Technology*; Xiaohuan Zhou, *Beijing University of Technology*;

Graphene reinforced aluminum composites (GRACs) show significant strengthening and toughening effects. The graphene nanoplates effectively prevent the slippage of dislocations within the Al matrix. In this study, molecular and dislocation dynamics simulations of dislocation motions in graphene reinforced aluminum composites are carried out. Molecular dynamics simulations are performed to analyze dislocation mobility of the GRACs. Then, dislocation dynamics uses the mobility data obtained from the molecular dynamics simulations to study the work hardening of the GRACs. The microstructure of the GRACs are obtained by reproducing the forming process. Controlling parameters include temperature, quench rate and compression are considered. The nucleation, expansion, and slippage of dislocations in the GRACs are investigated in detail. The results show that reinforcing of the GRACs is caused by an increased dislocation density and shear-stress transfer, while the toughening effect stems from a decrease of the plastic strain rate. Misorientation angle of Al matrix at the grain boundary also play an important role in dislocation motions in the GRACs. The variations of yield stress and strain with misorientation angle are analyzed as well. The present study reveal the dislocation mechanisms in the GRACs and explore the relations of work hardening and microstructure.

15th U.S. National Congress on Computational Mechanics
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Title: Deep Convolutional Neural Networks for Heterogeneous Material Homogenization

Author(s): Yanhui Jiang, *Northeastern University*; Chengping Rao, *Northeastern University*; Ruiyang Zhang, *Northeastern University*; *Yang (Emily) Liu, *Northeastern University*;

Homogenization, which passes information from a lower scale (e.g., microscale) to a higher scale (e.g., macroscale), exhibits a critical component in multiscale computational modeling of heterogeneous materials. Typically, homogenization is performed on unit cells and yields effective material properties upon volume averaging based on the asymptotic theory. Recent advances in machine learning and data-driven methods offer an alternative to determine the homogenized properties of heterogeneous materials. We herein present a deep learning approach, based on 3D convolutional neural networks (3D-CNN), to map the unit cell property structured in a 4D matrix to the homogenized connectivity matrix with 21 independent components, for composite materials with various types of microstructures (e.g., randomly distributed inclusion/fiber-reinforced polymer/ceramic matrix composites). The model is trained with datasets prepared through computational modeling and simulations. Generalizability and robustness of the proposed method are tested and illustrated through a few examples.

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Title: A Homogenization-based Phase Field Approach to Fracture

Author(s): *Yangyuanchen Liu, *Shanghai Jiao Tong University*; Yongxing Shen, *Shanghai Jiao Tong University*;

The regularized variational theory of fracture (Bourdin et al., 2000), or so-called phase field approach to fracture, has gained popularity due to its ability to predict crack nucleation, propagation, and branching without extra criteria. This approach works by minimizing a total energy functional with the displacement field and phase field (0=intact material, 1=crack) as arguments, and eliminates the cumbersome geometric tracking compared with traditional discrete crack methods such as the extended finite element method. However, each of the prevailing models (Amor et al., 2009; Miehe et al. 2010) predicts a different crack path even under certain simple loadings. In order to get a model with proper tension-compression decomposition, we apply the homogenization theory to construct a phase field model, which predicts reasonable crack paths for the three-point bending test and through-crack shear test, among others. We will compare the prediction of our model with similar ones proposed by Stobl and Seelig (2015) and Steinke and Kaliske (2018). Bourdin, B., Francfort, G. A., Marigo, J.-J., 2000. Numerical experiments in revisited brittle fracture. Journal of the Mechanics and Physics of Solids 48 (4) 797–826. Steinke, C., Kaliske, M., 2018. A phase-field crack model based on directional stress decomposition. Computational Mechanics. https://doi.org/10.1007/s00466-018-1635-0 Strobl, M., Seelig, T., 2015. A novel treatment of crack boundary conditions in phase field models of fracture. Proceedings in Applied Mathematics and Mechanics 15 (1) 155–156.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Advances in Immersed Particle Method and Deep Material Network for Data-driven RVE Analysis

Author(s): *Zeliang Liu, *LSTC*; C.T. Wu, *LSTC*;

In the past decade, multi-scale simulation methods have demonstrated significant advantages for computational mechanics due to their ability to consider microscopic heterogeneities inside a material. This talk introduces a new three-dimensional computational homogenization method for heterogeneous material modeling based on the concept of the representative volume element (RVE). To minimize the meshing effort and overcome severe element distortion issues of RVE models using conforming finite element meshes, an immersed particle modeling technique proposed by Wu et al. [1] is utilized for the RVE modeling and homogenization under large deformation. To further reduce the computation time and avoid the numerical difficulty associated with large material distortion in conventional RVE approach, a mechanistic machine learning approach called deep material network (DMN) is developed by Liu et al [2] for general 2D and 3D problems. It discovers a new way of describing multiscale materials by a multi-layer network structure and mechanistic building blocks. The data-driven framework of DMN will be discussed in detail about the offline training and online extrapolation stages. Efficiency and accuracy of DMN on addressing the long-standing 3D RVE challenges with complex morphologies and material laws are validated through numerical experiments, including the immersed particle method. In particular, we will demonstrate a three-scale homogenization procedure of CFRP system by concatenating the microscale and mesoscale material networks, while DNS is limited to two-scale homogenization due to its high computational cost. The complete learning and extrapolation procedures of DMN establish a reliable data-driven framework for multiscale material modeling and design. [1] C. T. Wu, D. Wang, Y. Guo, An immersed particle modeling technique for the three-dimensional large strain simulation of particulate-reinforced metal-matrix composites, Applied Mathematical Modelling 404 (2016) 2500-2513. [2] Z. Liu, C. T. Wu, M. Koishi, A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials, Computer Methods in Applied Mechanics and Engineering 345 (2019) 1138–1168.

15th U.S. National Congress on Computational Mechanics
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Title: Phase-field Modeling of Fatigue Crack Growth

Author(s): *Yu-sheng Lo, *University of Texas at Austin*; Chad Landis, *University of Texas at Austin*; Michael Borden, *Coreform*;

A phase-field fatigue model is presented for the study of fatigue crack growth. A crack growth viscosity parameter is introduced into the standard phase-field model for brittle fracture to account for rate- or cycle-dependent crack growth phenomena. A modified J-integral is developed to demonstrate how the phase-field approach can be used to generate Paris-law type crack growth rates. In order to model more general crack growth versus applied loading behaviors that are not a simple Paris-law, steady-state finite element calculations are performed to calibrate fits of the phase-field model to measured crack growth rates found in da/dN curves. Transient time or cycle dependent calculations are then performed and compared to experimental measurements on samples where crack turning is induced by the presence of a hole in the vicinity of the crack.

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Title: Thermodynamically Consistent Mathematical Models for Plates and Shells with Damping

Author(s): Karan Surana, *University of Kansas*; Sai Mathi, *University of Kansas*; J. N. Reddy, *Texas A&M University*; *Stephen Long, *University of Kansas*;

In a recent paper [1] the authors have shown that the currently used plate and shell mathematical models cannot be derived using the conservation and the balance laws of classical or non-classical continuum mechanics, hence are thermodynamically inconsistent. The authors also presented a thermodynamically consistent formulation for plates and shells for linear elastic reversible mechanical deformation in which the kinematic assumption is variable and hierarchical and is not chosen a priori. This formulation remains valid and accurate for thin as well as thick plates and shells. In this paper we extend the work presented in reference [1] to include dissipation mechanism in the derivation of the mathematical model. The conservation and the balance laws in R3 in Lagrangian description are utilized in conjunction with variable and hierarchical cross-section deformation mechanism. The ordered rate constitutive theories are derived using conjugate pairs in the entropy inequality in conjunction with representation theorem that considers strain rate tensors upto an arbitrary order n. The thermodynamically consistent formulation presented in this paper for plates and shells remains valid and accurate for very thin as well as thick plates and shells. Space-time coupled as well as space-time decoupled (with and without modal basis) methods of approximations are considered for obtaining numerical solutions of model problems. The results are compared with theoretical solution and the published works. References: [1] Surana, K. S. and Mathi, S.S.C. and Reddy, J. N. Thermodynamic Consistency of Plate and Shell Mathematical Models in the Context of Classical and Non-classical Continuum Mechanics and a Thermodynamically Consistent New Formulation. 15th U.S. National Congress on Computational Mechanics, Austin, TX, 2019.

15th U.S. National Congress on Computational Mechanics
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Title: Data-based Stochastic Model Reduction for Complex Dynamical Systems

Author(s): *Fei Lu, *Johns Hopkins Unversity*; Alexandre Chorin, *UC Berkeley*; Kevin Lin, *University of Arizona*; Xuemin Tu, *University of Kansas*;

We present a statistical inference approach to construct discrete-time reduced models for complex dynamics (such as chaotic dynamical systems, Kuramoto-Sivashinsky equations and stochastic Burgers equations), using only data consisting of discrete-time observation of the low-dimensional dynamical variables of direct interest. The reduced models are parametric time series models based on (Galerkin) schemes for these low-dimensional variables, and can have a time step-size which can be too large for the full system to be accurately/stably integrated. Therefore the reduced models are low-dimensional and greatly reduce the computational cost. The reduced models can capture the statistical-dynamical properties of these variables of interest, and can be used for prediction and uncertainty quantification. References: — F. Lu, X. Tu and A. J. Chorin. Accounting for model error from unresolved scales in ensemble Kalman filters by stochastic parametrization. Mon. Wea. Rev., 145(2017), no. 9, 3709--3723. — F. Lu, K. K. Lin and A. J. Chorin. Data-based stochastic model reduction for the Kuramoto--Sivashinsky equation. Physica D, 340 (2017), 46--57. — A. J. Chorin and F. Lu. Discrete approach to stochastic parametrization and dimension reduction in nonlinear dynamics. Proc. Natl. Acad. Sci. USA, 112 (2015), no. 32, 9804--9809.

15th U.S. National Congress on Computational Mechanics
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Title: Fully Resolved Simulations of Polymer Additive Manufacturing Processes

Author(s): *Jiacai Lu, *Johns Hopkins University*; Huanxiong Xia, *Beijing Institute of Technology*; Gretar Tryggvason, *Johns Hopkins University*;

Additive manufacturing processes include complex multiphysics and multiscale processes, and an evaluation of suitable material/process models require accurate solutions of the governing equations to determine how well the predictions of the model agree with experimental results. For complex processes where many physical effects must be accounted for, it is imperative to find solutions for situations that mimic the circumstances for which the model is intended. Ideally, we solve the equations for exactly the process we are interested in modeling. Fully resolved simulations are therefore an essential link in the modeling process since without them it is impossible to assess how well mathematical models of the various physical processes agree with experimental results in all but the simplest of circumstances. Here, a numerical method for fully resolved simulations of Fused Deposition Modeling, or Fusion Filament Fabrication, where a filament of hot polymer is deposited onto substrata where it cools down and solidifies, is described. The method is based on a the finite volume/front tracking method used earlier for a large number of multiphase systems, where the conservation equations for mass, momentum, and energy are solved on a fixed structured and staggered grid discretizing a domain containing two or more fluids, and the interface between the different fluids is tracked using connected marker particles. The method is extended by making it implicit to handle realistic material parameters, the viscosity of the melt is taken to be a function of temperature and shear rate, and a volume source enclosed in an immersed boundary is incorporated to model the nozzle. The polymer is modeled as an elastoplastic material whose properties depend on the temperature. The residual stresses due to the cooling and shrinking of the polymer as it cools down, the solidification and the deformation due to residual stresses are, in particular, captured. The method is implemented for a rectangular domain initially containing air and the behavior of both the polymer and the air is simulated. The performance and accuracy of the method were tested in several ways using simple injection of two short filaments, one on top of the other, and it was found that for governing parameters similar to those encountered under realistic conditions a converged solution could be obtained using about thirty control volumes across the filament diameter. A more complex geometry, consisting of a two-layer infilled rectangle was also simulated to show the capability of the method.

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Title: Time-discontinuous Material Point Method for Nonlinear Transient Problems involving Plastic and Large Deformations

Author(s): *Mengkai Lu, *Ningbo University*; Yonggang Zheng, *Dalian University of Technology*; Hongwu Zhang, *Dalian University of Technology*; Zhen Chen, *University of Missouri*;

Material point method (MPM) is an attractive computational method simulating the transient problems involving plastic and large deformations. When dealing with the blast/impact loadings, the stress responses obtained from the original MPM usually suffer from the spurious numerical oscillations. In order to overcome this deficiency, a time-discontinuous material point method (TDMPM) for the nonlinear transient problems is proposed. With the time-discontinuous Galerkin technique and the algebraic equilibrium equations based on the grid cells, the time-discontinuous formulation of the TDMPM for nonlinear problems can be derived. In the framework, the displacement and velocity fields within a discrete time interval are interpolated with the polynomial functions. Meanwhile, the discontinuous velocity field at each time instant is allowed, which ensures the proposed method could properly capture the discontinuous characteristics and alleviating the spurious numerical oscillations. Several representative wave propagation problems with plastic/large deformations are presented for demonstration and verification of the TDMPM comparing with that of the original MPM. In addition, the performances of CPDI and CPDI2 interpolations in the TDMPM are investigated in the numerical examples. Supports from NSFC (11672062 and 11772082), Research Foundation (No.GZ18110) of State Key Laboratory of Structural Analysis for Industrial Equipment, Dalian University of Technology are gratefully acknowledged. Keywords: Material point method, Time-discontinuous formulation, Wave propagations, Elastoplastic, Large deformation, Interpolations References:
[1] M.K. Lu, J.Y. Zhang, H.W. Zhang, Y.G. Zheng*, Z. Chen, Time-discontinuous material point method for transient problems. Computer Methods in Applied Mechanics and Engineering 2018, 328, pp. 663–685. [2] Y.G. Zheng, F. Gao, H.W. Zhang*, M.K. Lu, Improved convected particle domain interpolation method for coupled dynamic analysis of fully saturated porous media involving large deformation. Computer Methods in Applied Mechanics and Engineering 2013, 257, pp, 150–163. [3] J. Tao, H.W. Zhang, Y.G. Zheng, Z. Chen*, Development of generalized interpolation material point method for simulating fully coupled thermomechanical failure evolution. Computer Methods in Applied Mechanics and Engineering 2018, 332, pp, 325–342.

15th U.S. National Congress on Computational Mechanics
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Title: Simulation of the PBF Process Using a Mechanism Based Constitutive Model

Author(s): *Andreas Lundbäck, *Luleå University of Technology*; Andreas Malmelöv, *Luleå University of Technology*; Johan Lindwall, *Luleå University of Technology*; Lars-Erik Lindgren, *Luleå University of Technology*;

The talk describes the model and results for the AM-bench class 1 challenge (CHAL-AMB2018-01-PD, https://www.nist.gov/ambench/challenges-and-descriptions) using an improved model compared with our previous work presented at AM-Bench 2018. The challenge is a bridge-like structure produced with the powder bed fusion (PBF) process. It is built by 600 layers in Alloy 625. We will focus on the distortions induced by the release of residual stresses when cutting the built part from the substrate. A coupled thermo-mechanical model was applied in the original simulation of the AM-bench challenge. The 600 layers were merged into 25 layers in order to reduce the computational time. Each added layer was born hot without any prior or subsequent heat input. Due to the lumping of layers, it was expected that the model would over-predict the deformations. This was also found to be the case. The model over-predicted the deformations with about 50%. However, later work with less lumping showed that this over-prediction was not due to the lumping. In the revised model a mechanism based constitutive model will be used. Simple table interpolation logic for the flow stress was used in the previous model. It is assumed by the authors that a mechanism based material model including relaxation at elevated temperatures will reduce the residual stresses and thereby the post-cut deformations and thereby improve the accuracy of the results.

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Title: A Method-of-lines Approach to Moving and Deforming Meshes

Author(s): *Tomas Lundquist, *Paul Sabatier University*;

In modern applications of computational mathematics, unsteady simulations often involve a movement of the domain boundaries in such a way that the mesh is deformed continuously over time. The formal stability and convergence theory for numerical methods applied to deforming meshes is still mostly lacking, or limited to some specialized forms of schemes. In [1], a space-time approach using SBP type operators in both space and time was proposed, leading to provable stability with the energy method for high order schemes by satisfying a discrete geometric conservation law. In this presentation, building on the recent success of generalized SBP formulations in physical space [2], we propose a new method-of-lines approach to moving and deforming meshes. Discrete geometric conservation is achieved by construction already in the semi-discretized form of the equations. In this way, properties such as linear stability and free-stream preservation can be guaranteed using standard explicit and implicit time integration schemes. The added flexibility in the choice of time integration is a significant practical improvement to the previous space-time techniques, and constitutes the main novel contribution from the present work. The talk will focus mostly on the theoretical aspects of the new method-of-lines technique for deforming meshes, corroborated where appropriate with numerical calculations to confirm the practical advantages. By utilizing a generalized definition of SBP operators in space, we will in particular demonstrate that a simple Lagrangian formulation is sufficient to develop a unified stability theory for diverse classes of methods such as finite volume, finite difference and discontinuous Galerkin methods. [1] S. Nikkar, J. Nordstr■öm, “Fully discrete energy stable high order finite difference methods for hyperbolic problems in deforming domains”, Journal of Computational Physics 291 (2015) [2] T. Lundquist, A. Malan, J. Nordstr■öm, “A hybrid framework for coupling arbitrary summation-by-parts schemes on general meshes”, Journal of Computational Physics 362 (2018)

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Title: Inverse Mixed and Enhanced Strain Methods for Vascular Stress Analysis

Author(s): *Yuanming Luo, *the University of Iowa*; Jia Lu, *the University of Iowa*;

Inverse finite element method, which solves problems wherein a deformed state is given at the onset, has demonstrated its capability in stress analysis of vascular systems structures [1]. However, pure displacement formulation is known to suffer from volumetric locking in the impressibility limit and shear locking in bending-dominated deformations. To overcome the issue, mixed and enhanced formulations have been developed for forward finite element analysis [2, 3]. These methods have been widely accepted and demonstrated the effectiveness in resolving the locking issues. Recently, we introduced a family of finite strain inverse mixed methods and an inverse enhanced strain method for large deformation analysis of hyperelastic material. The methods draw on existing forward formulations and are designed in such a way that the deformation predicted by forward elements can be exactly reverted. Stability of the inverse mixed and enhanced strain formulation are investigated. Dependence of stress solution on material parameters are numerical investigated. Examples of vascular analysis show that, compared with displacement formulation, there are significant accuracy improvements upon using the methods. It has been reported that for thin-walled vascular structures (cerebral aneurysms for example) the wall stress is statically determined, and that the inverse method can capture the static determinacy. It is showed that the inverse mixed and enhanced formulations can capture this feature even better. References [1] Lu, J., Zhou, X. and Raghavan, M.L., 2007. Inverse elastostatic stress analysis in pre-deformed biological structures: demonstration using abdominal aortic aneurysms. Journal of biomechanics, 40(3), pp.693-696. [2] Simo, J.C., Taylor, R.L. and Pister, K.S., 1985. Variational and projection methods for the volume constraint in finite deformation elasto-plasticity. Computer methods in applied mechanics and engineering, 51(1-3), pp.177-208. [3] Simo, J.C. and Armero, F., 1992. Geometrically nonlinear enhanced strain mixed methods and the method of incompatible modes. International Journal for Numerical Methods in Engineering, 33(7), pp.1413-1449.

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Title: Discretizing Closed Smooth Surface with a Single High-Order Smooth Element

Author(s): *Hang Ma, *Shanghai University*;

Particles/voids in solids with closed smooth shapes are conventionally discretized by low-order elements in either the FEM or BEM in material simulations, resulting in large solution scales of the problem. Based on Lagrange interpolation polynomials, such closed shapes can be modeled more efficiently by using a single high-order closure element [1] with much few nodes. However, the drawback is that the end node/line exists in closure elements, across which the derivatives of shape functions and field variables have jumps, deteriorating the fitting accuracy of closure elements. By making full use of geometrical features of spheroid such as the periodicity, symmetry and smoothness, the high-order smooth element are constructed in the present work with the use of real nodes repeatedly as auxiliary nodes of interpolation in both the latitude and meridian directions, of which the curvilinear coordinates of the spheroid surface consist. The parametric plane of the smooth element is then broadened without adding fictitious nodes while the region of numerical quadrature remains unchanged. The fitting accuracy of the smooth element can be raised by one to two orders of magnitude, resulted from the raise of the order of interpolation polynomials and the surface smoothing or the removal of the end node/line effect of closure elements. In addition, the coefficients of shape functions are generated automatically in computer program to get rid of tedious manual work encountered in the construction of a variety of high order elements with different node numbers and node distributions. The accuracy and efficiency of high order smooth elements are demonstrated through a number of numerical examples, by checking the geometric fitting accuracy, the computation cost and some bench mark tests in elasticity [2], compared with the traditional closure elements and the quadratic elements. Keywords: high order element; closure element; smooth element; interpolation; end node/line effect

*E-mail address: hangma@staff.shu.edu.cn (H.Ma) Acknowledgement: The work was supported by the National Natural Science Foundation of China (Nos. 11672173, 11272195).

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Title: Modeling Earthquake Ruptures with High-resolution Fault-zone Physics: An Adaptive Asynchronous Space-time Discontinuous Galerkin Approach

Author(s): *Xiao Ma, *University of Illinois Urbana Champaign*; Amit Madhukar, *University of Illinois Urbana Champaign*; Robert Haber, *University of Illinois Urbana Champaign*; Reza Abedi, *University of Tennessee Space Institute*; Ahmed Elbanna, *University of Illinois Urbana Chamapaign*;

Earthquakes are among the most destructive natural hazards to mankind with losses exceeding thousands of lives and billions of US dollars annually. An outstanding challenge in computational seismology is to model accurately earthquake nucleation, propagation, and arrest and to predict the development of stress-accumulation patterns across regional fault networks and over the full seismic cycle. These capabilities would enable the development of physics-based seismic hazard models in support of informed risk analysis and policy making. The wide range of length and time scales involved in earthquake processes (from sub-millimeter scales to hundreds of kilometers and from milliseconds to centuries) poses a critical barrier to addressing these needs with conventional numerical schemes such as time-marching finite element and finite difference methods on non-adaptive meshes. The multi-scale character renders solutions by these methods computationally intractable, even on state-of-the-art supercomputing platforms. We propose an asynchronous space-time Discontinuous-Galerkin (aSDG) method with dynamic adaptive meshing to meet this challenge. The aSDG method easily accommodates variations of spatial and temporal resolution of several orders of magnitude across the solution domain. We demonstrate the capabilities of the aSDG method for resolving rupture propagation across complex fault zones using a unique model with explicit representations of pre-existing small-scale secondary faults and branches. This model enables new insights into earthquake rupture dynamics that might not be realizable in homogenized isotropic plasticity or damage models that typically smear out the secondary cracks. Specifically, we show that in addition to acting as energy sinks, secondary faults can also be energy sources that promote transient accelerations of rupture-propagation speeds and slip rates on the main fault. We also show that these secondary features significantly affect the stress state on the main fault and contribute to the enhanced generation of high frequency radiation. The aSDG method accurately resolves the different phases of rupture growth and arrest as well as the radiation fields associated with the non-uniform propagation. The method’s dynamic adaptive meshing provides unprecedented resolution of rupture process zones and global elastodynamic fields. We discuss the potential of the aSDG scheme to provide a unique computational pathway to efficient multiscale dynamic rupture simulations in seismology and a critical missing link for transitioning between physics-based simulation and societal risk management.

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Title: Multiphysics Simulations of Drug Adsorption in the Chemofilter Device

Author(s): *Nazanin Maani, *Purdue University*; Tyler Diorio, *Purdue University*; Steven W. Hetts, *University of California, San Francisco*; Vitaliy L. Rayz, *Purdue University*;

Introduction: Intra-Arterial Chemotherapy (IAC) is a preferred treatment for unresectable primary liver cancer. A significant amount of chemotherapy agents, e.g. Doxorubicin, injected into blood vessels supplying a tumor, pass into the systemic circulation, causing cardiac toxicity and limiting the effectiveness of IAC. These excessive drugs can be captured by the Chemofilter – a 3D-printable, catheter-based device deployed in a vein downstream of the liver during the IAC. The Chemofilter chemically binds Doxorubicin to decrease the amount of toxins in the blood stream, thereby increasing the effectiveness of IAC as higher drug doses can be safely administered. In this study, alternative prototypes of the Chemofilter were compared by evaluating their hemodynamic and filtration performance through multiphysics CFD simulations. Methods: A “honeycomb” Chemofilter design consists of an array of hexagonal channels which can be twisted and/or perforated for enhanced mixing. A strutted Chemofilter consists of a lattice of tessellated cubic cells. The flow through the device is simulated with ANSYS, solving the coupled Navier-Stokes and advection-diffusion equations in order to model the multiscale adsorption of Doxorubicin to the ionic resin surface. Electrochemical binding is represented by a source term, which is modeled using concentrated solution theory. A steady drug adsorption is assumed, as the saturation of the surface binding sites can be neglected for the duration of the injection. In addition, the transport of Doxorubicin is assessed using a heat transfer analogy to facilitate the optimization of the device prototypes. The effective diffusion coefficient of the drug remains to be determined from experiments, however, a comparative study of alternative designs is conducted by keeping the same coefficient in all simulations. Blood is modeled as a Newtonian fluid with the Reynolds number of 300 and Peclet number around 1000 for both heat and mass transport. Results/Discussion: Enhanced mixing provided by the twisted and perforated channels decreased the Doxorubicin concentration by 45.7% greater than that of the straight channel design. The honeycomb and the strutted Chemofilter provided a 61.8% and 40.4% decrease in the Doxorubicin concentration with a 2.7 and 2.5 mm Hg pressure drop, respectively. The Doxorubicin transport simulations predicted the effectiveness of the Chemofilter in removing excess drugs from circulation while eliminating flow stagnation regions prone to thrombosis. Conclusion: These results demonstrate the value of the multiphysics modeling approach in optimizing the design of the Chemofilter device and reducing the number of required in-vitro experiments and animal studies. Acknowledgements: NIH NCI-R01CA194533 award.

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Title: Non-ordinary State-based Peridynamics Free of Zero Energy Modes

Author(s): *Erdogan Madenci, *University of Arizona*; Mehmet Dorduncu, *University of Arizona*; Xin Gu, *Hohai University*;

The non-ordinary state-based peridynamics (NOSB PD) is attractive because of its ability to employ existing constitutive relations for material models. The deformation gradient tensor and the force density vector appearing in the equilibrium equations are expressed in terms of nonlocal integrals. Their definitions affect the accuracy and stability of PD predictions and suffer from the presence of zero energy modes. Therefore, this study introduces a more accurate representation of the deformation gradient and the force density vector by using the concept of peridynamic differential operator (PDDO). Also, it presents both the weak and strong forms of NOSB PD simulations using implicit linear and nonlinear solvers. The numerical results demonstrate the numerical accuracy without numerical instability by considering a two-dimensional rectangular plate with and without a hole under quasi-static tension.

15th U.S. National Congress on Computational Mechanics
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Title: Performance and Scalability of Parallel–Adaptive Asynchronous Spacetime Discontinuous Galerkin Methods

Author(s): *Amit Madhukar, *University of Illinois at Urbana-Champaign*; Robert Haber, *University of Illinois at Urbana-Champaign*; Reza Abedi, *University of Tennessee Knoxville (UTK) / Space Institute (UTSI)*; Volodymyr Kindratenko, *University of Illinois at Urbana-Champaign*;

The asynchronous Spacetime Discontinuous Galerkin (aSDG) method [1] is a powerful solution scheme for hyperbolic systems. It features unconditional stability, conservation over every spacetime cell, linear computational complexity, and support for arbitrarily high-order elements. However, its most powerful potential advantages are compatibility with an extremely powerful and dynamic form of adaptive spacetime meshing and a nearly perfect structure for parallel implementations. Ideally, these features would be exploited simultaneously. Unfortunately, it was not possible to evolve domain decompositions fast enough to maintain load balance in the face of dynamic adaptive meshing. Faced with a choice between serial adaptive solutions and parallel solutions on non-adaptive meshes, we chose the former more powerful option. Indeed, serial adaptive aSDG solvers typically outperformed conventional solvers running in parallel on large clusters, especially for multi-scale problems or problems with rapidly evolving domain geometry; cf. recent work on dynamic fracture [2]. This presentation describes recent work on a new approach to parallel–adaptive aSDG computations in which individual patch solutions, the basic unit of computation in aSDG solvers, replace subdomains as the means to define parallel solution tasks. A new ‘lazy’ adaptive meshing scheme parallelizes at the same patch-level granularity. The new parallel work unit comprises construction, solution, and local mesh adaptation for a single patch. A simple round-robin strategy preserves load balance by distributing these unit tasks across the available cores. We pin hyperthreaded meshing and solver threads to each core. The meshing thread handles patch construction and patch-local adaptive meshing; the solver thread carries out the more compute intensive patch solution. The software architecture operates asynchronously, at both the thread level within each core and the patch processing level across cores. We describe various optimizations for improved single-core performance and parallel scaling efficiency. For shared-memory parallel platforms we report parallel scaling efficiencies of 97% or better for non-adaptive runs and efficiencies above 90% for parallel–adaptive runs. We close with a discussion of continuing work, including a new implementation for large-scale distributed platforms. References: [1] R. Abedi, R. B. Haber, B. Petracovici. A spacetime discontinuous Galerkin method for elastodynamics with element-level balance of linear momentum, ?Comput. Methods Appl. Mech. Eng. 195 (2006) 3247–3273. [2] R. Abedi, and R. Haber. Spacetime simulation of dynamic fracture with crack closure and frictional sliding, Advanced Modeling and Simulation in Engineering Sciences 5 (2018). doi:10.1186/s40323-018-0116-5

15th U.S. National Congress on Computational Mechanics
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Title: Semantically Valid Deep-learning Classification of Fracture Morphology in High-strength Concrete

Author(s): *Anna Madra, *Pennsylvania State University*; Colin Loeffler, *Southern Methodist University*; Xu Nie, *Southern Methodist University*; William Heard, *U.S. Army Engineer Research and Development Center*; Jesse Sherburn, *U.S. Army Engineer Research and Development Center*; Michael Hillman, *Pennsylvania State University*;

The classification of fracture geometry is crucial in identifying damage mechanisms in concrete. While existing 3D imaging techniques such as X-ray micro-tomography permit examination of fracture at increasingly high-resolution, the complexity of damage morphology makes it challenging to manually define the range of geometrical features for classification. Moreover, the measurement of features such as length, aspect ratio, and tortuosity is ill-defined for bifurcating and compound geometry. We propose to combine the low-level geometric features into higher-level descriptors while preserving their semantic validity, i.e., physical interpretation, and use them to calibrate a deep-learning neural network to perform classification of damage morphology. The resulting model is then applied to compare fracture mechanisms observed in specimens subject to different loading parameters.

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Title: Generalized Summation-by-Parts for Entropy Stable Weighted Essentially Non-Oscillatory High-Order Finite Difference Scheme in Curvilinear Multi-Block Domains

Author(s): *Brad Maeng, *Sandia National Laboratories*; Travis Fisher, *Sandia National Laboratories*; Mark Carpenter, *NASA Langley Research Center*;

High-order numerical methods have been gaining continued interest for high-fidelity flow simulations because of the potential to handle complex flows effectively and efficiently. In this study, we extend the entropy stable weighted essentially non-oscillatory (SSWENO) scheme [1] using the generalized summation-by-parts (SBP) with simultaneous approximation term (SAT) framework [2]. In the generalized SBP-SAT framework, a point-wise stable SBP dual-flux operator can be established for the SSWENO scheme with a strong interface coupling formulation and stencil biasing mechanics across the interface. The resulting scheme exhibits better shock capturing across domain interfaces than a conventional SSWENO operator. We also introduce a hybrid operator where an entropy-stable artificial dissipation SBP operator [3] is used in conjunction with the HOFD scheme to reduce the computational overhead and limit excessive dissipation of turbulence. We present that the entropy stability property is maintained for all operators studied in this research in one- and higher-dimensions, including curvilinear body-fitted meshes. We verify the new scheme using canonical one-dimensional problems as well as turbulent boundary layer flows in three-dimensions. References [1] Travis C Fisher and Mark H Carpenter. High-order entropy stable finite difference schemes for nonlinear conservation laws: Finite domains. Journal of Computational Physics, 252:518–557, 2013. [2] David C Del Rey Fern ?andez, Jason E Hicken, and David W Zingg. Review of summation-by-parts operators with simultaneous approximation terms for the numerical solution of partial differential equations. Computers & Fluids, 95:171–196, 2014. [3] Ken Mattsson, Magnus Svard, and Jan Nordstrom. Stable and accurate artificial dissipation. Journal of Scientific Computing, 21(1):57–79, 2004.

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Title: The Role of Interface in Mechanical Properties of Organic-Inorganic Biological Nanocomposites: a 3-D Computational Investigation

Author(s): *Mohammad Maghsoudi-Ganjeh, *University of Texas at San Antonio*; Xiaodu Wang, *University of Texas at San Antonio*; Xiaowei Zeng, *University of Texas at San Antonio*;

The structural biological materials such as bone and nacre often exhibit mechanical properties far superior than their individual constituents. This has been associated with several toughening mechanisms originating from their intricate architecture and composite nature. At nanoscale, their building block is mostly a hybrid nanocomposite made of intertwined interaction of brittle/hard inorganic compound bonded via thin layers of ductile/soft organic matter. For instance, hydroxyapatite crystals joint by non-collagenous proteins or calcium carbonate nanograins bond by a network of chitin are essentially the material of bone extrafibrillar matrix and nacre tablet, respectively. It is most interesting and essential to learn how the small amount of ductile organic interface (<5%v.f) can give rise to a damage-tolerant nanocomposite material. To address this question, finite element models of a 3-D nanocomposite was developed in which randomly distributed elastic nanograins are connected by thin interface layers modeled as cohesive elements. To investigate the role of interface, ultimate strength and fracture energy of interfacial materials were varied in a range covering strong-tough, strong-brittle, weak-tough, weak-brittle, and intermediate-intermediate scenarios. The mechanical properties of the nanocomposite including ultimate stress, failure strain, toughness, and damage dissipation energy are discussed as a function of interface properties. It was found that tough interface results in appreciable amount of plastic deformation and significant enhancement of nanocomposites mechanical competencies through involvement of a majority of interfaces in load-bearing and energy-dissipation accompanying significant crack path deviation and irregular fracture surface. The unique finding of this study can help us better understand material basis of biological tissues with the insight to design better biomimetic material systems.

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Title: Near-wall Biological Transport Processes in Coronary Artery Atherosclerosis

Author(s): *Mostafa Mahmoudi, *Northern Arizona University*; Ali Farghadan, *Northern Arizona University*; Amirhossein Arzani, *Northern Arizona University*;

In the present study, image-based computational fluid dynamics (CFD) models have been used to non-invasively characterize the effect of wall shear stress (WSS) vectors on biochemical/cell-specific mass transport processes in stenosed coronary arteries. WSS is arguably the most important parameter in biomechanics of atherosclerosis and its importance in the pathology of atherosclerosis has been well accepted within the research community. WSS acts as a link between the fluid mechanics of blood flow and the biology of atherosclerosis. It has been recently shown that Lagrangian WSS structures govern near-wall transport in high Schmidt and Peclet number flows. The main aim of the present study is to investigate and provide additional insight into the connection between WSS and near-wall transport of some the prominent biochemicals/cells involved in atherosclerosis. Near-wall transport of these biochemicals and cells plays an important role in promoting or preventing atherosclerosis. The diseased coronary artery models are extracted from CT-angiography (CTA) images and image-based CFD simulations using Oasis (a minimally dissipative solver) is performed to obtain time-resolved WSS and velocity data in several coronary arteries. The Lagrangian coherent structures in WSS (WSS LCS) are calculated in the regions with soft and calcified plaques. WSS LCS is calculated from stable and unstable manifolds of the time-average WSS vector field. Prominent biological transport processes involved in atherosclerosis (low-density lipoprotein, monocyte, adenosine triphosphate, and nitric oxide) are modeled. Namely, biochemical/cell-specific continuum advection-diffusion-reaction equations with appropriate boundary conditions are solved to quantify the surface concentration patterns. Continuum transport models are implemented in FEniCS (an open-source finite element solver). The results are compared with WSS LCS and WSS magnitude. Our study shows a complex relationship between WSS and surface concentration patterns in atherosclerosis. Our computational framework could be used to study the often overlooked role of WSS in biological transport processes during prominent cardiovascular complications such as atherosclerosis and thrombosis.

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Title: Recent Theoretical and Numerical Advances in Modeling Biological Membranes

Author(s): *Kranthi Mandadapu, *University of California, Berkeley*; Amaresh Sahu, *University of California, Berkeley*; Yannick Omar, *University of California, Berkeley*; Roger Sauer, *RWTH Aachen University, Aachen*;

Biological membranes comprised of lipids and proteins make up the boundary of the cell, as well as the boundaries of internal organelles such as the nucleus, endoplasmic reticulum, and Golgi complex. Lipid membranes and their interactions with proteins play an important role in many cellular processes, including endocytosis, exocytosis, intracellular trafficking, membrane fusion, and cell-cell signaling. Membrane behavior is complex—they are elastic in bending, fluid in plane, and undergo several shape transitions. These shape changes include morphological transitions such as formation of invaginations, buds, and tubules from planar shapes in endocytosis and rearranging tubular networks in the endoplasmic reticulum. While these processes are well characterized by experiments in cell biology, the underlying mechanisms are poorly understood in a quantitative manner. One reason for this is the complex interplay between elastic bending and thermodynamically irreversible processes such as intra-membrane lipid flow, protein diffusion, and chemical reactions involved in protein binding. Modeling these processes pose mathematical challenges as all these processes occur on arbitrarily curving lipid membranes. In this talk, I will discuss recent advances in both the theoretical and numerical advances in modeling lipid membranes. To this end, I will discuss irreversible/non-equilibiurm thermodynamics formalism for arbitrarily curved lipid membranes in the differential geometric setting to determine their dynamical equations of motion [1]. Using this framework, we find relevant constitutive relations and use them to understand how bending, intra-membrane flows, diffusion of multiple transmembrane species, in-plane phase transitions and surface chemical reactions are coupled. I will also discuss the development of advanced numerical methods based on finite element (FE) methods that couple different processes such as out-of-plane bending with in-plane fluid flow and in-plane phase transitions on arbitrarily curving surfaces [2, 4]. To this end, I will talk on the Lagrangian and an arbitrary Lagrangian–Eulerian FE methods for arbitrarily curved and deforming interfaces. With these theories and numerical methodologies, I will discuss the physical insights gained from the morphological transitions encoded in the biological process of endocytosis. References: 1. Sahu, A., Sauer, R. A., and Mandadapu K. K., Physical Review E. 96, 042409 (2017). 2. Sauer, R. A., Duong, T. X., Mandadapu, K. K., and Steigmann, D. J., Journal of Computational Physics, 330, 436-466 (2017). 3. Sahu, A., Omar, Y. A. D., Sauer, R. A., and Mandadapu, K. K., arXiv:1812.05086 (2018).

15th U.S. National Congress on Computational Mechanics
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Title: Storm Surge Computational Methods in the World of Uncertainty Quantification and Optimization

Author(s): *Kyle Mandli, *Columbia University*;

Coastal hazards related to strong storms are one of the most frequently recurring and wide spread hazards to coastal communities today. In particular storm surge, the rise of the sea surface in response to wind and pressure forcing from these storms, can have a devastating effect on the coastline. Furthermore, with the addition of climate change related effects, the ability to predict these events quickly and accurately is critical to the protection and sustainability of these coastal areas. This talk will focus on two aspects of the coastal flooding problem, quantification of uncertainty and optimization of coastal protections, both of which require large ensembles of storm surge simulations. Approaches to this class of problems must then be both computational tractable as well as accurate enough to represent the relevant dynamics. We will therefore discuss approaches and ideas we have developed that hopefully may lead to ways to address these problems. This will includes resolution adaptation, multiscale modeling, reduced order models and new modeling approaches.

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Title: Modelling Fibrin Networks Using Spatial Euler-Bernoulli IGA Beams

Author(s): *Soham Mane, *The University of Texas at Austin*; Chad Landis, *The University of Texas at Austin*; Manuel Rausch, *The University of Texas at Austin*;

Modelling Fibrin networks using Spatial Euler-Bernoulli IGA beams Soham M. Mane1, Chad Landis, Manuel Rausch The University of Texas at Austin Thrombus is vital to our well-being as blood coagulation prevents bleeding after vascular injury. However, thrombus role is diametrical in that pathological coagulation also causes deep vein thrombosis, heart attacks, and strokes. Thrombus' propensity to detach and embolizes, and thus cause havoc, is strongly linked to its mechanical properties, which are primarily determine by its fibrin backbone initially and its fibrin/collagen co-network after maturation. To understand how thrombus macro-mechanics (such as its failure behavior) are linked to its microstructure, we develop mathematical/numerical models of thrombus' 3D microstructure. Specifically, we build representative volume elements (RVEs) containing 3D fiber networks. In turn, the networks are comprised of individual fibers (ostensibly fibrin or collagen), which are each modeled as spatial Euler-Bernoulli beam within the Isogeometric Analysis (IGA) framework. To verify our beam implementation we simulate three beam benchmark problems that have been widely used for verification: the Mainspring problem, the shallow arc snap-through problem, and the 45 degree Cantilevered Bend problem. Specifically, we solve those beam problems using single NURBS patches and multipatch beams. To connect multiple patches for the latter networks, we adopt the bending strip method that has previously been applied to multipatch IGA shells. Moreover, we implement a discretization algorithm that allows connecting more than two beams at a point, enabling network bifurcations as observed in natural and synthetic fibrin/collagen meshes. After verification of our implementation, we study two classes of networks: i) networks comprised of straight fibers and ii) networks comprised of undulated fibers. We test both types of networks under uniaxial extension, planar biaxial extension, simple shear and confined/unconfined compression. In our analysis of these tests, we focus on studying sensitivity to network parameters such as characteristic network length, degrees of anisotropy, bifurcation ratios, degree of undulation, and fiber stiffness. In our talk, we will present an in-depth analysis of how various modes of deformation at the fiber level give rise to the macroscopic properties of the network including fiber re-orientation, fiber bending, and fiber stretch. REFERENCES [1] A.M.Bauer, et.al, Nonlinear isogeometric spatial Bernoulli beam, Comput. Methods Appl. Mech. Engrg, 303, 101-127, 2016. [2] S.B. Raknes, et.al, Isogeometric rotation-free bending-stabilized cables, Comput. Methods Appl. Mech. Engrg, 263, 127-143, 2013.

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Title: Mathematical Modeling and Prediction of Plasmonic Photothermal Nanoparticle-Mediated Therapy for Targeted Pancreatic Cancer Treatment Planning

Author(s): *Santiago Manrique-Bedoya, *UT Antonio*; Chris Moreau, *UT Health San Antonio*; Sandeep Patel, *UT Health San Antonio*; Kathryn Mayer, *UT San Antonio*; Yusheng Feng, *UT San Antonio*;

Pancreatic cancer is one of the deadliest cancers, with a 7% survival rate at five years from diagnosis. Limited treatment options for patients who are diagnosed with late-stage disease is a major contributor to this problem. Endoscopic ablation is possible, but devices and methods must have high specificity for diseased tissue due to risk of debilitating pancreatitis. Gold nanoparticles may improve targeting of thermal therapy, but human studies carry unknown risks. We propose a computational model of plasmonic photothermal therapy (PPTT) to better characterize thermodynamics prior to in-vivo studies. This model may also serve as a future treatment planning tool for physicians. The three-dimensional model of the pancreas is constructed in SolidWorks using anatomically accurate illustrations. A model of a single nanoparticle was created using the same software and SEM images. Three different nanoparticle geometries were compared to determine the best shape for transferring heat: nano-rods, nano-spheres, and nano-bipyramids. COMSOL's LiveLink feature was used to import the geometry from SolidWorks and the power absorbed by the nanoparticles under laser irradiation is calculated using the RF Module. The PDE Module is used to calculate the total energy transferred from the nanoparticles to the surrounding media. Under laser illumination (808 nm and 20 mW), the nano-rods yield the highest temperature increase among the three shapes, making it the optimal choice for precise heat transfer in sensitive tissue. Clusters of nanoparticles are simulated to resemble aggregation after injection. Tissue damage is assessed by incorporating thermal properties of pancreatic tissue through solving the Penne's bioheat transfer equation and the Arrhenius equation. The computational results are compared with ex-vivo porcine pancreas experimental results, which shows very good agreement.

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Title: Virtual Element Methods for Elliptic and Parabolic Problems

Author(s): *Gianmarco Manzini, *Los Alamos National Laboratory*;

We present the Virtual Element Method (VEM) for the numerical treatment of elliptic and parabolic problems. This formulation works on very general unstructured meshes in 2D and 3D for arbitrary order of accuracy. Examples of applications are for Poisson, Stokes and biharmonic problems as well as general diffusion problems (advection-diffusion-reaction equations) and time-dependent problems. Numerical experiments verify the theory and validate the performance of the proposed method. References: - B. Ayuso de Dios, K. Lipnikov, and G. Manzini. The non-conforming virtual element method. ESAIM: Mathematical Modelling and Numerical Analysis, 50(3):879–904, 2016. - G. Manzini, G. Vacca, Design, analysis and preliminary numerical results for the nonconforming VEM for parabolic problems Technical Report N. LA-UR-18-29150 Los Alamos National Lab.(LANL), Los Alamos, NM (United States) - A. Cangiani, G. Manzini, and O. Sutton. Conforming and nonconforming virtual element methods for elliptic problems. IMA Journal on Numerical Analysis, 37:1317–1354, 2016

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Title: Deep Learning with Per-Voxel Uncertainty Quantification for Volumetric Segmentation of Battery Electrode Images

Author(s): *Cari Martinez, *Sandia National Laboratories*; Kevin Potter, *Sandia National Laboratories*; Matthew D. Smith, *Sandia National Laboratories*; Scott A. Roberts, *Sandia National Laboratories*;

Numerical simulations that model complex physical systems require accurate models of each system component. Recent advances in computed tomography (CT) have enabled imaging of specific as-built parts; however, for these images to be used in simulations, experts must perform volumetric segmentation of these scans. Each voxel in the data must be individually labeled by material before simulation of system performance is possible. Expert-driven segmentation is both time consuming and error prone. While image filtering and thresholding techniques are used to partially automate the segmentation process, they result in inaccurate segmentations due to artifacts and noise typically found in CT scans. Also, variability among human expert interpretations of the boundaries between materials introduces uncertainty into models, potentially leading to inaccurate simulations. In this work, we apply deep learning algorithms to automatically segment CT scans of lithium ion batteries, and we apply dropout layers to quantify the uncertainty in our model's segmentation for each voxel. Deep learning has been applied to 3D segmentation problems extensively, primarily in the medical imaging domain, and has shown to outperform existing methods. We modify a VNet architecture [2] to extend to larger volumes with potential class imbalances to segment battery CT scans. We incorporate dropout layers [1] that are active during both training and inference time to characterize the uncertainty in our model's prediction for each voxel. In addition to achieving human-level accuracy in a fraction of the time, our model maps uncertainty to inform the geometric variability in numerical simulations. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. References [1] Gal, Y. &. (2016). Dropout as a Bayesian approximation: Representing model uncertainty in deep learning. International Conference on Machine Learning, (pp. 1050-1059). [2] Milletari, F. N. (2016). V-net: Fully convolutional neural networks for volumetric medical image segmentation. 3D Vision (3DV), 2016 Fourth International Conference on. IEEE, (pp. 565-571).

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Title: Closure Models for Incompressible Navier-Stokes Equations with Variable Density

Author(s): *Arif Masud, *University of Illinois at Urbana-Champaign*; Lixing Zhu, *University of Illinois at Urbana-Champaign*;

The paper presents Residual-based closure models for variable density incompressible Navier-Stokes equations. When density is no longer constant, certain driving and/or destabilizing forces arise that can introduce instability mechanisms, that are discussed. We extend our earlier works on constant density incompressible fluids to the case of variable density fluids by consistently deriving the closure models via the Variational Multiscale (VMS) ideas. We decompose the governing system of equations for balance of momentum and conservation of mass into coarse-scale (mean flow) and fine-scale (centered fluctuations) variational sub-problems. We then apply Weak Galerkin (WG) ideas directly to the fine-scale variational problem and solving locally we extract expressions for the velocity and density fine-scales that yield the closure model. Weak continuity of fine-scale functions results in fine-scale models that inherit features of non-locality, which plays an important role in adequately representing a larger spectrum of scales in the computed flow. Representative numerical examples are presented to show the range of applicability of the method. References [1] Masud A., Calderer R. A Variational Multiscale Method for Incompressible Turbulent Flows: Bubble functions and Fine Scale Fields. Computer Meth Appl. Mech Eng, vol. 200, 2577-2593, 2011. [2] H. Gajendran, R.B. Hall, A. Masud, K.R. Rajagopal, Chemo-mechanical coupling in curing and material-interphase evolution in multi-constituent materials. Acta Mechanica, 229, 3393–3414, 2018.

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Title: Thermodynamic Consistency of Plate and Shell Mathematical Models in the context of Classical and Non-classical Continuum Mechanics and a Thermodynamically Consistent New Formulation

Author(s): Karan Surana, *University of Kansas*; *Sai Mathi, *University of Kansas*; J. N. Reddy, *Texas A&M University*;

This paper establishes that the currently used plate mathematical models such as those using Kirchhoff hypothesis, first order shear deformation assumption and higher order shear deformation assumption based on specific kinematic assumptions and their extensions to shell theories all derived using the energy methods or the principle of virtual work cannot be supported by the conservation and the balance laws of classical or the non-classical continuum mechanics. Furthermore if the deformation physics in the plates and shells requires incorporating dissipation and memory mechanisms, then the use of energy methods or the principle of virtual work is precluded for deriving the mathematical models as the mechanical deformation in such cases is not reversible. Thus, the main motivation for this work considered here is to derive a thermodynamically consistent description of the plate and shell deformation physics in which the kinematic considerations for the plate or the shell cross-sections are not chosen a priori, but instead are described in a variable and hierarchical fashion. This approach results in a single thermodynamically consistent mathematical model that remains valid and is accurate for extremely thin as well as thick plates and shells. The formulation presented in this paper intrinsically contains higher order shear deformation physics. Model problem studies and numerical results are presented for thin as well as thick plates and shells and are compared with theoretical and/or published results.

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Title: Imaging-based Reconstruction Methods for Patient-Specific Tricuspid Valve Models

Author(s): *Mrudang Mathur, *University of Texas at Austin*; Chen Shen, *University of Texas at Austin*; William Meador, *University of Texas at Austin*; Marcin Malinowski, *Spectrum Health*; Tomasz Jazwiec, *Spectrum Health*; Tomasz Timek, *Spectrum Health*; Manuel Rausch, *University of Texas at Austin*;

The tricuspid valve ensures unidirectional blood flow from the right atrium to the right ventricle. Its proper functioning depends on the well-orchestrated interplay between its three leaflets, the tricuspid annulus, and the tricuspid chordae tendineae, which connect the valve to the right ventricular endocardium. The specific role of each element of the valve is qualitatively understood but has not been captured in appropriate, patient-specific models. Doing so would be a huge step toward surgical simulations and predictive models. This is of particular interest to the surgical community given the large number of patients suffering from valve dysfunction, i.e., tricuspid regurgitation. Moreover, surgical outcomes for patients undergoing tricuspid valve repair are currently poor. To improve our quantitative understanding of tricuspid valve function and delineate the role of each member of this complex apparatus, we aim to build detailed, patient-specific finite element models of the human tricuspid valve. Toward this end, we collect sonomicrometry crystal data of tricuspid annular dynamics in explanted but beating healthy human hearts along-side hemodynamic data. We transform these data into continuous least-square cubic splines that approximate the tricuspid annulus and its dynamics throughout the cardiac cycle. Next, we explant the valve's leaflets, image them, and discretize their geometry. Subsequently, we non-rigidly transform the leaflet geometries onto the tricuspid annulus at end-diastole. Additionally, we use imaging data and literature data to reconstruct the chordae tendineae numbers and insertion sites to model complete human tricuspid valves in silico. We also identify material properties and microstructural information for leaflets and chordae via in vitro planar biaxial and uniaxial testing and 2-Photon microscopy, respectively. Finally, we apply transvalvular pressure gradients as collected in the explanted but beating healthy hearts. We solve the arising, non-linear boundary value problem in Abaqus Explicit and determine leaflet deformations and stresses for a total of eight human hearts. The valves show a complex closing behavior, with a Y-shaped coaptation line that originates from its three distinct leaflets. We find that the leaflet stresses are largest during systole and smallest during diastole with the belly regions showing maximal stresses. These findings agree well with our recent measurements of the in vivo tricuspid valve leaflet strains in the beating ovine heart. In conclusion, we developed a first patient-specific model of the TV and tested the feasibility of our combined in situ/in vitro/in silico framework.

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Title: Data-Driven Multiscale Modeling of Materials Synthesis

Author(s): *Karel Matous, *Department of Aerospace & Mechanical Engineering, University of Notre Dame, IN, USA.*;

With concentrated efforts from the materials science community to develop new multi-functional materials using unique processing conditions, the need for modeling tools that accurately describe the physical phenomena at each length scale has only further been emphasized. For example, additive manufacturing and shock synthesis lead to unique material morphologies that need to be understood for reliable engineering analysis and product safety assessments. Considering these material complexities, Direct Numerical Modeling (DNM) is accessible only for moderate system sizes. Thus, a multiscale strategy must recognize that just a relatively small part of the material will typically be instantaneously exposed to rapid material transformations. Macroscopic constitutive models obtained from homogenization, of the complex but slowly varying microstructure, may adequately describe the rest of the material. Nonlinear model reduction, pattern recognition and data-mining are a key to future on-the-fly modeling and rapid decision making. To address these challenges, we present an image-based multiscale framework for modeling the chemo-thermo-mechanical behavior of heterogeneous materials while capturing the large range of spatial and temporal scales [1]. This integrated computational approach for predicting the behavior of complex heterogeneous systems combines macro- and micro-continuum representations with statistical techniques, nonlinear model reduction and high-performance computing. Our approach exploits the instantaneous localization knowledge to decide where more advanced computations are required. Simulations involving this wide range of scales, O(106) from nm to mm, and billions of computational cells are inherently expensive, requiring use of high-performance computing. Therefore, we have developed a hierarchically parallel high-performance computational framework that executes on hundreds of thousands of processing cores with exceptional scaling performance. Any serious attempt to model a heterogeneous system must also include a strategy for constructing a complex computational domain. This work follows the concept of data-driven (image-based) modeling. We will delineate a procedure based on topology optimization and machine learning to construct a Representative Unit Cell (RUC) with the same statistics (n-point probability functions) to that of the original material. Our imaging sources come from micro-computed-tomography (micro-CT) and focused ion beam (FIB) sectioning. We show that high-performance DNM of these statistically meaningful RUCs coupled on-the-fly to a macroscopic domain is possible. Therefore, well-resolved microstructure-statistics-property (MSP) relationships can be obtained. References [1] K. Matous, M.G.D. Geers, V.G. Kouznetsova, A. Gillman, Journal of Computational Physics, 330 (2017) 192–220.

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Title: Towards Calibration of Fusion Fuel State Diagnostics

Author(s): *Kathryn Maupin, *Sandia National Labs*; Michael Glinsky, *Sandia National Labs*; Patrick Knapp, *Sandia National Labs*;

Computational modeling has advanced the study of mechanics in applications and regimes where experimentation or exploration may be dangerous or limited by cost or physical constraints. In such cases, computational models are derived using physical laws and calibrated with observational data. This process is often expensive, despite continuing advances in statistical inversion and the availability of cost-effective high-performance computing infrastructure, and can be nearly impossible if the observational data is sparse and is accompanied by large or poorly characterized uncertainties. These challenges give credence to the use of low fidelity models, such as surrogate models, which is often done in addition to higher fidelity models. Magnetized Linear Inertial Fusion (MagLIF) is a fusion concept that relies on the direct compression of magnetized, laser-heated fuel by a metal liner to achieve thermonuclear ignition. Plasma physicists rely on diagnostic metrics to infer the state of the fuel, as direct observation of the physical system is not possible. However, the calibration of these metrics is complicated by sparse experimental data and expensive high-fidelity neutron transport models. The use of a surrogate is therefore warranted, the development of which raises long-standing issues in modeling and simulation, including calibration, validation, and uncertainty quantification.

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Title: Adaptive Level-Set Topology Optimization with the eXtended Finite Element Method and Hierarchical Mesh Refinement

Author(s): *Kurt Maute, *University of Colorado Boulder*; John Evans, *University of Colorado Boulder*; Alireza Doostan, *University of Colorado Boulder*;

A broad range of topology optimization problems leads to designs with low volume fractions, i.e., the volume of the optimized design is much lower than the volume of the design domain. Using standard discretization approaches with uniformly refined meshes lead to impractical computational costs, in particular for 3D problems. Locally refining the mesh to resolve the geometry and the material layout as the design emerges in the optimization process has been identified a promising strategy and studied intensively in the past, mainly in the context of density methods. In this paper, we present a hierarchical mesh refinement scheme for level-set topology optimization. External boundaries and material interfaces are described by an explicit level-set method. The governing equations are discretized by eXtended finite element method. Starting with a coarse tensor mesh, hierarchical mesh refinement is a computationally efficient and robust method to generate 2D and 3D hexagonal and tetrahedral meshes. The refinement can be localized to regions of interest, such as in the vicinity of phase boundaries. Both, the level-set field and the state variables fields are discretized by hierarchically refined meshes, using the same or different interpolation orders. We will show with numerical examples that the proposed combination of methods leads to a computationally efficient approach to resolve local geometric features. Numerical examples include compliance and mass minimization problems with stress and eigen frequency constraints in 2D and 3D.

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Title: Data Assimilation for the Improved Modeling of Hurricane Storm Surges

Author(s): *Talea Mayo, *University of Central Florida*; Jeane Camelo, *University of Central Florida*;

Over the last century, numerical storm surge models have been developed and used for hindcasting, long-term risk assessment, and real-time forecasting of coastal flooding. In recent years, many research efforts have attempted to better resolve uncertain physical processes (e.g. wind driven waves and rainfall) that contribute to errors in storm surge forecasts. However, due to the current state of science, understanding and incorporating these physical processes into storm surge models remains a significant challenge. Furthermore, even if all processes were perfectly understood and modeled, storm surge forecasts are dependent on meteorological forcing, and are thus subject to the errors in hurricane forecasts. Here, we use observed water elevation data to compensate for these uncertainties. We develop a data assimilation framework for real-time forecasting of hurricane storm surges. Data assimilation methods combine observed data with numerical model output to improve the accuracy of modeled data, i.e. storm surge heights. Uncertain storm surge data is optimally estimated as a weighted average of what is modeled and what is observed. The weights are determined based on approximations of the respective errors of each. These methods have the advantage that they allow data to be assimilated sequentially, as data becomes available, making them particularly advantageous for real-time forecasting. This is a direct approach to reducing uncertainty in modeled data, as modeled storm surge heights are explicitly adjusted toward observed values in an optimal way. Additionally, the methods produce an estimate of the uncertainty in the improved storm surge forecast. In this work, we develop a framework to implement data assimilation methods for the Advanced Circulation (ADCIRC) model. ADCIRC is a high-fidelity numerical storm surge model that is often used for real-time storm surge guidance. We assess its performance through case studies of historical storms. We first “forecast” storm surges without implementing data assimilation. We then assimilate real-time water elevation data, e.g. tide gauge data provided by the National Oceanic and Atmospheric Administration. We compare the differences in the forecasts, those computed with and without data assimilation, to assess the potential of data assimilation to reduce uncertainties in storm surge forecasting and determine its feasibility for operational use in the future.

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Title: Three-Dimensional Fracture Propagation in Anisotropic Materials Using the Generalized Finite Element Method

Author(s): *Bryce Mazurowski, *University of Illinois at Urbana-Champaign*; C. Armando Duarte, *University of Illinois at Urbana-Champaign*;

Anisotropic materials are used extensively in many engineering applications. Single crystal and directionally solidified materials used in turbine blades and titanium alloys such as structural components composed of Ti-6242 exposed to extreme environments are known to exhibit orthotropic behavior. Settling for the assumption of isotropy is often not acceptable for the desired level of accuracy required in many applications. While there are several stress intensity factor (SIF) extraction methods for fractures in isotropic materials, extending these methods to the case of anisotropy is often not trivial. The Generalized Finite Element Method (GFEM) has shown good promise as a method for solving fracture mechanics problems when enriched with the asymptotic solution of elasticity in the neighborhood of a crack. Coupling GFEM with the Displacement Correlation Method (DCM) provides a methodology to accurately and efficiently extract SIFs in isotropic materials [1]. A reformulation of the DCM based on the mathematical framework of [2] to handle fully anisotropic materials is presented. Several quasi-static problems are analyzed showing the accuracy of the method compared to published results. A representative problem is examined using the orthotropic material properties of ti-6242 on a structural component. The results from this example problem using the anisotropic DCM are compared to those computed with the isotropic DCM to highlight the need to consider the orthotropic behavior of the material. Finally, propagation of a three-dimensional fracture in a structural component is explored. The fracture path from the simulation that considers the orthotropic properties is compared to the same problem when the directional properties are not considered. [1] Gupta, P., Duarte, C. A., & Dhankhar, A. (2017). Accuracy and robustness of stress intensity factor extraction methods for the generalized/eXtended Finite Element Method. Engineering Fracture Mechanics, 179, 120–153. https://doi.org/10.1016/j.engfracmech.2017.03.035 [2] Hoenig A. Near-tip behavior of a crack in a plane anisotropic elastic body. EngngFractMech 1982;16:393–403.

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Title: Model Reduction for Model Predictive Control of Automated Aircraft Landing

Author(s): *Andrew McClellan, *Stanford University*; Charbel Farhat, *Stanford University*; Joseph Lorenzetti, *Stanford University*; Marco Pavone, *Stanford University*;

A Model Predictive Control (MPC) algorithm seeks to produce a control law that optimizes the future behavior of a deployed system over a finite time horizon, by leveraging a real-time computational model of this system. For applications involving Fluid-Structure Interaction (FSI), this leveraging is challenging for two reasons: it implies the design of an accurate and yet real-time computational model for the prediction of the time-dependent flow-induced forces and moments acting on the system; it requires accounting for the modeling errors associated with such a computational model [1]. The projection-based reduction of CFD-based computational models for FSI provides one approach for addressing the first issue, albeit it complicates the task for addressing the second one. In this context, linear model reduction is adequate as the controller can be expected to maintain the system of interest within small perturbations around a pre-designed optimal trajectory. For applications involving FSI such as the automated landing of an aircraft considered in this talk, this requires the construction of a CFD-based Projection-based Reduced-Order Model (PROM) that is linearized not around a steady equilibrium position [2], but instead around a time-dependent trajectory. By necessity, such a CFD-based PROM is a parametric one, as it must accounts for the continuous changes of the atmospheric conditions during descent. A computational approach that addresses all these issues and is feasible for MPC will be presented in this talk, and illustrated with the PROM-based MPC of the mAEWing2 flying wing. References [1] M. Löhnig, M. Reble, J. Hasenauer, S. Yu, F. Allgöwer, Model Predictive Control using Reduced Order Models: Guaranteed Stability for Constrained Linear Systems, Journal of Process Control, vol. 24, no. 11, pp. 1647-1659, 2014. [2] T. Lieu, C. Farhat, M. Lesoinne, Reduced-Order Fluid/Structure Modeling of a Complete Aircraft Configuration, Computer Methods in Applied Mechanics and Engineering, vol. 195, nos. 41-43, pp. 5730-5742, 2006.

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Title: Finite Element Modeling of Soil Impact on the Army Combat Uniform for Design of Extremity Protection

Author(s): *Justin McKee, *US Army Research Laboratory*; Robert Spink, *US Army Research Laboratory*; David Fox, *US Army Research Laboratory*;

High-velocity soil propelled by buried explosives presents a threat to the dismounted Soldier that can cause extensive soft tissue damage to the extremities with poor treatment prognosis. These injuries can lead to long term physiological and psychological complications that reduce quality of life and require high health care costs. While it is desirable to add protection to reduce injury, extremities protection design is a challenge due to the need to keep weight low and maintain flexibility and comfort where joints such as the knee and hip require a large range of motion. Our approach is to optimize the uniform fabric, which is currently the only protection that covers much of the Soldier's extremities and has not been well characterized for soil blast loading. We have developed a yarn level model of the Fire-Resistant Army Combat Uniform (FR-ACU) with a soft backing to represent the underlying soft tissue. Simulations of impact from a soil cluster are performed to investigate how the soil, yarn, and backing interact and affect stress propagation and failure of the textile. First, a comparison is made between a 0 and 60 degree obliquity impact. Simulations show higher stress and failure in the 60 degree obliquity scenario resulting from the shape of the deflection profile and how the particles interact with the texture of the fabric formed by the yarn. Tension created by multiple soil particle impacts cause tears to propagate through the fabric along the yarn axes that would leave skin directly exposed to subsequent soil impacts. Next, fabric design is explored by changing the construction of the yarns. A simulation of fabric made of continuous filament yarns rather than staple yarns results in a reduction in tearing that would leave less skin exposed to soil flow. Similarly, replacing only ripstop yarns with higher strength continuous filament yarns was also effective at reducing tearing of the fabric. Both cases provide improvement in the performance of the FR-ACU fabric without additional weight. The FE model illustrate mechanisms of failure during soil loading that are unique compared to single projectile penetration of textiles and demonstrates potential improvement in protection that could be provided to the Soldier based on yarn construction.

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Title: Adaptive Seeding of Geometric Primitives in Topology Optimization Using the Topological Derivative

Author(s): *Pauline Menoret, *University of Connecticut*; Antonio Novotny, *Laboratório Nacional de Computação Científica (LNCC/MCT)*; Julian Norato, *University of Connecticut*;

Density-based and level-set methods for topology optimization typically result in organic designs that cannot be easily translated into manufacturable components and material systems, particularly when a structure made of primitives is desired. The geometry projection method circumvents this limitation by rendering optimal designs exclusively made of geometric primitives, such as cylindrical struts in a periodic lattice. To accomplish this, the geometry projection method smoothly maps a high-level parametric representation of the primitives onto a smooth density field. This field is subsequently discretized using a fixed finite element mesh for analysis, thus avoiding the need for re-meshing, just as in free-form topology optimization methods. In addition to its geometric parameters, each primitive is also ascribed with a size variable that, in the spirit of solid isotropic material penalization (SIMP), is penalized in the optimization so that a zero-size variable indicates the primitive can altogether be removed from the design. This feature of the geometry projection method greatly facilitates removing primitives from the design and therefore promoting convergence to optimal designs. To date, geometry projection techniques have employed arbitrary initial designs prescribed by the designer. That is, the designer must provide the location and dimensions for a fixed number of primitives. These primitives can be removed from the design during the optimization (by zeroing their size variables as aforementioned), however no strategy exists to adaptively seed new primitives. Here, we present a method to adaptively introduce geometric primitives of arbitrary shape in the topology optimization. To achieve this, we employ the topological derivative of the objective function with respect to the introduction of an infinitesimal inclusion with the same shape as the desired primitive. Primitives are then introduced at locations with the lowest topological derivative value. We demonstrate our method with the design of 2-dimensional structures made of bars. We first consider the minimization of thermal compliance in steady-state heat conduction, for which a closed-form expression of the topological derivative exists. We also consider the minimization of structural compliance in linear elasticity, which requires numerical construction of the topological derivative.

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Title: Variational Multiscale Error Estimates for Navier-Stokes Equations. Application to Anisotropic Mesh Adaptation

Author(s): *Youssef Mesri, *MINES ParisTech, PSL Research University, France*;

ABSTRACT This work is motivated by the success of the anisotropic adaptive finite element methods in accurately simulating complex physical systems in science and engineering. Anisotropic mesh adaptation is nowadays a mature tool to assist at a low computation cost the high-accuracy resolution. Thanks to error interpolation indicators and metric based adaptation, the mesh adaptation becomes a transparent black-box tool for a large panel of PDEs [2]. However, error interpolation indicators did not guarantee the robustness of the error estimation which leads to over-estimate the approximation error. This effect is accentuated in the context of the Navier-Stokes equations in particular for turbulent unsteady flows in which different scales interact. Recent works on variational multiscale error estimators for convection diffusion equation are shown the potential of such approaches in particular for dominated convection flows [5]. Indeed, the derived a posteriori error estimator takes into account the solution subscales as well. This approach was extended in [1.3] in order to be used for anisotropic mesh adaptation. The VMS error estimator is combined with the error interpolation error as a scaling function to derive a computable anisotropic error estimator. The latter is used to build variational multiscale metrics for anisotropic mesh adaptation. The focus of the present paper is on the construction of a VMS error estimator for the Navier-Stokes equations. The latter are discretized with the VMS finite element formulation in which the errors on velocity and pressure are modeled with respect to the equation residuals [4]. As in [1], the VMS error estimator is combined with the interpolation error to derive an anisotropic error estimator to be used in mesh adaptation. This paper in fine presents a new anisotropic a posteriori error estimator for the Navier-Stokes equations. It controls large and subscale errors in all space directions. From the VMS a posteriori error analysis, we get an optimal metric (optimal mesh) as a minimum of an error estimator function constrained by a given number of elements. The optimal metric obtained is used to build an optimal mesh for the given number of elements. Validation of the proposed approach on 2D and 3D benchmarks will be presented. REFERENCES [1] A Bazile, E Hachem, JC Larroya-Huguet, Y Mesri Variational Multiscale error estimator for anisotropic adaptive fluid mechanic simulations: Application to convection–diffusion problems. CMAME 331, 94-115. [2] Y, Mesri, M. Khalloufi, E. Hachem, On optimal simplicial meshes for minimizing the Hessian-based errors, APNUM, Vol. 109, pp. 235-249, 2016 [3] Y Mesri, A Bazile, JC Larroya-Huguet, E Hachem Parallel and adaptive VMS finite elements formulation for aerothermal problems. Computers & Fluids 173, 42-50 [4] E. Hachem, M. Khalloufi, J. Bruchon, R. Valette, Y. Mesri, Unified adaptive Variational MultiScale method for liquid-gas flows, CMAME, Vol. 308, pp. 238-255, 2016 [5] D. Irisarri, G. Hauke, A posteriori pointwise error computation for 2-D transport equations based on the variational multiscale method, CMAME 311 (2016) 648–670.

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Title: An Efficient Method for Computing Exact Sensitivities of Nonlinear History Dependent Material Models

Author(s): Van Tung Phan, *Argonne National Laboratory*; *Mark Messner, *Argonne National Laboratory*;

The mechanical response of an inelastic material is often described through a nonlinear model with some set of internal variables. Oftentimes we might want the sensitivities of such a material model -- the derivative of the model output with respect to the model parameters -- to perform sensitivity analysis on the parameters or to find optimal model parameters by comparison to experimental data using gradient-based methods. However, a dependence on internal, hidden variables makes computing the sensitivities difficult as the current state of the model depends not only on the current input but also on the entire chain of past internal variables leading up to the current state. This presentation describes a fast, numerically efficient method for computing the sensitivities of such models that does not require storing the entire past history of the internal variables. Instead, the method propagates the sensitivities along with the current state. The only additional storage required is the model sensitivity at the previous state and the sensitivity update only requires the factorized Jacobian of the current model state with respect to the input and internal variables, which is already available if the model update is computed with an implicit time integration. The method works for both stress driven and strain driven problems. We demonstrate the utility of this method by computing optimal model parameters from synthetic and actual experimental data and assess the benefits of a gradient-based optimization methods against other common methods of determining material parameters from data, including genetic algorithm optimization.

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Title: An Optimal Isogeometric Dual Mortar Method for Fourth Order Problems

Author(s): *Di Miao, *Brigham Young University*; Michael Scott, *Brigham Young University*; Michael Borden, *Coreform*; Dereck Thomas, *Coreform*;

Due to the tensor product structure, conventional non-uniform rational B-splines (NURBS) surfaces become inefficient when dealing with complex geometries. Though multi-patch NURBS can be used to discretize complicated domain, additional treatments are needed to handle couplings along patch interfaces. Among popular domain decomposition methods, mortar method is superior in that it neither introduces additional degrees of freedom nor requires the evaluation of penalty parameters. In this talk, we propose a dual mortar method, which allows us to apply weak C^1 constraint across patch interfaces to solve higher order PDEs. By using locally supported dual basis, the condensed stiffness matrix preserves sparsity and positive definiteness. Meanwhile, we propose a quadrature free algorithm to robustly construct the enriched dual basis. Whereas conventional dual basis does not reproduce all polynomials but constant, leading to a sub-optimal convergence; the enriched dual basis can reproduce polynomials up to a given order without losing their compact supports. The optimal approximation properties of the proposed method have been confirmed in biharmonic benchmarks. We also demonstrate the capacity of the proposed dual mortar method in solving Cahn-Hilliard problem and Kirchhoff-Love shell problem.

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Title: Shock Capturing with Deep Neural Networks

Author(s): *Craig Michoski, *University of Texas at Austin*; Miloš Milosavljevi?, *University of Texas at Austin*; David Hatch, *University of Texas at Austin*; Todd Oliver, *University of Texas at Austin*;

Capturing shock fronts and highly nonlinear features of PDEs has traditionally posed a challenging problem for numerical methods. Most shock-capturing schemes significantly degrade the accuracy of the solution in the regions of interest, or they exactly parameterize the moving front in a way that is only feasible in the simplest of cases; and all while increasing the computational cost of the underlying numerical method. We display an alternative formulation employing deep neural networks to capture shocks, where the computational cost of the method is not increased and the accuracy of the method is not degraded.

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Title: Analysis of Semi-Elliptical Fatigue Crack Propagation

Author(s): *Yozo Mikata, *Fluor*;

Introduction In this paper, fatigue crack propagation of a semi-elliptical crack under a uniform loading is investigated. The focus of this paper is to solve differential equations derived from Paris law [1]. Stress intensity factors are approximate. Those approximate stress intensity factors are based on empirical equations given in [3] and [4]. Mathematical formulations The governing equations for fatigue crack propagation of semi-elliptical cracks are derived from Paris law. By introducing an intermediate special function, it is shown that the governing equations can be semi-analytically solved. As an application of the mathematical result, numerical examples will be shown. Conclusion Semi-analytical solutions are obtained for fatigue crack propagation of semi-elliptical cracks based on the assumption that the crack shape stays self-similar. References 1. Paris, P.C., Erdogan, F. (1963). “Critical Analysis of Crack Propagation Laws,” Journal of Basic Engineering, Vol. 85, pp. 528-534. 2. Tada, H., Paris, P.C., Irwin, G.R. (1985). The Stress Analysis of Cracks Handbook (2nd Ed.), Paris Production Inc., St. Louis. 3. Newman, J.C., Raju, I.C. (1981). “An Empirical Stress-Intensity Factor Equation for the Surface Crack,” Engineering Fracture Mechanics, Vol. 15, pp. 185-192. 4. Anderson, T.L. (1995). Fracture Mechanics, Second Edition, CRC Press.

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Title: Towards the Development of a Growth and Remodeling Model to Elucidate Vaginal Prolapse

Author(s): Akinjide Akintunde, *Tulane University*; Gabrielle Clark, *Tulane University*; *Kristin Miller, *Tulane University*;

Pelvic organ prolapse (POP) is the descent of the female pelvic organs including through the vagina. Although the underlying mechanisms of POP remain unknown, we hypothesize that elastic fiber fragmentation precipitates decreased structural integrity and increased risk of POP. Additionally, smooth muscle cell (SMC) contractility is decreased in vaginal tissue of women with POP and in vasculature of mice with defects in elastic fiber integrity [1]. The interactions between vaginal SMCs and elastic fibers, however, are not known. Further, the vagina is understudied from a biomechanical perspective, thus the structural mechanisms by which elastic fibers and SMCs contribute to POP are currently unknown. This lack of understanding impedes progress towards preventing POP and developing effective interventions. Towards this end, mathematical models–particularly growth and remodeling (G&R) models are effective tools to better understand the structural mechanisms of POP. In addition, such tools allow the evaluation of potential intervention strategies to impede POP progression in silico. To address these knowledge gaps, our recent research efforts are focused on understanding the role of (1) elastic fibers and (2) SMCs in the biaxial mechanical response of the murine vagina wall and remodeling as a function of age and pressure. In healthy vaginal tissue, elastic fibers provide tissue compliance and regulate collagen fiber recruitment with increasing load through maintenance of collagen crimp [2]. Along with SMCs, elastic fibers contribute to the maintenance of the vaginal caliber and overall tissue geometry. These findings provide fundamental knowledge towards understanding the underlying structural and ECM changes in POP. The results of these studies motivated the formulation of a first-generation G&R model for the vagina, that can be used to investigate the independent role and potential interaction of elastic fiber disruption and SMC contractility on POP progression. Validated strain-energy function and model parameters were implemented in the constrained mixture theory of G&R, employed to account for the mechano-mediated production and degradation of vaginal ECM and test multiple hypotheses regarding POP development [3]. Ongoing work on the model formulation and preliminary results will be presented. References [1] Boreham et al., 2002, Am J Obstet Gynecol. [2] Akintunde et al., 2018, J Biomech Eng. [3] Humphrey & Rajagopal, 2002, Math Model Methods Appl Sci.

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Title: Simulation of a Surrogate Head Model Subjected to Blast

Author(s): *Scott T. Miller, *Sandia National Laboratories*; Candice Cooper, *Sandia National Laboratories*; Adam Willis, *San Antonio Military Medical Center*; Ricardo Mejia-Alvarez, *Michigan State University*;

Blast-induced Traumatic Brain Injury (bTBI) is a signature wound of modern warfare. Resulting persistent neurologic/behavioral symptomatology includes headaches, sleep disorder, cognitive impairment and mood disturbance. The physical damage mechanisms of bTBI are not yet understood, but clinical experience and neuropathologic analysis seems to indicate that it is an interface problem. In particular, astroglial scarring at multiple intracranial interfaces is observed clinically. This talk presents an on-going project whose goal is to build a simplified head model which reproduces the human intracranial injury after blast exposure in order to isolate the mechanism(s) of injury. After presenting background information on bTBI and the experimental side of the project, we introduce our surrogate head model (i.e., test object) and identify the clinical observations we intend to reproduce. Our computational simulations use an explicit Lagrangian finite element model for the test object coupled to an Eulerian shock-physics code to deliver the incident blast. Metrics such as strain, strain rate, pressure, etc, are evaluated and examined near the fluid-structure interfaces. Intracranial cavitation is investigated, and skull vibrations are examined as a driver of intracranial pressure waves.

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Title: The Complex and Hypercomplex Finite Element Method for Computational Fracture

Author(s): *Harry Millwater, *University of Texas at San Antonio*; Arturo Montoya, *University of Texas at San Antonio*; Daniel Ramirez, *University of Texas at San Antonio*; Andres Aguirre, *University of Texas at San Antonio*; Manuel Garcia, *Angelo State University*;

The complex-variable finite element method, ZFEM, provides a convenient and accurate approach to computing shape, material, and loading sensitivities. The traditional finite element method is augmented with imaginary nodes and degrees of freedom (DOF). Perturbations of the model are then applied along the imaginary direction. After solving the system of equations, sensitivities of the displacement field are then contained in the imaginary DOF. This approach also scales to higher order derivatives through the use of hypercomplex variables with additional imaginary axes. The application of ZFEM in fracture mechanics provides a new, robust, and highly accurate method for computing the energy release rate (ERR) through the imaginary perturbation of the crack surface. The method has been verified for LEFM, EPFM, thermoelastic, FGMs, mixed mode, interface cracks, and others. The results have been shown to be as accurate as the J integral but more general. In addition, derivatives of the ERR with respect to structural parameters, e.g., geometric features (notch radius, hole size) and material properties can be computed using second order sensitivity analysis. This presentation will focus on new extensions of the methodology, in particular, - Extension to higher order (second and higher) using multicomplex or multidual algebra - Efficiency improvements using a local stiffness derivative approach - A new “block-solver” methodology for solving the hypercomplex system of equations - New application areas such as interacting cracks and thermally-driven progressive fracture H.R. Millwater, D. Wagner, A. Baines, and A. Montoya, “A Virtual Crack Extension Method to Compute Energy Release Rates using a Complex Variable Finite Element Method,” Engineering Fracture Mechanics 162 (2016) 95–111, http://dx.doi.org/10.1016/j.engfracmech.2016.04.002 D. Ramirez Tamayo, A. Montoya, H.R. Millwater, “Application of the Complex-variable Finite Element Method to Mixed Mode Fracture and Interface Cracks”, AIAA Journal, V 56, No. 11 (2018), https://arc.aiaa.org/doi/abs/10.2514/1.J057231 A. Montoya, D. Ramirez Tamayo, H.R. Millwater, and M. Kirby, “A Complex-Variable Virtual Crack Extension Finite Element Method for Elastic-Plastic Fracture Mechanics, Engineering Fracture Mechanics”, 202 (2018) 242-258 https://doi.org/10.1016/j.engfracmech.2018.09.023

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Title: From an Efficient A posteriori Algebraic Error Estimator to a p-robust Multilevel Solver

Author(s): *Ani Miraçi, *Inria, 2 rue Simone Iff, 75589 Paris, France & Université Paris-Est, CERMICS (ENPC), 77455 Marne-la-Vallée 2, France*; Jan Papež, *Inria, 2 rue Simone Iff, 75589 Paris, France & Sorbonne Université, Univ. Paris-Diderot SPC, CNRS, Laboratoire Jacques-Louis Lions, France*; Martin Vohralík, *Inria, 2 rue Simone Iff, 75589 Paris, France & Université Paris-Est, CERMICS (ENPC), 77455 Marne-la-Vallée 2, France*;

In this work, we consider conforming finite element discretizations of arbitrary polynomial degree p ? 1 of the Poisson problem. We propose a multilevel iterative algebraic solver and an a posteriori estimator on the algebraic error. We prove that the algebraic error estimate is reliable and efficient (represents a two-sided bound of the error), with a constant independent of p. We show that the iterative solver contracts the algebraic error on each iteration with a factor bounded independently of the degree p. Actually, these two results are equivalent. The p-robustness results rely on the work of Schöberl et al. [2] for one given mesh. We combine this with the design of an algebraic residual lifting constructed over a hierarchy of meshes, in the spirit of Papež et al. [1]. This construction is obtained by employing one multigrid-type iteration to approximate the algebraic error. This includes a global coarse level lowest-order (p = 1) solve with local higher-order (p) contributions from the subsequent mesh levels. The higher-order contributions are given as solutions of Dirichlet problems posed over patches of elements around vertices, that are mutually independent and thus naturally parallelizable. This residual lifting is the core of our a posteriori estimator and determines the descent direction for the next iteration of our multilevel solver. Numerical tests are presented to illustrate these theoretical findings. REFERENCES [1] J. Papež, U. Rüde, M. Vohralík, and B. Wohlmuth, Sharp algebraic and total a posteriori error bounds for h and p finite elements via a multilevel approach. HAL Preprint 01662944, 2017. URL https://hal.inria.fr/hal-01662944. [2] J. Schöberl, J. M. Melenk, C. Pechstein, and S. Zaglmayr, Additive Schwarz preconditioning for p-version triangular and tetrahedral finite elements, IMA J. Numer. Anal., 28 (2008), pp. 1–24.

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Title: Damage Detection via Embedded Sensory Particles – Effect of Particle/Matrix Interphase Properties

Author(s): *Mirmilad Mirsayar, *Aerospace Eng Department, Texas A&M University*; Darren Hartl, *Aerospace Eng Department, Texas A&M University*;

The use of novel composites in various engineering applications offers multifunctional benefits in both cost and time efficiency for structural reinforcement and other purposes (e.g., self-sensing, self-healing, etc.) simultaneously. Recent studies corroborate the use of embedded sensory particles made of magnetic shape memory alloys (MSMAs) as a new technique of non-destructive evaluation and health monitoring of metallic structures. Due to the applied mechanical load, stress-induced phase transformation occurs at a certain stress level in the embedded particles changing their mechanical and magnetic properties. The location of a crack, which causes the highest stress concentration, can then be detected via this technique by monitoring the localized changes in the magnetic properties of the composite. The feasibility of this approach strongly relies on the particle/matrix interphase properties playing a significant role in transferring the far-field applied stress from the matrix to the embedded particles. Using the finite element analysis, this work investigates the effects of material properties and thickness of the interphase on the phase transformation response in embedded SMA particles in the vicinity of a crack. Depending on the interphase elastic and cohesive properties, the interphase thickness, and the operational temperature, it is found that interphase damage may occur at different stress levels affecting phase transformation response in SMA particles. The effect of particle position relative to the crack tip on interphase damage as well as particle transformation response is studied by a full factorial design of experiments. Finally, to manifest the feasibility of the technique, the changes in magnetic permeability and thus changes in magnetic field strength due to the applied stress field is evaluated.

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Title: Electrode Microstructural Origins of Hot Spot Formation in Lithium-Ion Batteries

Author(s): *Aashutosh Mistry, *School of Mechanical Engineering, Purdue University*; Mukul Parmananda, *School of Mechanical Engineering, Purdue University*; Partha Mukherjee, *School of Mechanical Engineering, Purdue University*;

Thermal interaction is an inescapable trait of high energy lithium-ion cells. Heat generation and undesirable local thermal excursion represent a considerable safety concern for modern-day Li-ion batteries, e.g., in electric vehicles. Self-heating owing to electrode microstructural resistances to multi-modal transport mechanisms is an intrinsic characteristic of porous electrodes1. Such electrodes exhibit considerable spatial inhomogeneity which translates to heterogeneous heat generation rates, effectively causing hot spot formations during operation. This work presents a mesoscale analytics based on tomographic image-based reconstruction of porous electrodes and thermo-electrochemical interactions to comprehend the correlation between microstructure-scale spatial variability on the local thermal signature evolution.

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Title: Conditional Mutual Information to Quantify Information Content of Sequential Synthetic MRI Acquisitions

Author(s): *Drew Mitchell, *The University of Texas MD Anderson Cancer Center*; Ken-Pin Hwang, *The University of Texas MD Anderson Cancer Center*; Jason Stafford, *The University of Texas MD Anderson Cancer Center*; James Bankson, *The University of Texas MD Anderson Cancer Center*; David Fuentes, *The University of Texas MD Anderson Cancer Center*;

Introduction: We model an adaptation of 3D QALAS (3D-quantification using an interleaved Look-Locker acquisition sequence with T2 preparation pulse) for 3D multi-parameter quantification in the brain.[1] 3D QALAS is a novel technique that is based on a multi-acquisition 3D gradient echo sequence. The primary drawbacks of quantification methods are scan time and accuracy. Many existing methods require clinically unacceptable scan times, while fast methods typically have a narrow range of accuracy or require high SNR to obtain adequate estimates.[2] Information theory addresses these two drawbacks by quantifying the information content of potential acquisitions. Mutual information is a measure of information gained about final parametric map reconstructions from acquisitions with specific acquisition and subsampling parameters. Optimizing this metric allows selection of parameters which maximize synthetic MRI reproducibility. Methods: A mathematical model of the 3D QALAS sequence represents the uncertainty in parametric map reconstruction and machine noise during acquisition. A recursive conditional mutual information formulation quantifies information content of a new measurement given any number of previous acquisitions with independent parameters. Mutual information is calculated using Markov chain Monte Carlo to compute the required high-dimensional integration. A representative in silico phantom is used to estimate mutual information and predict optimal acquisition parameters. To test acquisition parameter optimization, two scans were performed on a System Standard Model 130 phantom (QalibreMD, Boulder, CO) with a 3T scanner (MR750, GE Healthcare, Waukesha, WI). Results: Reconstruction uncertainty is measured by the standard deviation of parametric map values within the phantom elements. For M0, T1, and T2 maps, the standard deviation of reconstructed values is negatively correlated with mutual information. A reconstruction from an acquisition conditioned on a low-resolution pre-scan image also demonstrates reduced reconstruction uncertainty compared to an image from an unconditioned acquisition. Conclusion: This information theoretic analysis enables quantitative guidance of synthetic MRI acquisitions across multiple applications. It is a novel quantitative understanding of parametric map reconstruction uncertainty in terms of acquisition and subsampling parameters, which is currently understood only heuristically. This quantitative optimization has potential applications in corrective updates to acquisitions in real time, which could range in complexity from updating new measurements locations in undersampled acquisitions to altering pulse sequence parameters mid-scan to maximize information acquired within clinical constraints. References: 1. Kvernby et al. (2014). Simultaneous three-dimensional myocardial T1 and T2 mapping in one breath hold with 3D-QALAS. 2. Odrobina et al. (2005). MR properties of excised neural tissue following experimentally induced demyelination.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Flow-induced Vibration of a Circular Cylinder with Attached Flexible Splitter Plate

Author(s): Mohd Furquan, *IIT Kanpur*; Tulsi Sahu, *IIT Kanpur*; *Sanjay Mittal, *IIT Kanpur*;

Flow-induced vibration (FIV) of an elastically mounted circular cylinder with an attached splitter plate in a uniform flow is studied in the laminar regime. Two different reduced speeds are defined to quantify the compliance of the elastic support and flexibility of the splitter plate. The vibration response of the flexible plate, and a stationary cylinder, exhibits lock-in with various eigenmodes of the plate in different ranges of reduced speed. The onset of these lock-in regions is abrupt and hysteretic. The elastically mounted cylinder, without the splitter plate, undergoes large amplitude vortex-induced vibration (VIV). A rigid splitter plate attached to the cylinder reduces the peak amplitude during VIV significantly. However, galloping is observed beyond a critical reduced speed. The flexibility of the plate, profoundly, affects the vibration response of the system. In the limit of infinite flexibility, the system behaves like an isolated cylinder. It is associated with large amplitude VIV but is devoid of galloping. It is found that the galloping instability sets in when the flexibility of the plate is less than a certain value. Interestingly, VIV and galloping are separated by a regime of steady flow. In the VIV regime, the plate-tip and cylinder vibrate in phase for low reduced speed; they are out of phase for larger reduced speed. The change in phase is also associated with change in the frequency of vibration. At low speed the frequency of vibration is close to the first natural frequency of the system, while at high reduced speed it is closer to the second natural frequency. Optimal flexibility of the splitter plate is estimated for which the VIV is low and the system is not prone to galloping instability. The idea has promise in design of devices for suppression of VIV in off-shore applications. A stabilized space-time finite element method is used for carrying out the flow computations [1]. [1] Furquan, M. & Mittal, S. 2015 Flow past two square cylinders with flexible splitter plates. Comput. Mech. 55 (6), 1155-1166.

15th U.S. National Congress on Computational Mechanics
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Title: The Complex- and Hypercomplex- Variable Finite Element Method in Nonlinear Fracture Mechanics Problems

Author(s): *Arturo Montoya, *The University of Texas at San Antonio*; Daniel Ramirez, *The University of Texas at San Antonio*; Harry Millwater, *The University of Texas at San Antonio*;

The complex variable finite element method, ZFEM, has been extended for computing the nonlinear energy release rate (ERR) of materials undergoing plastic deformation. Contour-based approaches, such as the J-integral, are known to exhibit contour path dependency and monotonic loading limitations in elastic-plastic fracture problems. ZFEM computes the numerical derivative of the potential energy with respect to a crack extension by implementing the complex Taylor series expansion method (CTSE) within the finite element formulation for nonlinear problems. A virtual crack extension is introduced by elongating the imaginary component of complex-nodal coordinates surrounding the crack tip. The verification of the ZFEM method consisted of simulating experimental tests of compact tension specimens using material models based on the deformation and incremental theory of plasticity and comparing the results against the J-integral solution and ASTM standards approximation. The specimens were exposed to a loading/unloading cycle. The following conclusions were obtained from these simulations: • ZFEM provides an accurate, single ERR estimate at all levels of plasticity, i.e. small scale, contained, and large scale yielding. On the contrary, the J-integral results are contour dependent for incremental plasticity. A saturated J-integral value is reached at different contours for varying load levels. • ZFEM does not depend on the existence of a strain energy density formulation to compute the ERR. • ZFEM provides accurate ERR estimates under loading/unloading conditions, while the J-integral is inaccurate during unloading. In addition, extending a finite element model into a hypercomplex domain allows the computation of high-order derivatives of strain energy with respect to a crack path extension, which can be used to predict the crack growth direction under a given loading. Reference 1. A. Montoya, D. Ramirez Tamayo*, H.R. Millwater, and M. Kirby*, “A Complex-Variable Virtual Crack Extension Finite Element Method for Elastic-Plastic Fracture Mechanics, Engineering Fracture Mechanics”, 202 (2018) 242-258. https://doi.org/10.1016/j.engfracmech.2018.09.023

15th U.S. National Congress on Computational Mechanics
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Title: Polytopal Discontinuous Petrov-Galerkin (PolyDPG) Applied to Linear Elasticity

Author(s): *Jaime Mora Paz, *University of Texas at Austin*; Leszek Demkowicz, *University of Texas at Austin*; Mohamed Ebeida, *Sandia National Laboratories*;

As a continuation of the Discontinuous Petrov-Galerkin (DPG) finite element methodology for polygonal meshes, labeled PolyDPG, initially derived in 2D as a conforming discretization of the ultraweak variational formulation of Poisson's equation [1], we now present PolyDPG for polyhedra. This 3D version is characterized by a non-conforming discretization of traces. A convergence proof of the proposed method for the linear elasticity equations is given. The method shows the expected convergence rates in numerical experiments with different polyhedral meshes, including Voronoi partitions generated by VoroCrust [2]. As an application of the method, we investigate a linear elasticity model of a composite material with an incompressible matrix and large material contrast, inspired by the research on elastomeric syntactic foams at Sandia National Laboratories [3]. REFERENCES [1] Vaziri Astaneh, A., Fuentes, F., Mora, J., and Demkowicz, L. (2018). High-order polygonal discontinuous Petrov–Galerkin (PolyDPG) methods using ultraweak formulations. Computer Methods in Applied Mechanics and Engineering, 332:686–711. [2] Abdelkader, A., Bajaj, C. L., Ebeida, M. S., Mahmoud, A. H., Mitchell, S. A., Owens, J. D., and Rushdi, A. A. (2018). Sampling conditions for conforming Voronoi meshing by the VoroCrust algorithm. arXiv preprint arXiv:1803.06078. [3] Brown, J., Carroll, J., Huddleston, B., Casias, Z., and Long, K. (2018). A multiscale study of damage in elastomeric syntactic foams. J. Mater. Sci., 53(14):10479–10498.

15th U.S. National Congress on Computational Mechanics
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Title: Multiscale Design and Fabrication of a Reliably Manufacturable Negative Stiffness Metamaterial

Author(s): Carolyn Seepersad, *UT Austin*; *Clinton Morris, *PARC*; Michael Haberman, *UT Austin*;

A negative stiffness metamaterial is designed to demonstrate mechanical stiffness and loss properties that exceed those of its constituent materials. The metamaterial is designed with a multi-level, set-based design approach that leverages machine learning algorithms, specifically Bayesian network classifiers, to create inverse maps of the design space at each level, thereby supporting design exploration. The resulting metamaterials are comprised of micron-scale negative stiffness inclusions embedded within a viscoelastic matrix. The inclusions are fabricated with a micro-stereolithography process. To ensure that resulting designs are reliably manufacturable, manufacturing variability is quantified and incorporated into the design process. The metamaterial is assembled and tested, and results demonstrate broadband damping capabilities from a passive, mechanically tunable metamaterial.

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Title: Simulation and Experimental Validation of Fracture, Fragmentation, and Debris Field Formation of Glass Lite Specimens under Blast Loading Using the Applied Element Method

Author(s): *Jonathan Moss, *University of North Carolina at Charlotte*; Matthew Whelan, *University of North Carolina at Charlotte*; David Weggel, *University of North Carolina at Charlotte*;

Numerical simulation of blast events, specifically those involving debris field formation, presents a complex set of modeling challenges. A relatively new method of analysis, the Applied Element Method (Meguro and Tagel-Din, 2000) has been demonstrated to be an effective alternative to the commonly used Finite Element Method and shows promise for simulation of the response of structural components under blast loading, specifically for those involving brittle fracture and debris field formation. The relative ease with which element separation and collision, two critical aspects of debris field formation, can be modeled using the Applied Element Method underscore its suitability for such problems. In this study, the effectiveness of the Applied Element Method for predictive simulations of debris field formation, specifically as a tool for hypothesis testing in a post-blast investigative environment, is evaluated through comparison to experimental databases compiled through open-arena blast testing of conventional glass lite specimens. An overview of the Applied Element Method will be presented with specific detail given to the development of a model for simulation of debris field formation resulting from blast loading of conventional building fenestration systems. Experimental data compiled over a series of six open-arena blast tests performed on a conventional façade structure featuring six glass lite specimens mounted to aluminum mullions on a steel reaction frame backed by an enclosure specifically constructed for tracking debris field formation will be used for comparison to Applied Element Method simulations. Experimental measurements obtained across the set of open-arena blast tests include measurement of the incident and reflected blast pressures, high-speed videography, and debris field measurements across the floor of the building enclosure as well as a witness panel on the rear wall. The results of the Applied Element Method simulations will be compared to the experimental databases, with specific emphasis on the predictive accuracy of the fragmentation and debris field formation of the glass lite specimens under blast loading. Meguro, K. and Tagel-Din, H. (2000) “Applied Element Method for Structural Analysis: Theory and Applications for Linear Material,” Structural Engineering/Earthquake Engineering JSCE, 17(1). 21-35.

15th U.S. National Congress on Computational Mechanics
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Title: DFT-FE: Parallel Adaptive Finite-element Code for Material Modeling Using Density Functional Theory

Author(s): *Phani Motamarri, *University of Michigan Ann Arbor*; Sambit Das, *University of Michigan Ann Arbor*; Vikram Gavini, *University of Michigan Ann Arbor*;

Large-scale DFT calculations are very crucial to improve the predictive capabilities of computation based design of new materials in a variety of application areas. For example, accurate determination of dislocation core properties in metals and semiconductors, understanding ion conduction mechanisms and computing diffusivities in solid-state electrolytes, and large-scale bio-molecular simulations, all require the ability to conduct accurate and computationally efficient DFT calculations involving many thousands of atoms on both metallic and insulating systems. However, the solution to governing equations in DFT demands significant computational resources, and accurate DFT calculations are routinely limited to material systems with at most few thousands of electrons restricting the system sizes to a few hundred atoms. This computational complexity is of bigger concern in the context of ab-initio molecular dynamics with long time-scales and atomic relaxations with large number of relaxation steps. To overcome the above limitations, an open-source code DFT-FE based on adaptive finite-element discretization of DFT has been released recently, and this talk will present the recent research efforts in enabling systematically convergent and computationally efficient large-scale DFT calculations on material systems with tens of thousands of electrons for both metallic and insulating systems, on massively parallel computing architectures, while allowing for arbitrary boundary conditions and complex geometries using DFT-FE. Key computational ideas involved in the development of DFT-FE will be discussed: (i) unified real-space formulation for DFT (ii) a-posteriori mesh adaption for optimal finite-element meshes (iii) adaptive higher-order spectral finite-element framework in conjunction with Chebyshev acceleration, spectrum splitting based Rayleigh procedure combined with mixed precision arithmetic (iv) configurational force approach for geometry optimization. The numerical investigations conducted with DFT-FE on representative benchmark examples will be discussed along with performance comparisons with other widely used DFT codes like Quantum espresso and ABINIT.

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Title: A Thermodynamically Consistent Discontinuous Galerkin Formulation for Interface Separation

Author(s): Daniele Versino, *Los Alamos National Laboratory*; *Hashem Mourad, *Los Alamos National Laboratory*;

The formulation of an interface damage model, based on the discontinuous Galerkin (DG) method, is presented. This interface model is used for the simulation of failure and crack propagation in homogeneous and laminated structures in both static and dynamic analyses. The DG formulation avoids common difficulties associated with cohesive elements. Specifically, it does not introduce any artificial interfacial compliance and, in explicit dynamic analysis, it leads to a stable time increment size which is unaffected by the presence of stiff massless interfaces. The proposed method is implemented in a finite element setting. Convergence and accuracy are demonstrated in Mode I and mixed-mode delamination. Significantly, numerical results obtained using the proposed interface model are found to be independent of the value of the penalty factor that characterizes the DG formulation. By contrast, numerical results obtained using a classical cohesive method are found to be dependent on the cohesive penalty stiffnesses. As a result of this notable advantage, the proposed approach is shown to yield more accurate predictions pertaining to crack propagation under mixed-mode fracture. Furthermore, in explicit dynamic analysis, the stable time increment size calculated with the proposed method is found to be an order of magnitude larger than the maximum allowable value for classical cohesive elements.

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Title: A General Decomposition of Two-Dimensional Peridynamic Force States with Applications to Plasticity

Author(s): *Farzaneh Mousavi, *University of Nebraska-Lincoln*; Florin Bobaru, *University of Nebraska-Lincoln*;

Peridynamics is a non-local theory that can model evolving discontinuities like cracks initiating, growing, and interacting in a body, since it uses integrals instead of spatial derivatives in the equations of motion. Several works have been recently published on simulating two- and three-dimensional elasto-plastic deformation with ordinary state-based peridynamics. While using a two-dimensional peridynamic model to simulate elasto-plastic behavior of material is more efficient computationally for certain problems, only a couple of these studies focus on two-dimensional peridynamic plasticity theory. We find that some formulations in the literature are not sufficiently general and we introduce a new decomposition of the force state, crucial in modeling plastic deformation. We introduce a general decomposition of 2D peridynamic force state into co-isotropic and co-deviatoric parts for ordinary state-based peridynamics for the first time, based on relationship between the stress tensor and peridynamic force state. Our approach is objective and can be used in both small and large rotation. We present several examples of elasto-plastic deformations to verify our formulation.

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Title: A Coupled Immersed-meshfree Framework for Air-Blast-Structure Interaction

Author(s): *Georgios Moutsanidis, *Brown University*; Yuri Bazilevs, *Brown University*;

We present a coupled immersed-meshfree formulation for air-blast-structure interaction [1]. A background discretization provides the basis functions to approximate the unknowns of the coupled air-blast-structure interaction problem, while foreground lagrangian particles are used to track the position of the solid, store history dependent variables, and perform numerical quadrature on the solid terms. We also present a newly developed hyperbolic phase field model for brittle fracture, which we couple with the air-blast-structure interaction framework [2]. Isogeometric basis functions are used to discretize the background domain, while reproducing kernel shape functions are assigned to the particles and approximate the damage field. The presented numerical examples demonstrate the method's ability to simulate damage and fracture under extreme conditions. References: [1] Bazilevs, Y., Moutsanidis, G., Bueno, J., Kamran, K., Kamensky, D., Hillman, M.C., Gomez, H. and Chen, J.S., 2017. A new formulation for air-blast fluid–structure interaction using an immersed approach: part II—coupling of IGA and meshfree discretizations. Computational Mechanics, pp.1-16. [2] Georgios Moutsanidis, David Kamensky, J.S. Chen, Yuri Bazilevs, Hyperbolic phase field modeling of brittle fracture: part II—immersed IGA–RKPM coupling for air-blast–structure interaction, Journal of the Mechanics and Physics of Solids, 2018, ISSN 0022-5096, https://doi.org/10.1016/j.jmps.2018.07.008.

15th U.S. National Congress on Computational Mechanics
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Title: Computational Investigations on Cerebral Vasculature Anatomy and Its Role in Embolic Stroke

Author(s): *Debanjan Mukherjee, *University of Colorado Boulder*; Neel Jani, *University of California, Berkeley*; Jared Narvid, *University of California, San Francisco*; Shawn C. Shadden, *University of California, Berkeley*;

Stroke caused due to the occlusion of a cerebral artery by a fragmented piece of clot or acellular debris (embolus) accounts for close to half of all reported stroke cases. Identifying the source of the embolus is a key step in diagnosis and long-term treatment for an embolic stroke patient. However, this often constitutes a challenging task, requiring a predictive understanding of embolus transport across complex hemodynamic flow patterns via a large arterial pathway from the heart to the brain. An added complexity lies in inter-patient variability in vascular anatomy. Specifically for cerebral vasculature, the Circle of Willis – a ring like network connecting the six major cerebral arteries at the base of the brain – shows significant variability in its topology and anastomoses. Only about 30 percent of population has the typical anastomoses with all connecting segments of the Circle being fully developed. The remaining segments of population have variants of an incomplete Circle anastomoses. Here we present a computational investigation into elucidating how this anatomical variability influences embolus distribution to the brain, and consequently, embolic stroke risks. We have developed an image-based modeling framework to computationally vary the Circle of Willis anatomy via iterative modification of various arterial segment geometries. This was coupled with a three-dimensional computational fluid dynamics model and a discrete particle dynamics model for embolus transport. Our study comprised systematic computations for embolus transport for a cohort of four patients with six different Circle anatomy variants – leading to a total of 24 different anatomical models. Numerical data from these simulations demonstrated that the Circle anatomy has a notable influence in distribution of emboli into the six major cerebral arteries. Results also provided quantitative insights into the proximal collateral flow routing occurring in the various Circle anastomoses, and indicated a hemodynamically based rationale for the variance in embolus distribution seen across different anatomical models. Finally, continued investigations have provided significant insights into clinical implications of this relation between anatomy and embolus distribution, including discerning between left-right contralateral cerebro-embolic events in patients with carotid artery disease.

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Title: Development and Validation of Human Knee Joint Finite Element Model under Various Experimental Loading Conditions

Author(s): *Sayak Mukherjee, *Center for Applied Biomechanics, University of Virginia, Charlottesville, VA 22911, USA*; Wei Zeng, *Center for Applied Biomechanics, University of Virginia, Charlottesville, VA 22911, USA*; Adrian Caudillo, *Center for Applied Biomechanics, University of Virginia, Charlottesville, VA 22911, USA*; J. Sebastian Giudice, *Center for Applied Biomechanics, University of Virginia, Charlottesville, VA 22911, USA*; Matthew Panzer, *Center for Applied Biomechanics, University of Virginia, Charlottesville, VA 22911, USA*;

Various studies suggest that a large portion of lower extremity injuries caused by traffic accidents occur at the knee joint. During accidents the knee is subjected to a combination of bending moments and shear loading, which have been identified as primary mechanisms of injury. The knee response under such conditions largely depends on the interactions of the cruciate and collateral ligaments, articular cartilage, and menisci. Thus proper characterization of these parts become necessary to evaluate the behavior of the knee under various loads. The structural and material behavior of these components have been extensively tested and their response have been well documented in available literatures. The present study aims to redevelop the Global Human Body Model Consortium (GHBMC) owned 50th percentile seated male finite element (FE) knee and validate it against the experimental data available in literature. This work constitutes a nearly complete overhaul of the original knee joint, with mesh and material changes to the femur, tibia, articular cartilage, menisci, and ligaments, while maintaining the anatomical geometry derived from imaging data from the GHBMC volunteer. Accurate material models of different anatomical components of the knee were developed based on response curve to particular loading and injury tolerances available in literature, with many sources published after the original model development. After the geometric and material modeling of individual knee parts were finalized, simulations were performed on the FE model of knee under various combinations of bending and shear loads. Two load cases of valgus bending were performed: four-point bending, which consists only of bending loads, and three-point bending, which combined bending with shear loading. A sensitivity analysis was performed on orientation, material properties and failure criteria of different knee components to assess the validity of the FE model under the combined bending and shear loads. A range of motion study was also performed with the knee in flexion and extension, and validated against experimental data. The validation of the range of motion was an important contribution to improve the biofidelity of the model for positioning of the knee. This detailed knee model was then integrated into whole body GHBMC model to better estimate the lower extremity injuries during automotive collisions. Keywords: Finite Element Model (FEM); cruciate and collateral ligaments; computational modeling; sensitivity analysis;

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Title: High-Order Hybridized Discontinuous Galerkin Method and Scalable Solution Strategies for Incompressible Magnetohydrodynamics

Author(s): *Sriramkrishnan Muralikrishnan, *The University of Texas at Austin*; Stephen Shannon, *Schlumberger*; Tan Bui-Thanh, *The University of Texas at Austin*; John Shadid, *Sandia National Labs*;

We present a high-order hybridized discontinuous Galerkin (HDG) method and scalable linear and nonlinear solution strategies for incompressible resistive magnetohydrodynamics (MHD). Incompressible resistive MHD presents several challenges in terms of nonlinearity, coupled fluid and magnetic physics, incompressibility constraints in both velocity and magnetic fields to name a few. As a step forward to addressing these challenges in the context of high-order methods, we present an IMEX-HDG-DG nonlinear solution strategy (compared against a Picard iteration strategy) for various benchmark problems in incompressible MHD including, but not limited to, the island coalescence problem which is of significant interest to the MHD/plasma physics community. For linear solvers, we will explore block preconditioning strategies and also show the applicability of a newly developed multilevel solver for HDG trace system in the context of incompressible MHD. Various large scale numerical results in both 2D and 3D will be presented.

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Title: A Re-examination of Wave Dispersion in Bond-based Peridynamics bar

Author(s): *Venkata Mutnuri, *Indian Institute of Science Bangalore*; Srinivasan Gopalakrishnan, *Indian Institute of Science Bangalore*;

In this paper, elastic wave dispersion characteristics in a bond-based peridynamic (BBPD) bar is critically examined. These characteristics are known to strongly depend on two BBPD material parameters: micro-modulus function (C) and horizon (H). In literature, characteristics of frequency – wavenumber relation have been studied [1] establishing, in general, the following facts: dispersive nature of waves; waves at lower and higher frequencies behave as homogenous (propagating) and in-homogenous (attenuating) waves, respectively. Most of the literature has considered either a uniform C within H or a linear variation C that goes to zero at end of H. In these C (and also others [1]), homogenous waves show existence of a set of frequencies at which wavenumber is multi-valued. Further, in any linear form of C, there exists a single frequency at which wavenumbers are infinite in number. An examination of this behaviour of multi-valued nature of wavenumbers is the subject of this paper. For a given frequency, owing to transcendental nature of dispersion relation, there exist infinite roots to wavenumber. Each root corresponds to a single wave mode [2]. By considering various forms to C in the dispersion relation, all possible wave modes are clearly separated and their characteristics are studied. Utilizing the concept of group speeds of waves, it is established that not all wave modes are physically admissible. For certain C, it is known that negative group speeds exists in certain regions of wavenumber [3]. However, these regions of wavenumber are shown to be part of physically inadmissible wave modes. References [1] O. Weckner and R. Abeyaratne, “The effect of long-range forces on the dynamics of a bar”, Journal of the Mechanics and Physics of solids, 53 (2005), pp. 705-725. [2] Karl F. Graff, “Wave motion in elastic solids”, Dover publicaions, Inc., New York, 1975. [3] Y. Mikata, “Analytical solutions of peristaltic and peridynamics problems for a 1D infinite rod”, International Journal of Solids and Structures, 49 (2012), pp. 2887-2897.

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Title: Thermodynamically Consistent Mathematical Models for Bending of Beams with Dissipation Mechanism

Author(s): Karan Surana, *University of Kansas*; *Dhaval Mysore, *University of Kansas*; J. N. Reddy, *Texas A&M University*;

In a recent paper [1] the authors have shown that currently used mathematical models for bending of beams such as Euler-Bernoulli, Timoshenko and higher shear deformation beam models derived based on kinematic assumptions in conjunction with energy methods or principle of virtual work cannot be derived using conservation and balance laws of either classical or non-classical continuum mechanics, thus these mathematical models are thermodynamically inconsistent. Additionally, this approach precludes derivations of mathematical models incorporating dissipation and memory mechanism as in such cases the mechanical deformation is not reversible. In reference [1] authors have also presented a thermodynamically consistent formulation for bending of beam in R2 for linear elastic behavior that incorporates slender as well as deep beam deformation physics in a single formulation. This paper extends the work of reference [1] to include dissipation mechanism. The conservation and balance laws in R2 or R3 constitute mathematical model in which the kinematics of beam cross-section deformation physics is incorporated hierarchically. The ordered rate constitutive theory is derived using entropy inequality, integrity and higher order strain rate measures. Space-time coupled as well as space-time decoupled methodologies are presented for obtaining solution of the resulting mathematical model. Details of modal basis technique and its use in decoupling Ordinary Differential Equations in time resulting from space-time decoupling are presented. Numerical results are presented for model problems including comparison between results from the space-coupled methodology and those obtained using the space-time decoupled approach. References: [1] Surana, K. S. and Mysore, D. and Reddy, J. N. Thermodynamic consistency of beam theories in the context of classical and non-classical continuum mechanics and a thermodynamically consistent new formulation. Continuum Mechanics and Thermodynamics, Accepted, 2019.

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Title: A Conforming to Interface Structured Adaptive Mesh Refinement Technique for Modeling Complex Morphologies

Author(s): *Anand Nagarajan, *Department of Mechanical and Aerospace Engineering , The Ohio State University*; Bowen Liang, *Department of Mechanical and Aerospace Engineering , The Ohio State University*; Ming Yang, *Department of Mechanical and Aerospace Engineering , The Ohio State University*; Mohamad Mohamadsalehi, *Department of Mechanical and Aerospace Engineering , The Ohio State University*; Soheil Soghrati, *Department of Mechanical and Aerospace Engineering , Department of Material Sciences and Engineering, The Ohio State University*;

Conforming mesh generation for complex geometries such as fiber composites, structural adhesives, and pitting corrosion present a significant challenge for modeling engineering problems using the Finite Element (FE) method. Controlling the size and shape metrics of the finite elements is key to mitigating problems associated with accuracy, stability and even the efficiency of the simulation, but can be computationally demanding. This problem is compounded for large-scale simulations involving millions of degrees of freedom (dofs), which necessitates the need for a parallel mesh generation framework. A new non-iterative mesh generation algorithm named Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) is introduced for generating high-quality 3D conforming FE models of problems involving complex morphologies [1]. Using a four-step transformation, CISAMR transforms a structured tetrahedral mesh into a conforming mesh with low element aspect ratios. A Structured Adaptive Mesh Refinement (SAMR) is first performed near the vicinity of material interfaces. This is followed by an r-adaptivity operation to relocate selected nodes of nonconforming elements, and the small fraction of highly deformed tetrahedrons is eliminated using a face-swapping operation. A sub-tetrahedralization procedure is subsequently performed, which constructs the final conforming mesh by subdividing remaining nonconforming elements, as well as tetrahedrons with hanging nodes. The CISAMR also introduces a hierarchical r-adaptivity algorithm for discretizing material interfaces intersecting one another (e.g., in polycrystalline materials). In addition to the handling of material interfaces in close proximity or those intersecting with one another, CISAMR also facilitates the construction of periodic meshes, which are often used for micromechanical and multiscale analyses of materials. It also facilitates conforming mesh generation in a parallel computing framework with minimal communication cost between processors, and nearly 100% code reuse from the sequential algorithm [2]. The parallel CISAMR algorithm is observed to yield ideal scalability (linear speedup) at worst, and achieves even better scalability in most cases. In this work, we analyze the quality of meshes generated using CISAMR for complex microstructures, introduce new algorithmic aspects such as higher-order mesh generation, discuss the scalability of the parallel CISAMR, and show its application for simulating micromechanical behavior and failure response of various materials systems. References: 1. A. Nagarajan, and S. Soghrati. "Conforming to interface structured adaptive mesh refinement: 3D algorithm and implementation." Computational Mechanics (2018): 1-26. 2. B. Liang, A. Nagarajan, and S. Soghrati. "Scalable parallel implementation of CISAMR: a non-iterative mesh generation algorithm." Computational Mechanics(2018): 1-23.

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Title: Contemporary Computational Geometries in LS-DYNA

Author(s): *Attila Nagy, *LSTC*; Liping Li, *LSTC*; Stefan Hartmann, *DYNAmore GmbH*; Marco Pigazzini, *LSTC*; David Benson, *LSTC*;

The support of novel computer-aided geometric descriptions forming a potential future basis of isogeometric analysis LS-DYNA is discussed. We present an interface that enables the import and analysis of virtually any computational geometry constructed using a Bernstein-like basis e.g., hierarchical B-splines, analysis suitable T-splines, U-splines. The interface is flexible to accommodate eventual future extensions and allows the use of ASCII as well as binary formats in order to address the very different requirements of research prototyping and production grade industrial deployment. Selected examples will demonstrate the applicability of the method.

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Title: Hybrid Topology/Shape Optimization of Microvascular Composite Using an Analytic Sensitivity Analysis over a Stationary Mesh

Author(s): Reza Pejman, *Drexel University*; Marcus H.Y. Tan, *N/A*; Sherif H. Aboubakr, *North Carolina State University*; William H. Martin, *North Carolina State University*; Jason F. Patrick, *North Carolina State University*; *Ahmad Najafi, *Drexel University*;

We present a gradient-based topology/shape optimization of microvascular composites over a stationary mesh using the Interface-enriched Generalized Finite Element Method (IGFEM). The emphasis of this presentation is placed on the novel scheme which simultaneously can perform the topological change as well as the shape optimization of microvascular composites. We previously developed a fully analytical sensitivity analysis of the shape optimization of microvascular composites in IGFEM framework over a fixed mesh. The developed analytical sensitivity analysis circumvents the problems frequently observed in finite differences and semi-analytical sensitivity approaches. In the current study, we present a new feature which enables the optimizer to appear/disappear the microchannels and change the topology of the network during the optimization process. This task has been carried out by introducing a new set of design parameters which act analogous to the penalization factor of Solid Isotropic Material with Penalization (SIMP) method. The analytical sensitivity of the newly introduced design parameters has been developed and their accuracy is verified against the finite difference method. Reduced-order thermal and hydraulic models are implemented in this analysis. Using these simplified thermal and hydraulic models result in significant reduction in the computational cost. Furthermore, the produced network configurations are suitable for large-scale manufacturing without the essence of post-processing because the microchannel boundaries are precisely represented in the proposed model. The method has been validated by experiment and three sets of application problems have been solved to demonstrate the benefits of using the suggested hybrid topology/shape optimization scheme rather than using only the shape optimization method for microvascular materials. In the first set of examples, we have shown that in contrast to the shape optimization scheme the design space in the topology/shape optimization method is not locked down to the topology of the initial configuration. The second set of problems represent the ability of the topology/shape optimization method to handle strict constraints. Finally, the third set of examples have illustrated how topological changes and network branching can lead to vascular redundancy, which is of great importance in designing microvascular cooling networks for blockage tolerance.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Data-Driven Approach to Composite Material Characterization Using Bayesian Calibration

Author(s): *David Najera, *ATA Engineering*; Eric Jayson, *ATA Engineering*; Doug Melville, *ATA Engineering*; Tommy Board, *ATA Engineering*;

Fiber-reinforced composite materials continue to rapidly improve in terms of structural performance. These materials offer the promise of significant weight reduction in many products—particularly aerospace structures, where weight minimization is critical to both cost and performance. However, the introduction of new materials is a slow and expensive process that requires dependable material property data early in the design cycle, and it takes a rigorous, comprehensive testing program to fully characterize the properties first at the ply level, then at the laminate level, and finally at the product or component level. The ability to reliably predict laminate material properties using limited ply-level material property data early on, and an understanding of the accuracy of those predictions, can dramatically shorten the design cycle. We propose a data-driven approach to obtain material properties for newly developed composite materials. The proposed approach uses limited ply-level property test data to generate finite element model parameters that best fit the statistical distributions from test data. The material model correlation process uses neural networks to act as surrogates of high-fidelity finite element models. The surrogate model is then used to perform Bayesian calibration (via Markov Chain Monte Carlo) to directly find the optimal parameters that are a best fit for a given set of test data. At the end of the process, statistical distributions of all the parameters of interest are provided. This process provides a tractable and systematic approach for the selection of finite element model material parameters for a novel material with limited test data. In recent work, the approach has been validated using test data derived from a composite material that is typically used in space, defense, and missile applications. This technology could potentially enable accelerated development of new materials, and it could be extended to other kinds of materials beyond composites –especially those materials that exhibit high levels of statistical variability.

15th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification in Computational Models of Large Scale Physical Systems

Author(s): *Habib Najm, *Sandia National Labs*; Cosmin Safta, *Sandia National Labs*; Xun Huan, *Sandia National Labs*; Michael Eldred, *Sandia National Labs*; Gianluca Geraci, *Sandia National Labs*; Joseph Oefelein, *Sandia National Labs*; Guilhem Lacaze, *Sandia National Labs*;

Uncertainty quantification (UQ) in large scale computational models of complex physical systems faces the two key challenges of high dimensionality and high sample computational cost. Such models often involve a large number of uncertain parameters, associated with various modeling constructions, as well as uncertain initial/boundary conditions. Exploring such high dimensional spaces typically necessitates the use of a large number of computational samples, which, given the cost of large scale computational models, is prohibitively expensive and thus infeasible. We will discuss a set of UQ methods, and a UQ workflow, to address this challenge. The suite of methods includes global sensitivity analysis (GSA) with polynomial chaos (PC) regression and compressive sensing, coupled with multilevel Monte Carlo (MLMC) and/or multilevel multifidelity (MLMF) methods. The combination of these tools is often useful to reliably cut-down dimensionality with feasible computational costs, identifying a lower dimensional subspace on the uncertain parameters where subsequent adaptive sparse quadrature PC methods can be employed, with accurate estimation of predictive uncertainty. We will illustrate this UQ workflow on model problems, and on an application involving high-speed turbulent reacting flow.

15th U.S. National Congress on Computational Mechanics
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Title: A Nonlinear ALE-FSI Framework for Computational Hemodynamics of Patient-Specific In-Vivo Geometries

Author(s): *Nitesh Nama, *University of Michigan*; Miquel Aguirre, *Mines Saint-Etienne*; Jay D. Humphrey, *Yale University*; C. Alberto Figueroa, *University of Michigan*;

Over the recent decades, computational techniques have been widely employed to study blood flow in arteries owing to their unique capability to allow investigation of the interplay of different biomechanical factors. To model the three-dimensional blood flow in compliant arteries, various fluid-structure interaction (FSI) methods such as Arbitrary Lagrangian-Eulerian (ALE) methods and immersed methods have been proposed. However, the implementation of these methods in pre-existing Computational Fluid Dynamics (CFD) solvers results in a significant increase in the computational cost, making it challenging to achieve results in a clinically relevant time-frame. Here, the Coupled Momentum Method (CMM) proposed by Figueroa et al. [1] is especially attractive since it employs a membrane formulation for arterial walls, which does not add additional degrees of freedom to the rigid-wall CFD system and results in a minimal increase in computational cost. The membrane assumption for the arteries is reasonable in view of the long wavelength of the cardiac pulse compared to the diameters of arteries. Nonetheless, the CMM is limited due to the assumption of linearity for membrane behavior. To accurately capture the nonlinear behavior of the arterial walls for arteries experiencing large deformations, such as ascending thoracic aorta, the CMM needs to be extended for nonlinear membranes. In this work, we present a nonlinear ALE-FSI formulation that can account for large deformations of arterial walls, while preserving the computational efficiency of CMM to a large extent. In particular, we employ a moving mesh approach for the fluid-solid system to allow for large deformations of arterial wall while employing a nonlinear membrane description of arterial wall for computational efficiency. Another important issue concerning the development of patient-specific FSI simulations is the knowledge of state of stress in the medically-imaged in-vivo geometry. To this end, we integrate a forward incremental prestress approach within our nonlinear ALE-FSI framework to identify the in-vivo state of stress. We present benchmark results for a variety of constitutive models to ascertain the accuracy of both the prestress algorithm as well as subsequent FSI computations. We also present results to demonstrate the effect of inclusion of prestress in FSI simulations. Lastly, we present a quantitative comparison of the developed ALE-FSI formulation with the linear CMM to investigate the effect of nonlinear wall mechanics in cases with large deformations. [1] Figueroa, C. A. et al., Computer methods in applied mechanics and engineering, 195(41), 5685-5706, 2006.

15th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification of Fluid Structure Interactions Using Non-Intrusive Polynomial Chaos Expansion - A Coupled Framework of OpenIFEM and DAKOTA

Author(s): *Narendra Nanal, *Rensselaer Polytechnic Institute*; Lucy Zhang, *Rensselaer Polytechnic Institute*;

Simulation of fluid-structure interaction problems (FSI) has gained tremendous importance due to its vast number of practical applications. More realistic estimation of output can be obtained by considering uncertainties in different input parameters and boundary conditions. In this study effect of uncertainties in solid and fluid material properties on different outcomes of FSI simulation is analyzed. OpenIFEM was used to simulate FSI problems while DAKOTA toolkit was used for uncertainty quantification. Modular nature of OpenIFEM framework and non-intrusive UQ approach makes it very easy to implement different test cases. Three test cases were considered in this study: (i) Deflection of a cantilever beam consisting of a hyperelastic material. (ii) The drag coefficient of a cylinder in a flow. (iii) Deformable leaflet immersed in fluid flow in which, outputs analyzed were solid deflection, pressure, and velocity at different fluid locations. Non-intrusive Polynomial Chaos Expansion was used for uncertainty quantification. Anisotropic polynomial refinement is performed to determine the polynomial order for each stochastic dimension. For FSI test case, uncertainties in 5 different material parameters were considered. Even though 5 is not a very large number, it can be computationally expensive considering the cost of one FSI simulation. Hence a surrogate model was constructed for FSI test case using the kriging technique. Mean and variance of each relevant output was calculated for all the timesteps. Variance-based global sensitivity analysis was conducted. Sensitivity analysis provided insights about the impact of uncertainties in each input parameter on the output which can be extremely useful for analysis and designing of different complex systems.

15th U.S. National Congress on Computational Mechanics
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Title: Low-rank multifidelity approaches for quantifying uncertainty in topology optimization

Author(s): *Akil Narayan, *University of Utah*; Vahid Keshavarzzadeh, *University of Utah*; Robert Kirby, *Baylor University*;

We consider topology optimization under uncertainty with multiresolution finite element models. In our bifidelity setting, a coarse and fine mesh corresponding to low- and high-resolution models are available. The inexpensive low-resolution model is used to explore the parameter space and approximate the parameterized high-resolution model and its sensitivity, where parameters are considered in both structural load and stiffness. Error bounds on approximation errors and sensitivity errors are presented, along with numerical examples on benchmark problems.

15th U.S. National Congress on Computational Mechanics
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Title: The Effects of Episiotomy Technique on Pelvic Floor Muscles during a Childbirth

Author(s): *Renato Natal Jorge, *INEGI, Faculdade de Engenharia da Universidade do Porto, Portugal*; Dulce Oliveira, *INEGI, Faculdade de Engenharia da Universidade do Porto, Portugal*; Teresa Mascarenhas, *INEGI, Faculdade de Medicina da Universidade do Porto, Portugal*; Marco Parente, *INEGI, Faculdade de Engenharia da Universidade do Porto, Portugal*;

Vaginal childbirth is the main risk for pelvic floor muscles injury, contributing to pelvic floor dysfunction. The present work will analyze the influence of mediolateral episiotomies in the mechanics of the pelvic floor with the fetus in occiput posterior position when compared to the occiput anterior position. Numerical simulations of vaginal deliveries, with and without episiotomy, are performed based on the Finite Element Method [1]. The biomechanical model includes the pelvic floor muscles, a surface to delimit the anterior region of the birth canal and a fetus [2]. Fetal malposition induces greater extension of the muscle compared to the normal position, leading to increases of stretch [3]. The faster enlargement may be responsible for a prolonged second stage of labor. Regarding the force required to achieve delivery, which might justify the increased need of surgical interventions. Furthermore, episiotomy is essential in reducing the damage to values near the ones obtained with normal position, making the fetal position irrelevant. These biomechanical models have become extremely useful tools to provide some understanding of pelvic floor function during delivery helping in the development of preventative strategies. References [1]-DA Oliveira, MPL Parente, B Calvo, T Mascarenhas, RM Natal Jorge, “A holistic view of the effects of episiotomy on pelvic floor”, International Journal for Numerical Methods in Biomedical Engineering, 33:e2892, 2017. [2]-MP Lages Parente, RM Natal Jorge, T Mascarenhas, AA Fernandes, JAC Martins, "Deformation of the pelvic floor muscles during a vaginal delivery", International Urogynecology Journal, 19:65-71, 2008. [3]-MPL Parente, RM Natal Jorge, T Mascarenhas, AA Fernandes, JAC Martins, “The influence of an occipito-posterior malposition on the biomechanical behavior of the pelvic floor”, European Journal of Obstetrics, Gynecology & Reproductive Biology, 144S:S166-S169, 2009.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Certified Reduced Basis Methods for Variational Data Assimilation

Author(s): *Nicole Nellesen, *RWTH Aachen University*; Martin Grepl, *RWTH Aachen University*; Karen Veroy-Grepl, *RWTH Aachen University*;

In order to approximate the state of a physical system, data from physical measurements can be incorporated into a mathematical model to improve the state prediction. Discrepancies between data and models arise, since on the one hand, measurements are subject to errors and, on the other hand, a model can only approximate the actual physical phenomenon. In this talk, we present a model order reduction method for (an interpretation of) the 3D-method of variational data assimilation for parametrized partial differential equations. The classical 3D-VAR method makes informed perturbations in order to find a state closer to the observations while main physical laws described by the model are maintained. We take inspiration from recent developments in state and parameter estimation and analyse the influence of the measurement space on the amplification of noise. Here, we prove a necessary and sufficient condition for the identification of a “good” measurement space which can, in turn, be used for a stability-based selection of measurement functionals. We propose a certified reduced basis (RB) method for the estimation of the model correction, the state prediction, the adjoint solution, and the observable misfit. Finally, we introduce different approaches for the generation of the RB spaces suited for different applications, and present numerical results testing their performance.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Survey of DAKOTA’s V&V Capabilities in the Simulation of Residual Stresses in a Simple Composite Structure

Author(s): *Stacy Nelson, *Sandia National Laboratories*; Alexander Hanson, *Sandia Natioanl Laboratories*;

Process-induced residual stresses occur in composite structures composed of dissimilar materials. As these residual stresses can result in fracture, their consideration when designing composite parts is necessary. However, the experimental determination of residual stresses in prototype parts can be time and cost prohibitive. Alternatively, it is possible for computational tools to predict potential residual stresses. However, to develop confidence in these predictions, they must be rigorously validated. Specifically, sensitivity studies should be completed to define which model parameters are critical to the residual stress predictions. Then, the uncertainty associated with those critical parameters should be quantified and processed through the model to develop stress-state predictions encompassing the most important sources of physical variability. Numerous sensitivity analysis and uncertainty quantification methods exist, each offering specific strengths and weaknesses. Therefore, the objective of this study is to compare the performance of several validation methods during the manufacturing process simulation of a composite structure. The examined methods include simple sampling techniques, as well as more sophisticated surrogate approaches. The computational costs are assessed for each of the examined methods, and the results of the study indicate that the surrogate techniques are potentially much more efficient than the more widely used sampling methods.

15th U.S. National Congress on Computational Mechanics
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Title: Image Texture-Based Elastography of the Intranuclear Space

Author(s): Soham Ghosh, *University of Colorado Boulder*; Benjamin Seelbinder, *University of Colorado Boulder*; *Corey Neu, *University of Colorado Boulder*;

The cell nucleus is known to contain, maintain, and organize the genomic information. The chromatin in the nucleus is a highly organized structure that organizes for efficient DNA replication and transcription. The heterochromatin is a compact region with high DNA density, while the euchromatin is a less compacted region that is believed to contain most transcriptionally active genes. The relative mechanical role of the euchromatin and heterochromatin regions can reveal the mechanobiological function of the chromatin. However, intranuclear mechanics (e.g. stiffness of subnuclear domains) is not well understood, in part due to technical challenges of measurement inside the subcellular organelles. We propose a noninvasive image texture-based elastography technique that can elucidate relative stiffness of euchromatin and heterochromatin regions. We utilized cardiomyocytes (CM) from embryonic H2b-eGFP mice that were seeded on silicon substrates with soft (15 kPa) and stiff (400 kPa) elastic properties to mimic normal and fibrotic cardiac environments. The histone tag present in all nucleosome complexes rendered the image texture. During spontaneous CM beating, the deforming nuclei were imaged by epifluorescenece microscopy. Deformation microscopy was applied to the reference undeformed and deformed images to quantify the spatial intranuclear displacement map. We further segmented and defined euchromatin and heterochromatin regions of interest that were assumed to have uniform stiffness. We solved an inverse problem to quantify the relative stiffness of the two intranuclear regions, with known displacements defined as boundary conditions, and minimization of nodal displacements obtained from finite element forward simulation and the deformation microscopy. A linear elastic material model was used to calculate the Young's Modulus with an estimated Poison's ratio. Known forward simulations were used to validate the technique and to quantify the sensitivity to noise. We found that CM cultured on soft substrates resulted in a ratio of heterochromatin to euchromatin stiffness of ~5, while for stiff substrates, the ratio was ~25% lower, indicating that the intranuclear stiffness was relatively more homogeneous in fibrotic model. Further, downregulating the expression of the nuclear membrane proteins KASH and nesprin 3 altered intranuclear stiffness distribution. The reported technique can be applied to broader application areas on any images that have inherent texture expressed a function of the stiffness.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Phase-Field Modeling of Chemically-Driven Fracture

Author(s): Louis Schuler, *The University of Utah*; *Pania Newell, *The University of Utah*;

Subsurface systems are highly heterogeneous systems containing fracture and fracture networks which control fluid flow and transport phenomena. However, reactions at the fluid-mineral interfaces can influence the fracture behavior. The important interaction between mechanically-driven and chemically-driven processes in such porous media has been recognized as a mean in controlling the evolution of the mechanical and transport phenomena. The phase-field fracture technique is a geometrical approach, in which the crack discontinuity is smoothed into a diffusive crack zone governed by a continuum damage variable. This variable, defined in the solid, can be interpreted as a phase change between the unbroken and broken state of the material. Phase-field technique enables to overcome the difficulties of other classical numerical techniques, such as crack branching or remeshing. In this work, we utilize the non-local, phase field method to show the evolution of chemically-driven fractures. We are mainly focused at the crack tip and how the crack propagation is driven by chemical reactions. We develop a thermo-dynamically consistent approach in which mechanical properties depend on the chemical reaction rate. The method is numerically implemented and tested based on benchmark examples, such as a single edge crack in a finite width plate. The results obtained with and without chemistry are compared and quantified.

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Title: Modeling the Effects of Helium-Vacancy Clusters on the Stress-Strain Response of an Iron Bicrystal by a Mechanistic Finite Element Approach Informed by Molecular Dynamics Data

Author(s): *Ba Nghiep Nguyen, *Pacific Northwest National Laboratory, Richland, WA 99352, USA*; Richard Kurtz, *Pacific Northwest National Laboratory, Richland, WA 99352, USA*; Fei Gao, *University of Michigan, Ann Arbor, MI 48109, USA*;

In future fusion reactor applications, prime candidate materials such as ferritic/martensitic steels will be exposed to high-energy neutrons leading to helium (He) generation due to transmutation reactions. Formation of He is of particular concern because it has negligible solubility in metals and is strongly trapped by lattice defects with excess free volume such as vacancies, dislocations, grain boundaries (GBs) and particle-matrix interfaces. Helium can cause hardening and increases in the ductile-to-brittle transition temperature and swelling as a result of nucleation and growth of He bubbles. It also weakens GBs by lowering the GB cohesive stress or by promoting nucleation, growth and coalescence of GB cavities, which can lead to intergranular fracture. As it is very difficult to experimentally quantify the effects of nano-scale He-vacancy clusters on material integrity, computational methods such as MD simulations have been useful for elucidating the degradation mechanisms associated with He bubble nucleation and growth. We investigate the effects of He bubbles on the stress-strain behavior of an iron (?-Fe) bicrystal by a mechanistic finite element (FE) approach using a continuum damage mechanics (CDM) description of the material behavior informed by MD data. First, MD analyses of single crystal and bicrystal lattice configurations (?11 <110> {332} orientation) were performed to compute the uniaxial responses of the ?-Fe single crystal and GB. MD results were then used in FE analyses of the same systems to identify parameters for the CDM constitutive relations for the crystal and the traction-separation law for the GB depicted by cohesive elements. Next, a 3D FE model of the ?-Fe bicrystal system with an imperfect GB subjected to uniaxial tensile loading was developed. This model includes an equivalent hollow sphere representing the system with two vacancies under internal pressure in the middle of the GB to model the effects of pressurized He bubbles at 5 K and room temperature on stress, strain and damage distributions. Finally, MD stress/strain data of the same bicrystal system with He bubbles were compared to the corresponding FE results to validate this mechanistic approach that appears to be very efficient in terms of computational time.

15th U.S. National Congress on Computational Mechanics
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Title: Discontinuous Galerkin Methods for Turbulent Flows

Author(s): *Cuong Nguyen, *MIT*; Jaime Peraire, *MIT*; Sebastien Terrana, *MIT*; Pablo Fernandez, *MIT*;

We present the recent development of hybridized discontinuous Galerkin (HDG) methods for numerical simulation of turbulent flows in hydrodynamics (HD) and magnetohydrodynamics (MHD). The main ingredients in devising HDG methods are ({\em i}) a local Galerkin projection of the underlying partial differential equations at the element level onto spaces of polynomials of degree k to parametrize the numerical solution in terms of the numerical trace; ({\em ii}) a judicious choice of the numerical flux to provide stability and consistency; and ({\em iii}) a global jump condition that enforces the continuity of the numerical flux to obtain a global system in terms of the numerical trace. HDG share many common advantages of DG methods and possess some unique features that make them well-suited to simulating turbulent flows. However, like other DG methods, HDG methods may suffer from numerical stability issues in the presence of shock waves, other types of discontinuities, and singularities. In order to improve robustness of HDG methods, we propose a physics-based shock capturing method and an entropy-variable scheme. We extend our approach to ideal and resistive MHD systems coupled with a generalized Lagrange multiplier for hyperbolic-parabolic divergence cleaning. Furthermore, we develop matrix-free iterative solvers and preconditioners for solving nonlinear systems arising from the numerical discretization of HD/MHD equations on GPU architectures. The performance and robustness of the proposed approach are illustrated through a series of turbulent flows in subsonic, transonic, and supersonic, and hypersonic regimes.

15th U.S. National Congress on Computational Mechanics
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Title: On Peridynamic Modeling of Crack Nucleation

Author(s): *Sina Niazi, *University of Nebraska-Lincoln*; Florin Bobaru, *University of Nebraska-Lincoln*;

Brittle and quasi-brittle crack propagation under static or dynamic loading has been successfully analyzed using peridynamics (PD). PD models converge in terms of nonlocal region (horizon) size going to zero when pre-cracks are present (excluding problems in which material length-scale enforce a specific horizon size). However, existing PD models based on a single fracture parameter, associated with the critical fracture energy, produce different strengths for different horizon sizes in modeling of crack nucleation from sites other than pre-cracks, and under quasi-static loading conditions. To introduce an independent parameter from the one linked to the critical fracture energy into the PD bonds behavior, one can use a bi-linear bond force-strain relationship and relate the extra parameter to the ultimate strength of the material. Recent works ([1,2]) focused on crack propagation based on such bi-linear behavior of PD bonds. We study the nucleation of crack in a plate with a hole under tensile quasi-static loading. We utilize the bi-linear model with two PD models, one that fully homogenizes the material (the fully homogenized peridynamic model, FH-PD) and one that performs a partial homogenization based on a stochastic procedure (the intermediately homogenized peridynamic model, IH-PD model [3]). The simulation results show that convergence is achieved for crack nucleation under horizon going to zero in both models, and that with the IH-PD model, by accounting for the presence of defects, one obtains a faster convergence. The obtained simulation results match well with the results published in the experimental literature. Notably, the proposed PD approach does not depend on the location, shape, or number of holes in the plate. The recent model introduced in [4] is valid only for the special case of a plate with a hole. References [1] Zaccariotto, M., Luongo, F., & Galvanetto, U. (2015). Examples of applications of the peridynamic theory to the solution of static equilibrium problems. The Aeronautical Journal, 119(1216), 677-700. [2] Yang, D., Dong, W., Liu, X., Yi, S., He, X. (2018). Investigation on mode-I crack propagation in concrete using bond/-based peridynamics with a new damage model. Eng Fract Mech, 199, 567-581. [3] Chen, Z., Niazi, S., Zhang, G., & Bobaru, F. (2017). Peridynamic functionally graded and porous materials: Modeling fracture and damage. Handbook of Nonlocal Continuum Mechanics for Materials and Structures, 1-35. [4] Zhang, H., & Qiao, P. (2018). A coupled peridynamic strength and fracture criterion for open-hole failure analysis of plates under tensile load. Engineering Fracture Mechanics, 204, 103-118.

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Title: A Nonlocal Matching Boundary Condition for Coupling Peridynamics with Finite Element

Author(s): *Clint Nicely, *Raytheon Space and Airborne Systems*; Rui Zhang, *University of Texas at Dallas*; Shaoqiang Tang, *Peking University*; Dong Qian, *University of Texas at Dallas*;

Since the inception it has been desirable to couple Peridynamics with a more established discretization model in order to utilize the benefits of both models. In this presentation a coupling approach has been established between Peridynamics and the finite element method. In order to minimize the artificial wave reflection that is present within coupling methods a Non-Local Matching Boundary Condition (NMBC) is used for treating the numerical peridynamic/finite element interface. The NMBC is cast in the form of a parameterized expression that involves the displacements and their higher-order time derivatives of peridynamic nodes at and near the numerical interface. The application of NMBC will be shown for the three prominent forms of Peridynamics in 1D with a demonstration in 2D using non ordinary Peridynamics with a correspondence material for both unidirectional and multidirectional waves. The interface transfer is determined by a projection of the PD results onto the FEM domain using the shape functions inherent within finite element to interpolate the PD results to the finite element domain. Multiple examples are given to demonstrate the effectiveness of the coupling method by comparing a direct coupling, a coupling with only projection of the PD result, and finally a method using the projection and NMBC combined. These examples demonstrate the high effectiveness of the NMBC coupling approach.

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Title: Monotone Embedded Discrete Fracture Method for Flows in Porous Media

Author(s): *Kirill Nikitin, *Marchuk Institute of Numerical Mathematics of Russian Academy of Sciences*; Yuri Vassilevski, *Marchuk Institute of Numerical Mathematics of Russian Academy of Sciences*; Ruslan Yanbarisov, *Marchuk Institute of Numerical Mathematics of Russian Academy of Sciences*;

Porous media may contain fractures of different types and scales. Small fractures can be accounted in the permeability tensor during the upscaling procedure within a mesh cell, while large fractures intersect several mesh cells and can dramatically affect the subsurface flow. We propose a FV method for the single- and multiphase flows in fractured media. The method combines the Embedded Discrete Fracture approach with advanced monotone FV schemes for the porous media. For extremum-preserving FV schemes [1,2] it can be shown that the monotone Embedded Discrete Fracture Method (mEDFM) for the matrix-fracture system is extremum-preserving as well. Numerical experiments demonstrate good agreement of the mEDFM with the reference fine grid solution and with the discrete fracture method. [1] Nikitin K., Terekhov K., Vassilevski Y. A monotone nonlinear finite volume method for diffusion equations and multiphase flows. // Computational Geosciences, 2014, 18(3), 311–324. [2] Chernyshenko A., Vassilevski Y. A finite volume scheme with the discrete maximum principle for diffusion equations on polyhedral meshes. // Finite Volumes for Complex Applications VII-Methods and Theoretical Aspects, Springer International Publishing Switzerland, 2014, 197–205.

15th U.S. National Congress on Computational Mechanics
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Title: Producing Credible Discretizations by Combining Conformal Decomposition and Incremental Mesh Improvement

Author(s): *David Noble, *Sandia National Laboratories*; Scott Roberts, *Sandia National Laboratories*; Matthew Staten, *Sandia National Laboratories*; Corey McBride, *Sandia National Laboratories*; C. Riley Wilson, *Sandia National Laboratories*;

Normally, the performance of a part is simulated using a discretized model that conforms to the geometry of the part, as the part was originally designed. However, when there is significant variation from part-to-part, we would like to produce models using the as-manufactured part geometry. For the same reason, it is desirable to use the patient-specific geometry when analyzing biological systems. To this end, we seek to produce credible discretizations using experimentally obtained images of actual parts and microstructures. Previous work has verified the use of Conformal Decomposition Finite Element Methods (CDFEM) for simulating the transport in experimentally imaged domains of multiple materials [1]. CDFEM is an enriched finite element method that can be used to describe discontinuous physics across fluid-fluid interfaces. Level sets are used to describe the domain of each fluid. Nodes are added at the intersection of each level set surface with the edges of the input mesh, and a conforming mesh is generated automatically. CDFEM can be used for producing discretization of as-manufactured parts by using levels sets that are generated from segmented images obtained using methods such as X-ray computed topography. However, CDFEM produces poorly conditioned systems of equations when the interfaces come close to the background mesh nodes. The current work seeks to circumvent this liability by using incremental mesh improvement to improve the quality of the discretization produced by CDFEM. Specifically, small edges are collapsed, and internal edges are swapped on the mesh, eliminating the poor-quality elements produced by the conformal decomposition. These operations are designed to act on a mesh that is stored in distributed memory. The quality of the resulting discretization is assessed for multiple demonstration problems. The resulting discretization is shown to have much better conditioning and improved mesh quality compared to standard CDFEM discretizations.
[1] Scott A. Roberts, Hector Mendoza, Victor E. Brunini, David R. Noble, “A verified conformal decomposition finite element method for implicit, many-material geometries”, Journal of Computational Physics, Volume 375, 2018
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15th U.S. National Congress on Computational Mechanics
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Title: A Coupled Multi-physics Model for Chronic Traumatic Encephalopathy

Author(s): *Lise Noel, *University of Colorado Boulder*; Ellen Kuhl, *Stanford University*;

Chronic traumatic encephalopathy is a progressive neurodegenerative disorder, caused by repetitive mild traumatic brain injuries. It affects patients, mainly contact-sport athletes, at an early age. The pathology manifests itself in an accumulation of abnormally phosphorylated tau proteins within the brain. The first stage of the disease is associated with focal deposition of tau protein tangles especially at the depth of cortical sulci. Later, abnormal proteins propagate to adjacent cortical tissues and finally to the entire brain and trigger severe brain degradation and atrophy. Contrary to other neurodegenerative diseases, chronic traumatic encephalopathy results from the combination of both short-term biomechanical and long-term biochemical damage of the brain tissues. To date the only reliable diagnosis is obtained through post-mortem histopathology. Therefore, numerical methods have been used to simulate the initiation and to track the progression of the disease. So far, numerical models have mainly focused on the immediate response to a single trauma or on the propagation of abnormal proteins following an artificial seeding. Here we propose a coupled multi-physics framework to model both the initiation of the pathology and its propagation to the entire brain. The model simultaneously solves a mechanical equilibrium and a diffusion equation and handles the interplay between three fields. First, a displacement field allows us to model the effect of traumatic injuries. A concentration field keeps track of tau protein deposition in the tissues. We assume that protein misfolding can be triggered by two mechanisms: tau protein tangles can be generated in cerebral tissues as they experience high strains (biomechanical source) or proliferate as a result of aging (biochemical source). The protein propagation is modelled through anisotropic diffusion in gray and white matter. Finally, as tau protein tangles disrupt the stability of microtubules and eventually of the axons, a degradation of the brain mechanical properties is assumed in colonized tissues. This degradation is represented by a gradient-enhanced damage model which requires the introduction of an additional nonlocal strain energy field. We illustrate the features of our model using two-dimensional sagittal brain slices built from MRI and discretized with the finite element method. We solve the resulting coupled system of equations iteratively and calibrate the model parameters with experimental data from the literature. We explore different loading scenarios and demonstrate the influence of repetitive mild traumatic brain injuries on early aging.

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Title: Multiscale Modeling of Damage Accumulation and Permeability Variation in Shale Rocks under Mechanical Loading

Author(s): Vasav Dubey, *Texas A&M University, College Station, USA*; Sara Abedi, *Texas A&M University, College Station, USA*; *Arash Noshadravan, *Texas A&M University, College Station, USA*;

Understanding the poromechanical and fluid transport properties of rocks such as petroleum shales is critical and relevant in many disciplines including petrophysics, hydrology, and subsurface engineering. Due to the presence of various sources of heterogeneities, spanning across multiple length scales, these formations are suitable for multiscale modeling framework. The inherent complex multiscale and heterogeneous structure of organic-rich shale presents challenge in the development of physics-based predictive model for poromechanical and transport properties. The aim of this work is to introduce a framework of experimental characterization, micromechanical modeling, and uncertainty quantification to improve the predictive capability of physics-based model for microcrack induced poromechanical, damage, and transport properties. A multilevel structural ‘‘thought model’’ is utilized within the framework of micromechanics, as a basis to link the relevant textural and compositional features to the bulk poromechanical properties. Different effective medium approximations based on assumptions about subscale morphology are employed to introduce a homogenized poromechanical property at a given microstructural level. The nonlinear and hydraulic response of shale rocks are strongly influenced by the presence and evolution of microcracks. The Linear Elastic Fracture Mechanics (LEFM) framework is used to construct damage criterion in terms of thermodynamics force associated with crack density and formulation is developed for damage evolution in the transversely isotropic medium. The damage model is further extended to account for the effect of microcrack growth in the permeability variation. To account for statistical fluctuation of poromechanical, damage and transport properties at the macroscale, probabilistic description is assigned to key model input parameters at different length scales. Moreover, in order to calibrate model parameters associated with the damage growth and permeability variation model, we conduct direct tensile experiments using a miniature tensile module which can be analyzed under a scanning electron microscope (SEM). Using a miniature tensile module with small sample size makes it feasible to conduct more tests, in comparison to a typical direct tension test for brittle rocks with large sample size. The proposed framework can be used to inform and study the degradation of stiffness, crack growth and permeability variation for organic-rich shales under direct tensile loading. The multiscale model along with stochastic upscaling presented in this work provides an important step forward in extending the existing multiscale poromechanical models of shale by incorporating the effect of microcracks and their evolution with loading.

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Title: Isogeometric Mesher for Eye-Specific Geometries of the Optic Nerve Head Based on Optical Coherence Tomography (OCT) Data

Author(s): *Fred Nugen, *The University of Alabama at Birmingham*; Mustapha El Hamaoudi, *The University of Alabama at Birmingham*; Preston Fuchs, *The University of Alabama at Birmingham*; Massimo Fazio, *The University of Alabama at Birmingham*; Brian Samuels, *The University of Alabama at Birmingham*; Rafael Grytz, *The University of Alabama at Birmingham*;

Isogeometric analysis offers several advantages over classical FEM methods but remains mostly unused in biomechanical applications including ocular biomechanics. One major difficulty for biological applications is patient-specific mesh generation based on image data. We have designed a software tool to generate isogeometric meshes of the optic nerve head (ONH) from incomplete in vivo 3D optical coherence tomography (OCT) data. A detailed understanding of the eye-specific biomechanical response of the ONH is needed to gain insight into the susceptibility of individuals to pathological remodeling and mechanical insult to axons in glaucoma, where glaucoma is second leading cause of blindness worldwide. OCT imaging of the ONH can provide detailed information of the 3D in vivo anatomy but the data is often incomplete due to blood vessel shadowing and limitations in penetration depth of the imaging layer. The OCT data used here was collected in tree shrew eyes at variable intraocular pressure (IOP) levels. Our method is based on an initial, generic mesh, which is morphed to match 3D point clouds from segmented OCT data. The geometry incorporates the eye-specific axial length and details of the ONH tissues including features for the peripapillary sclera, retina, lamina cribrosa, and pia. The software tool offers convenient mesh parameterization for characteristic measurements like tissue thicknesses, scleral canal opening, location and attachment of the lamina cribrosa. It also creates separate meshes where appropriate. Tying constraints are used at mesh interfaces to allow for independent and robust meshing of the complex anatomy of the ONH tissues. A microstructure-based constitutive model is used to account for collagen fiber crimping and anisotropic fiber distribution. Eye-specific material parameters are obtained by matching IOP-dependent changes of characteristic model variables (scleral canal opening, lamina cribrosa position, and peripapillary sclera deformation). The model replicates the IOP-dependent deformations measured by OCT well. Furthermore, the model can be used to estimate the biomechanical response in regions that are not visible in the OCT data. As seen in other applications, the isogeometric elements produce smooth strain and stress predictions using significantly less degrees of freedom as compared to classical linear or quadratic volume elements. We present a robust meshing tool to generate eye-specific models of the tree shrew eye using isogeometric elements. Isogeometric analysis presents a new and promising approach for eye-specific modeling in ocular biomechanics.

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Title: A Novel Transient Diffuse Source Algorithm for Multiscale Simulation in Porous Media

Author(s): *Krishna Nunna, *Texas A&M University*; Michael King, *Texas A&M University*; Ching-Hsien Liu, *Texas A&M University*;

A novel upscaling approach was previously introduced using pressure transient concepts which allowed us to distinguish between well-connected, weakly connected and disconnected pay in the local upscaling region. The current work applies these same concepts to multiscale multiphase simulation using diffuse source basis functions which generate high resolution velocity fields that capture the subgrid heterogeneity and multiphase flow effects. The local flow field generated for coarse transmissibility calculation is based on transients approaching pseudo steady state as opposed to steady state or pseudo steady state. Transients allow us to assess the impact of localization and degree of local connectivity on overall multiscale simulation performance. The concept of diffusive time of flight together with transient basis functions allow us to assess the error in localization for a particular local flow problem. The upscaling step draws upon its similarity to pressure transient well testing concepts to set up local flow problems to obtain coarse transmissibilities. After solving for flow on the coarse scale, superposition allows us to downscale the coarse flow, generating a fine scale velocity field. The downscaled flow may be utilized for solving transport on the fine grid. The approach is tested on the SPE10 synthetic reservoir model.

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Title: Implementation of Biofidelic Bone-Ligament Interaction in a Lower Extremity Finite Element Model

Author(s): *Cody O'Cain, *University of Virginia*; Bronislaw Gepner, *University of Virginia*; John-Paul Donlon, *University of Virginia*; Meade Spratley, *University of Virginia*; Jason Kerrigan, *University of Virginia*; Richard Kent, *University of Virginia*;

Ligaments, bands of fibrous connective tissue, often provide kinematic constraint and stability to complex joints inside the human body. Proper modeling of ligaments needs to account for their fibrous nature with complex origin/insertion geometry and allow for transverse loading from bony surfaces to provide biofidelic joint constraint. Previous work has been done to model the proper attachment sites of each ligament by using many tension only elements in parallel fiber bundles to connect multiple points along the attachment sites1. However, since each connection used only a single cable element, this approach still failed to incorporate transverse loading. The goal of this study was to compare several formulations of ligaments to identify which allowed for both complex geometry, and transverse loading while maximizing efficiency. To improve upon previous work, the parallel fiber bundles were modeled using multiple tension only elements connected in series to allow for contouring over bony surfaces and carrying transverse loading through contact. Four forms were modeled and implemented. The first was comprised of multiple parallel chains, each comprised of serial discrete cable elements. The second used the same as the first but added additional cross-linking beams between each chain. The third used low stiffness isotropic shells to connect the chains instead of cross-linking beams. The final form used transversely isotropic shells, effectively replacing cable elements. All forms of the ligaments were generated with identical numbers of nodes and respective elements in order to test efficiency. Finally, an automated method was used to implement all four formulations into the detailed finite element lower extremity, to ensure that all ligaments could properly contour their respective bony surfaces and could provide transverse loading through contact. Results showed that the serial chains of discrete beams in parallel were the most computationally efficient, followed by the parallel chains with cross-linking beams, which were 1.29x as costly. The parallel chains with isotropic shells were found to be 1.5x as costly, and the transversely isotropic shells were found to be 1.36x as costly. Although all forms of the ligament could provide transverse loading to the bone surface, the first form had the potential to slip off the bone surface. This was not the case for the other forms that could share load through either cross-linking or shells elements. References 1. Nie, Bingbing, et al. "Determination of the in situ mechanical behavior of ankle ligaments." J. Mech Behav Biomed Materials (2017).

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Title: Non-Intrusive, Multi-Scale Generalized Finite Element Approach for Accurate Resolution of Structural Fasteners

Author(s): Haoyang Li, *University of Illinois*; *Patrick O'Hara, *Air Force Research Laboratory*; Armando Duarte, *University of Illinois*;

Many applications in civil and aerospace engineering utilize structural components in which the overall behavior is dependent upon structural details at multiple length scales of interest. In many cases, even if the overall response of a structural component is insensitive to fastener details, the usable service life of the component is likely to depend greatly upon the localized stress fields in these regions. As such, it is important to enable accurate resolution of the localized stress fields in the region near structural fasteners so as to accurately predict the service life of a structural component. The unfortunate reality is that detailed models of structural components with sufficient localized mesh densities, particularly when analyzing complex structural components, pose a serious challenge, and are infeasible for use in many instances. The computational expense grows rapidly with the disparity in scales as well as with the number of fasteners; with the additional reality that creating such meshes is time-consuming, and in some cases not possible with an acceptable element size. The methodology presented here describes a concerted effort to alleviate the intense modeling requirements for this class of problems, while still maintaining high levels of accuracy in the local stress fields. The methodology presented in this talk is a multi-scale extension of the standard global-local FEM in which the Iterative Global-Local Algorithm is used to tightly couple a coarse, standard finite element representation of a global/component-level model, with a highly-adapted local finite element model extracted from the region near a localized feature – structural fasteners, in the current context. The Generalized FEM with numerically-generated global-local enrichment functions is used for the highly adapted local models, and a standard, low order finite element model is used at the component level. The coupling algorithm relies upon only the transfer of standard finite element output quantities, such as displacement fields, and residual forces, and is thus non-intrusive in nature. In this talk, the basic algorithm is detailed, as well as its sensitivity to key parameters of the structural fastener layout – such as number and relative placement of fasteners. The method is applied to a spot-welded, hat-stiffened panel model, and the localized stress fields computed near the critical spot weld are compared against those computed with two alternative approaches often used in practice – 1) fastener elements 2) sub-modeling. The approaches are compared against a direct finite element analysis in terms of accuracy and computational efficiency.

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Title: Reduced-order Modeling through Machine Learning and Graph-theoretic Approaches for Brittle Fracture Applications

Author(s): *Daniel O'Malley, *Los Alamos National Laboratory*;

Typically, thousands of computationally expensive micro-scale simulations of brittle crack propagation are needed to upscale lower length scale phenomena to the macro-continuum scale. Running such a large number of crack propagation simulations presents a significant computational challenge, making reduced-order models (ROMs) attractive for this task. The ultimate goal of this research is to develop ROMs that have sufficient accuracy and low computational cost so that these upscaling simulations can be readily performed. However, constructing ROMs for these complex simulations presents its own challenge. Here, we present and compare four different approaches for reduced-order modeling of brittle crack propagation in geomaterials. These methods rely on machine learning (ML) and graph-theoretic algorithms to approximate key aspects of the brittle crack problem. These methods also incorporate different physics-based assumptions in order to reduce the training requirements while maintaining accurate physics as much as possible. Results from the ROMs are directly compared against a high-fidelity model of brittle crack propagation. Further, the strengths and weaknesses of the ROMs are discussed, and we conclude that combining smart physics-informed feature engineering with highly trainable ML models provides the best performance. The ROMs considered here have computational costs that are orders-of-magnitude less than the cost associated with high-fidelity physical models while maintaining good accuracy.

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Title: In Search of Basis Functions That Give Rise to High Order Finite Difference Methods

Author(s): *Ossian O'Reilly, *University of Southern California*;

The summation-by-parts approach has become a valuable tool for obtaining provably stable numerical methods by analyzing properties at the discrete level. Basic linear algebra concepts such as commutativity, skew-symmetry, and positive definiteness play a crucial role in the analysis. Some schemes that belong to this framework can be derived at the continuous level, starting from a set of basis functions via Galerkin's method, e.g., spectral element and discontinuous Galerkin schemes. But within the SBP framework there are also high order finite difference methods - for which no basis functions are known. An open question is if there is an underlying basis for all SBP schemes. This work aims to begin bridging this gap in knowledge by showing that there exist piecewise polynomial functions that, when inserted into Galerkin's method with mass lumping, give rise to high order SBP finite difference operators of the first derivative.

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Title: Finite Element Discretization of the Graph Laplacian in the Limit of Large Data

Author(s): *Assad Oberai, *USC*; Franca Hoffmann, *Caltech*; Zhi Ren, *Caltech*; Bamdad Hosseini, *Caltech*; Andrew Stuart, *Caltech*;

Graph Laplacian approaches are often used to solve problems in unsupervised and semi-supervised learning. For specific scalings, the large data limit of the Graph Laplacian has been shown to converge to a differential operator [1,2]. We consider the discretization of this operator using the finite element method, and demonstrate how this discretization may be used to (a) understand the properties of the eigenspectrum of this operator and (b) to develop numerical methods to solve semi-supervised learning problem in the limit of large data. References [1] Trillos NG, Slep?ev D. A variational approach to the consistency of spectral clustering. Applied and Computational Harmonic Analysis. 2018 Sep 1;45(2):239-81. [2] Dunlop MM, Slep?ev D, Stuart AM, Thorpe M. Large data and zero noise limits of graph-based semi-supervised learning algorithms. arXiv preprint arXiv:1805.09450. 2018 May 23.

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Title: Three-Dimensional J-Integral and ?J Based on a Domain Integral Method for Finite Strain Elastic-Plastic Fracture Problems under Cyclic Loads

Author(s): Koichiro Arai, *Tokyo University of Science*; *Hiroshi Okada, *Tokyo University of Science*; Yasunori Yusa, *Tokyo University of Science*;

In this presentation, we discuss about a new three-dimensional J-integral based on the virtual crack extension and the domain integral method. It is the three-dimensional version of the T*? (see, Atluri et al. [1] and Okada et al. [2]) which represents the energy dissipation into a small volume surrounding the crack front, per unit crack extension. Engineering structures sometimes undergo large deformations prior to their failures. Koshima and Okada [3] pointed out that the so-called path independent property was lost due to the effect of finite rotation. To retain the path-independent property, an additional term must be included. Such formulation was presented as the T*? integral by Atluri, et al. [1]. Arai et al. [4] recently proposed a new three-dimensional J-integral formulation considering the virtual crack extension. They also included the additional term. The J-integral of Arai et al. was extended to the ?J [5] to characterize crack propagation phenomena under cyclic loads. In this presentation, we will present the derivations of new J-integral and ?J. Some numerical examples on the evaluation of J-integral and a ductile crack propagation analysis under a large cyclic load will be shown. REFERENCES [1] S. N. Atluri, T. Nishioka, and M. Nakagaki, “Incremental path-independent integrals in inelastic and dynamic fracture mechanics”, Engrg. Fract. Mech., Vol. 20, pp. 209-244, (1984). [2] H. Okada and S. N. Atluri, “Further studies on the characteristics of the T*-? integral: plane stress stable crack propagation in ductile materials, Comp. Mech., Vol. 23/4, pp. 339-352, (1999). [3] T. Koshima and H. Okada, “Three-dimensional J-integral evaluation for finite strain elastic-plastic solid using the quadratic tetrahedral finite element and automatic meshing methodology”, Engrg. Fract. Mech., Vol. 135, pp. 34-63, (2015). [4] K. Arai, H. Okada and Y. Yusa, “A new three-dimensional J-integral formulation for arbitrary load history and finite deformation”, Trans. of JSME (in Japanese), Vol. 84, No. 863, pp. 18-00115, (2018). [5] K. Arai, H. Okada, Y. Yusa, A new formulation of J-integral range ?J using three-dimensional equivalent domain integral for finite deformation elastic-plastic problem, Transaction of JSME (in Japanese), Vol. 84 (2018), No. 864, p. 18-00309.

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Title: Topology Optimization of Flow Machine Impellers Using the Finite Volume Method

Author(s): *Carlos Massaiti Okubo Júnior, *Polytechnic School of University of São Paulo, São Paulo, Brazil*; Emílio Silva, *Polytechnic School of University of São Paulo, São Paulo, Brazil*;

The design of impellers for ?ow machines is a difficult task due to the large number of free geometrical parameters involved. Numerical simulations can provide very precise information about the behavior of ?uid ?ow inside these machines. In this context, optimization arises as an option to reduce time in the development of an impeller for flow machines. The Topology Optimization Method (TOM) is used to design flow machine impellers for the first time in [1]. A rotating domain is considered and designs of radial pumps and turbines are generated for Newtonian laminar flow cases. In [2], a similar approach is presented, however this time to design radial pumps to work with Non-newtonian fluids. In the previous works, impellers are designed by optimizing what can be considered as a rotating channel. Also, all the simulation work is performed with the Finite Element Method. In this work, a different approach using the Finite Volume Method is presented. Domain and boundary conditions are defined in such a way that the optimization results in guide vanes in a rotating flow, which can be interpreted as blades. A continuous adjoint formulation is used to calculate the sensitivities of the optimization problem. The numerical implementation is performed using an open source object oriented CFD code. The interpolation function presented in [3] is used. Centrifugal impeller design cases are presented, considering Newtonian and laminar flow. References 1. Romero J S and Silva E C N. A topology optimization approach applied to laminar ?ow machine rotor design. Comput. Methods Appl. Mech. Engrg. , 2014, 279: 268-300 2. Romero J S and Silva E C N. Non-newtonian laminar flow machine rotor design by using topology optimization. Struct Multidisc Optim. , 2017, 55: 1711-1732 3. Borrvall T and Petersson J. Topology optimization of fluids in Stokes flow. Int. J. Numer. Meth. Fluids, 2003, 41: 77–107

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Title: Neural-net Prediction of Stress Concentration at Fillets for Efficient Structural Analysis Using Simplified FEM Models

Author(s): Taichi Yamaguchi, *The University of Tokyo*; Gaku Hashimoto, *The University of Tokyo*; *Hiroshi Okuda, *The University of Tokyo*;

Parallel large-scale finite element method software has enabled us to analyze detailed models. However, to evaluate complicated small geometries efficiently are still difficult. A small fillet is one of complex shapes which is encountered in practical stress analysis. It makes mesh generation difficult. In addition, we need to refine the meshes to evaluate stress concentration at the fillet accurately. By contrast, it is easy to generate meshes for a simplified model without small fillets. So some pieces of software to remove fillets from a CAD model have been developed. Although it is easier to analysis simplified model, we have to evaluate stress singularity at a sharp corner without a fillet. As meshes are refined, the peak stress value increases. In finite element analysis a zooming method is used to evaluate stress concentration. They are efficient method to evaluate large structure including small and complex shape, but they require refining the shape until the stress converges. Analytical solutions for stress concentration factors at fillets are presented, but they are only applied to defined model shapes in defined loading conditions. Recently, as one of the soft computing approaches, a neural-net enhanced FEA has been used for solving inverse and/or optimization problems efficiently. Neural network is an effective technique for efficient finite element analysis. Therefore, we have developed neural-net prediction method of stress concentration at fillets. The method predicts stress concentrations at fillets in a model from stress distribution of the same model without fillets. We only once train the neural network by the relationship between the stress distribution at a sharp corner without a fillet and stress concentrations at various fillets of a representative model. The neural network could be applied to various model shapes in various loading conditions. We validated the method in three dimensional stress analysis. The method accurately predicted the stress concentration of the model which we didn’t use to train the neural network. It enables us to efficiently evaluate stress concentration using simplified FEM models.

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Title: Regularity Results for Defects in Complex Crystals and Applications in Materials Science

Author(s): *Derek Olson, *Rensselaer Polytechnic Institute*; Christoph Ortner, *University of Warwick*;

Defects are ubiquitous throughout naturally occurring crystals, and they play an important role in their mechanical and electrical properties. In this talk, we consider point defects and dislocation defects in complex crystals, or multilattices, and prove rigorous decay rates for the elastic-far fields generated by the defect. We then discuss how these decay rates may be used to show convergence of numerical simulations of single-defect computations in multlattices---including direct atomistic simulations and atomistic-to-continuum coupling algorithms.

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Title: Early Detection of Breast Cancer through an Inverse Problem Approach to Stiffness Mapping: Tissue Phantom Experiments with Improved Cost Functions

Author(s): *Lorraine Olson, *Rose-Hulman Institute of Technology*; Robert Throne, *Rose-Hulman Institute of Technology*;

Early detection of breast cancer will continue to be crucial in improving patient survival rates. Manual breast exams and mammograms are the most widely used early detection techniques. Manual breast exams are limited in their ability to detect tumors since they only produce qualitative information. Mammograms, while effective, expose the patient to radiation and do not quantify tissue stiffness, an identifying characteristic of breast tumors. Our ultimate goal is to develop a system that exploits this stiffness difference to automate, quantify, and enhance the resolution of the manual breast exam. An electro-mechanical device will gently indent the tissue surface in various locations, recording tissue surface deflections on the remainder of the surface. This deflection data will be used with inverse techniques involving finite element methods (FEM) and genetic algorithms (GA) to provide 3D maps of the elastic modulus of the interior of the breast tissue to identify suspicious sites. We have developed appropriate computational algorithms and experimentally validated the technique with 180 g gelatin tissue phantoms. The algorithm correctly identified the presence or absence of 2 g tumors (approximately 1.3 cm cubes) in 12 tumor-free phantoms and 14 tumor-containing phantoms. To put this in context, the American Joint Committee on Cancer grades cancers in part by their tumor size. Breast cancer tumors less than 2 cm where the cancer has not spread to other sites are collected into the lowest risk group for invasive cancers with a relative 5 year survival rate of 100%. These results are promising but clearly a great deal of work remains to be done before the method could be applied as a clinical screening tool. The genetic algorithm relies on a cost function to identify the “best” match between the finite element model and the experimental measurements—we initially used a one-norm. To improve the algorithm’s discriminating capabilities we tested different cost functions, such as a modified signal-to-noise ratio and a two-norm. Neither of these cost functions performs better than the one-norm. Since data near the indenter is likely to be more significant than data far from the indenter, we have also weighted the data by a significance factor. We will report on the performance of significance factors that decay with the radius, as well as windows that uniformly include all data within a certain radius of the indenter. Acknowledgements: This work used the Extreme Science and Engineering Discovery Environment (XSEDE), NSF ACI-1548562.

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Title: A Data-driven Reduced 1D Model for Prediction of Morphometric and Hemodynamic Remodeling in Pulmonary Hypertension

Author(s): *Mette Olufsen, *NC State University*; Megan Chambers, *NC State University*; Mitchel Colebank, *NC State University*; M. Umar Qureshi, *NC State University*;

Pulmonary hypertension (PH) is a complex disorder that encompasses five etiologies involving vascular remodeling of different parts of the pulmonary circulation. It is associated with stiffened large arteries and increased vascular resistance. However, it is not well understood how different parts of the system remodel during PH and how their remodeling contributes to the progression of the disease. In this talk, we will discuss how modern imaging technology, advancements in computational methods for image segmentation, and contemporary modeling approaches can be combined to explore these questions. Specifically, we develop a data-driven, 1D fluid dynamics network model, where imaging data are used to set up subject-specific geometry for both the large and small vessels. The large vessels are represented explicitly by their length and radii, while the small vessels are represented by subject-specific structured trees. This model is fitted to hemodynamic data from control and hypoxia-induced pulmonary hypertensive mice. Nominal parameter values for the vessel stiffness and hemodynamic quantities are calculated from morphometric and invasively measured hemodynamic data. We use Bayesian methods to estimate subject-specific parameters fitting the model to data. Posterior distributions for each parameter are used to propagate uncertainties to the model predictions. In addition to time-series predictions of pressure and flow, we validate our results in the frequency domain assessing changes in wave-propagation and wave-intensity with the disease. We use this model to characterize subject and disease-specific remodeling within the proximal and distal vasculature. Specifically, we quantify relative changes in vascular resistance, proximal and distal arterial stiffness, vascular compliance, and wave reflection amplitudes across the control and hypertensive mice. For the microvasculature, we conduct a morphometric analysis characterizing changes in vascular branching structure due to disease. This is done by extracting skeletonized networks from the micro-CT images and using a custom algorithm to represent the network as a connected graph. We use topological data analysis to determine subject specific fractal parameters and analyze how these change with PH. Our model and data analysis outcomes will be combined to understand the links between spatially distributed etiologies and global hemodynamics and shed light on the prospect of combining the model and graph-based morphometric analysis of vascular trees.

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Title: Non-oscillatory Finite Element Method for Free Surface Flows and Emergence of Cavities in Ducts

Author(s): *Pablo Ortiz, *University of Granada. Spain*; Jorge Molina, *University of Granada, Spain*;

Advanced simulation of free surface natural flows, and of combined free surface/pressurized flows in hydraulic structures, requires a proper numerical approach for the dynamics of interfaces, avoiding spurious residuals during interface propagation. In recent years we introduced a finite element model to simulate shallow flows with dry fronts [1] [2], and we extended the formulation to flows coupled with erodible–non erodible interfaces [3]. The method is developed by integrating a high order continuous finite element procedure with an independent conservative sign-preserving correction. Sign preservation proved to be a significant capability to reduce residuals on the interface. In this work we present an extended conservative finite element method for flows with interfaces based on flux limiters, with improved conservation properties after correction. We introduce demanding tests to discuss interaction and coalescence among nearby interfaces, as well as applications to severe frictional flows, such as experiments of dam–break flow type with and without erodible boundaries. Air cavity emergence and propagation in ducts is a stringent problem of flows with air/water interface. In this case, the interface is a combination of regions where transition air/water is well defined and zones where a diffuse transition between both phases appears, frequently due to a bore formation. We illustrate the suitability of the model for air/water propagation and cavity emergence in ducts, and compare numerical results with laboratory experiments for ducts with partial obstructions during pressurization. Acknowledgements: This research is supported by MICIIN Grant #BIA-2015-64994-P (MINECO/FEDER). REFERENCES [1] P.Ortiz, “Shallow water flows over flooding areas by a flux-corrected finite element method”, Journal of Hydraulic Research, 52, 2, 241-252 (2014). [2] P. Ortiz. ‘Non-oscillatory continuous FEM for transport and shallow water flows’. Comput. Meth. Appl. Mech. Engrg., 223-224, 55-69, (2012). [3] P. Ortiz, J. Anguita, M. Riveiro, “Free surface flows over partially erodible beds by a continuous finite element method”, Environ. Earth Sci., 74, 7357–7330 (2015).

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Title: Recent Advances in Topology Optimization Considering Additive Manufacturing Support Structures

Author(s): *Mikhail Osanov, *Johns Hopkins University*; Justin Unger, *Johns Hopkins University*; James Guest, *Johns Hopkins University*;

Additively manufactured components often require temporary support structures to prevent the component from collapsing or warping during fabrication. Whether these support materials are removed chemically as in the case of many polymer additive manufacturing processes, or mechanically as in the case of metallic processes such as (for example) Direct Metal Laser Sintering (DMLS), the use of sacrificial material increases total material usage, build time, and time required in post-fabrication treatments. Although manufacturing technology development and feedstock material development will play important roles in addressing this issue in the future, we explore here the role that computational design methods can play in reducing the use of support structures in additive manufacturing (AM). Recent advancements regarding topology optimization considering overhang constraints [1-2], part orientation optimization, and support structure design will be discussed. The presented approaches utilize projection-based methods with the key feature that underlying design objectives related to support structures are embedded within the topology optimization formulation and algorithm, creating a mathematically consistent design optimization approach that can be effectively solved with gradient-based optimization. Advantages and limitations of the approaches will be discussed, along with finer points related to computational efficiency, geometric control, and selective relaxation of various constraints. The resulting new approaches are demonstrated on 2D and 3D mechanical design problems. [1.] Gaynor A.T., Guest J.K. (2014). Topology Optimization for Additive Manufacturing: Considering Maximum Overhang Constraint. Proceedings of the 15th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Atlanta, GA, 1-8. [2.] Gaynor A.T., Guest J.K. (2016). Topology optimization considering overhang constraints: Eliminating sacrificial support material in additive manufacturing through design. Structural and Multidisciplinary Optimization, 54(5):1157–1172.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Monte Carlo Framework for Modeling Protein Assembly on Lipid Membranes

Author(s): *Carlos Osorio, *University of Houston*; Ashutosh Agrawal, *University of Houston*;

Proteins polymerize on lipid membranes and remodel them during numerous cellular processes. For example, enodcytic proteins continuously remodel plasma membrane for cellular transport. Various fission proteins polymerize in order to execute cell mitosis, nuclear division and vesicle fission. While continuum theories have been extensively used to model lipid-protein interactions and membrane shape changes, several fundamental questions still remain open ended. One excellent example is that of calthrin, a key protein that drives the most commonly used cellular transport pathway. Despite decades of research, the primary mechanism by which clathrin remodels plasma membrane is not yet established. To resolve this and similar issues, there is a critical need to develop a molecular scale computational framework to investigate protein-lipid interactions. In this work, we will present a new Monte Carlo framework that allows proteins to self-assemble on membranes and drive morphological changes. The fluid membrane is modeled as a 2D elastic surface using finite difference method. The proteins are modeled as discrete particles that interact with each other and with the membrane. The framework will be used to analyze the consequences of clathrin assembly on membrane geometry, which can potentially bring new insights into the ongoing debate on clathrin-mediated membrane remodeling.

15th U.S. National Congress on Computational Mechanics
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Title: Peridynamic Formulation for Beam Structures with an Application to Predict Damages in Offshore Structures

Author(s): *Selda Oterkus, *University of Strathclyde*; Cong Tien Nguyen, *University of Strathclyde*;

Peridynamic Formulation for Beam Structures with an Application to Predict Damages in Offshore Structures Cong Tien Nguyen1 and Selda Oterkus2 1University of Strathclyde, Glasgow, UK, e-mail: nguyen-tien-cong@strath.ac.uk 2University of Strathclyde, Glasgow, UK, e-mail: selda.oterkus@strath.ac.uk Engineering structures are usually complex and exact analysis of the structure may not be possible. In order to reduce computational time, structural simplification can be used to reduce the computational cost. As a result, structural simplification is necessary. Peridynamics is a new non-local continuum theory which uses the integral equations rather than differential equations. Peridynamics is suitable for damage prediction and can also be applicable for simplified structures [1-3]. This study presents a novel peridynamic model for a three-dimensional beam with 6 degrees of freedom based on Timoshenko beam theory. The accuracy of the peridynamic model is validated by considering offshore structures subjected to static and dynamic loading conditions. References [1] Silling, S. A. (2000). Reformulation of elasticity theory for discontinuities and long-range forces. Journal of the Mechanics and Physics of Solids, 48(1), 175-209. [2] Diyaroglu, C., Oterkus, E., & Oterkus, S. (2017). An Euler–Bernoulli beam formulation in an ordinary state-based peridynamic framework. Mathematics and Mechanics of Solids, 1081286517728424. [3] Yang, Z., Oterkus, E., Nguyen, C. T., & Oterkus, S. (2018). Implementation of peridynamic beam and plate formulations in finite element framework. Continuum Mechanics and Thermodynamics, 1-15.

15th U.S. National Congress on Computational Mechanics
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Title: Advancements in Overlay Grid-Based Hex Meshing from Noisy 3D Image Data

Author(s): *Steven Owen, *Sandia National Laboratories*; Corey Ernst, *Elemental Technologies*;

New methods for generating a quality conformal all-hex mesh for simulation based upon overlay grid procedures are presented. Noisy input data where interfaces between materials are not precisely known are the focus of this work. Applications including CT images of human anatomy, image-based RVE models of polycrystals, complex composite materials and rubber compounds are motivations for this study. We will introduce new methods for automatically defeaturing, thickening and non-manifold resolution to define clean interfaces. A new guaranteed quality smoothing approach will also be proposed to ensure a minimum prescribed mesh quality. The proposed methods build upon the Sculpt [1] tool, developed at Sandia National Labs, a parallel MPI-based overlay grid tool for hexahedral mesh generation. [1] S. J. Owen, M. L. Staten and M. C. Sorensen. Parallel hex meshing from volume fractions, Engineering with Computers 30 (2014). Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. SAND Number: SAND2019-1085 A

15th U.S. National Congress on Computational Mechanics
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Title: Accelerating Topology Optimization Using Reduced Order Models

Author(s): Youngsoo Choi, *Lawrence Livermore National Laboratory*; *Geoffrey Oxberry, *Lawrence Livermore National Laboratory*; Daniel White, *Lawrence Livermore National Laboratory*; Daniel Tortorelli, *Lawrence Livermore National Laboratory*;

Topology optimization automates the design process by solving an optimization problem that determines the material layout of an object subject to design constraints and PDEs describing the physics acting on the object. However, solving this optimization problem is computationally intensive because it requires solving these physics PDEs, which requires a sequence of large-scale linear solves, and slows down design computations for rapid prototyping parts in additive manufacturing. To accelerate these linear solves, we propose using projection-based model order reduction to both construct reduced order models (ROMs), and augmenting the Krylov subspace in preconditioned conjugate gradient (PCG) solves of original, “full order model” (FOM) physics PDEs required for training and updating ROMs. To the best of our knowledge, previous work using reduced order modeling to accelerate topology optimization only uses the first of these two steps to accelerate linear solves. Our work is most similar to that of Gogu [1], which trains ROMs of finite element models on the fly by solving FOMs using direct linear solvers. In that work, the ROM basis is updated using Gram-Schmidt orthogonalization; when the ROM basis reaches a specified maximum size, basis updates replace the oldest basis vector with a new basis vector. Our contributions are to (1) replace the Gram-Schmidt basis with a proper orthogonal decomposition (POD) basis computed using an incremental SVD, (2) use this POD basis to accelerate FOM solves required for ROM training by using an augmented PCG method, AUG-PCG [2], (3) implement a parallel version of our approach in C++ using MPI, and (4) show that our method generalizes beyond the linear compliance optimization problems used in Gogu’s work (e.g., stress-constrained optimization). Our proposed method is applied to several large-scale topology optimization problems to demonstrate a considerable reduction in PCG iterations required for FOM solves, and it generates optimal designs similar to solving FOMs without using AUG-PCG. These results suggest that augmenting PCG with a ROM basis is another opportunity to decrease computational costs in topology optimization for rapid prototyping in additive manufacturing applications. References [1] C. Gogu. “Improving the efficiency of large scale topology optimization through on-the-fly reduced order model construction.”International Journal for Numerical Methods in Engineering, 101 (2015): 281-304. [2] K. Carlberg, V. Forstall, and R. Tuminaro. “Krylov-subspace recycling via the POD-augmented conjugate-gradient method.” SIAM Journal on Matrix Analysis and Applications, 37.3 (2016): 1304-1336.

15th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification and Propagation in Parametrically Homogenized Constitutive Models

Author(s): *Deniz Ozturk, *Johns Hopkins University, Department of Civil Engineering*; Shravan Kotha, *Johns Hopkins University, Department of Civil Engineering*; Adam L. Pilchak, *Air Force Research Laboratory, Materials and Manufacturing Directorate*; Somnath Ghosh, *Johns Hopkins University, Departments of Civil and Mechanical Engineering*;

Parametrically Homogenized Constitutive Models (PHCMs) for Ti-Al alloys have been developed in [1,2,3] as a promising alternative to the computationally prohibitive homogenization methods. PHCMs are thermodynamically consistent, reduced-order models that have explicit representation of microstructural descriptors in their functional forms. Their general forms are similar to conventional phenomenological constitutive models of deformation that represent fundamental characteristics of the material's macroscopic response. PHCM's constitutive parameters are designed to have direct dependence on representative aggregated microstructural parameters (RAMPs), e.g. morphological and crystallographic variables of the microstructure. Machine learning is used with calibration databases generated from Crystal Plasticity Finite Element (CPFE) simulations to decipher the functional forms of PHCM constitutive parameters in terms of the RAMPs. PHCMs can be directly incorporated in any finite element code, e.g. ABAQUS through user defined material modeling windows such as UMAT. In this study, an uncertainty quantification and propagation (UQ-UP) framework is developed for PHCMs, in order to achieve probabilistic predictions of the macroscopic material response accounting for (i) material microstructural uncertainty, (ii) error due to model reduction and (iii) sparsity of the CPFE-based calibration data. Calibration dataset for the probabilistic PHCM is generated by performing CPFE analyses of virtual polycrystalline microstructures with a wide range of initial crystallographic and morphological parameters. Sensitivity analyses and machine learning methods are employed to identify the polynomial bases to represent the microstructural dependencies in the CPFE data. Bayesian inference is used to quantify the non-stationary error arising from model reduction and CPFE data sparsity. Uncertainty in the material microstructure is represented by the statistical moments of microstructural parameters, which are calculated from the multiple EBSD scans collected from different locations on the material. A Taylor series expansion based UP method is developed for PHCM for the propagation of uncertainty between the microstructural parameters (e.g. arising from natural variability due to the manufacturing process) and the output variables of interest, such as stress, plastic strain and macroscopic fatigue damage measures. References: 1. D. Ozturk, S. Kotha, A. Pilchak, S. Ghosh. J. Mech. Phys. Solids (2019) 2. S. Kotha, D. Ozturk, S. Ghosh. Int. J. Plast. (2019a) 3. S. Kotha, D. Ozturk, S. Ghosh. Int. J. Plast. (2019b)

15th U.S. National Congress on Computational Mechanics
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Title: On the Rate of Convergence of a Nonlinear Viscoelastic Constitutive Model

Author(s): Eyüp Can Kökan, *Bo?aziçi University*; *Sebnem Ozupek, *Bo?aziçi University*; Birkan Tunç, *ICES, UT Austin*;

Convergence characteristics of three nonlinear viscoelastic constitutive equations are compared. The first equation is a built-in material model of a commercial finite element software [1]. The other two equations are implemented in the software as a user material [2]. All three constitutive models are valid for finite deformations and represent viscoelastic effects. In addition to these, one model takes into account the effects of damage. In determining the convergence behavior both homogeneous and inhomogeneous deformation states are considered, and various element types are investigated. The calculation of convergence rate of Newton-Raphson method is emphasized. Residual force and largest correction to displacement are examined in the study. The effect of the time incrementation on the convergence rate is determined by considering both automatic and fixed time incrementation. The results show that the best convergence rate is achieved for the user material model without damage. This is followed by the user material model which takes damage into account. The slowest convergence rate is calculated for the built-in material model. [1] Simulia, ABAQUS User's Manual, Dassault Systems Simulia Corp., 2018. [2] B. Tunç, ?. Özüpek, E. Becker, Implementation and validation of a three dimensional damaging finite strain viscoelastic model, International Journal of Solids Structures 102-103 (2016) 275-285.

15th U.S. National Congress on Computational Mechanics
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Title: Experimental Analysis and Constitutive Modelling of the PC/ABS Glassy Polymeric Blend under Different Stress States

Author(s): *Fernando P.B. Macedo, *Faculty of Engineering, University of Porto*; Shenghua Wu, *Faculty of Engineering, University of Porto*; Francisco M.A. Pires, *Faculty of Engineering, University of Porto*;

Keywords: Mechanics of Solid Polymers; Amorphous Polymer Blends; Constitutive Modelling; Mechanical Testing. Abstract. The mechanical performance and physical specifications of individual polymeric materials can be highly improved through the mixture of two or more thermoplastics, and addition of fine dispersed rubber particles: the rubber-toughened polymeric blends. A case of interest is the ternary amorphous Polycarbonate/ABS blends – although neat PC has high ductility, thermal stability and durability, it lacks in high notch-sensitivity and fracture toughness, properties that are highly improved by the addition of ABS, a rubber-toughened polymer [1]. The fracture behaviour of rubber toughened polymers is known to be governed by matrix shear yielding and crazing, interconnected with cavitation of the rubber particles, and depends on the applied stress state. When the stress state is compressive, rubber-toughened polymers usually show plastic deformation by shear-yielding; when the stress state is tensile, a competition between shear-yielding and crazing takes place. The crazing phenomenon usually appears in geometries with sharp notches and is associated to be the outcome of internal cavitation. Many experiments also indicate that hydrostatic stress is a key feature in the nucleation of crazes [2]. This work starts to present the results of an experimental campaign performed to analyse the behaviour of PC/ABS blend with different volume fractions and under different stress states and strain rates. A constitutive model, based on the work of Ames [3] and in the Gearing-Anand model [2], is proposed in order to predict the mechanical behaviour of the PC/ABS blend, depending on the volume fraction of its constituents. The benchmark experimental results ensure the attainment of the material properties through a specialized parameter identification procedure. The constitutive model is implemented through an implicit integration scheme. A representative set of numerical examples is presented taking into account a wide range of mechanical conditions. The predictions of the model are appraised against the experimental set of results obtained by our group. References [1] Hund, J.; Naumann, J.; Seelig, T. (2018). An experimental and constitutive modeling study on the large strain deformation and fracture behavior of PC/ABS blends. Mechanics of Materials, 124, 132-142. [2] Gearing, B.P.; Anand, L. (2004). Notch-sensitive fracture of polycarbonate. International Journal of Solids and Structures, 41, 827-845. [3] Anand, L; Ames, N.M. (2006). On modeling the micro-indentation response of an amorphous polymer. International Journal of Plasticity, 22, 1123-1170.

15th U.S. National Congress on Computational Mechanics
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Title: Spheres Settling in Oldroyd-B Fluids

Author(s): *Tsorng-Whay Pan, *University of Houston, Department of Mathematics*; Roland Glowinski, *University of Houston, Department of Mathematics*;

In this talk we present a numerical study of two balls settling in a vertical channel with a square cross-section filled with an Oldroyd-B fluid. Two initial configurations have been studied: two balls released side by side and one atop the other. For the side by side initial configuration, two balls may stay apart and interact periodically or form a vertical chain up to the blockage ratio, elasticity number and the two terminal speeds as in [1]. For the initial configuration with one ball atop the other, we have obtained that either the trailing ball catches up the leading one to form a vertical chain or two balls separate with a stable final distance as observed experimentally in Boger fluids.
[1]. T.-W. Pan and R. Glowinski, Numerical study of spheres settling in Oldroyd-B fluids, Physics of Fluids 30 (2018), 113102.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Machine Learning for Emulating and Assimilation in Multi-scale Geophysical Simulations

Author(s): *Nishant Panda, *T-5, Los Alamos National Lab*; David Osthus, *CCS-6, Los Alamos National Lab*; Diane Oyen, *CCS-2, Los Alamos National Lab*; Gowri Srinivasan, *XCP-8, Los Alamos National Lab*; Humberto Godinez, *T-5, Los Alamos National Lab*;

Most simulations that model complex environmental process are multi-physics in nature with unknown or imprecise parameters. In this talk, we give an outline of how machine learning can be used to emulate meso-scale physics in environmental simulations. In particular, we show an example from subsurface simulation where the meso-scale fracture propagation is emulated using machine learning. Similar techniques can be employed for real-time simulation of coastal processes where shallow water models are employed for modeling offshore ocean waves and Boussinesq models are used to model near-shore physics. We will also talk about using machine learning to build surrogates for a data-driven assimilation approach to gain knowledge about unknown parameters. Examples will include convection-diffusion equation, Lorenz system and the shallow water equation. (LA-UR-19-20882)

15th U.S. National Congress on Computational Mechanics
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Title: Statistical Machine Learning Closures for Reduced-Order Models of Dynamical Systems

Author(s): *Eric Parish, *Sandia National Laboratories*; Kevin Carlberg, *Sandia National Laboratories*;

Projection-based reduced-order models (ROMs) are a practical tool for generating computationally efficient approximations to high-dimensional dynamical-system models. For practical deployment in applications such as design under uncertainty, it is critical to quantify (and hopefully reduce) the epistemic uncertainty introduced by such approximations. This work proposes a machine-learning framework for generating statistical closure models for projection-based ROMs of dynamical systems. The purpose of such closure models is to develop statistical predictions of the error induced a ROM approximation in an effort to both quantify and reduce the epistemic uncertainty introduced by a ROM. The presented framework is based on Long Short-Term Memory (LSTM) neural networks from deep learning. The recursive nature of LSTM networks allows them to capture non-Markovian effects; a feature that is essential for dynamical system closure modeling. We consider a wide range of candidate features and network architectures within a cross-validation framework for model selection. We present results on dynamical systems arising from fluid-dynamics applications, which highlight the ability of the proposed framework to both statistically quantify and substantially reduce the epistemic uncertainty introduced by model reduction.

15th U.S. National Congress on Computational Mechanics
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Title: On Arbitrarily-Shaped Polyhedra for Elastodynamic Virtual Element Methods

Author(s): *Kyoungsoo Park, *Yonsei University*; Heng Chi, *Georgia Institute of Technology*; Glaucio Paulino, *Georgia Institute of Technology*;

The literature on numerical methods (e.g. finite elements, virtual elements) concentrates on convex element types. However, the virtual element method is able to handle arbitrarily shaped elements, which offer unique features such as flexibility in discretization, easy treatment of representative volume elements, mesh refinement, coarsening and adaptivity. In this presentation, we focus on general convex and nonconvex virtual elements for elastodynamic problems with explicit time integration. Convergence of the solution is demonstrated in relation to stability, mass lumping scheme, element size and distortion for arbitrary virtual elements. The critical time step is approximated using two approaches, i.e., maximum eigenvalue of a system of mass and stiffness matrices, and an effective element length. Computational results demonstrate that small edges on convex polygonal elements do not significantly affect the critical time step, while convergence of the solution is observed regardless of the stability term and element shape. Thus, the virtual element method (VEM) is able to consistently handle general convex and nonconvex elements in both 2D and 3D.

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Title: Effect of Copolymer Composition on Thermomechanical Behavior of Shape-Memory Polyurethane via Coarse-grained Molecular Dynamics Simulation

Author(s): *Sungwoo Park, *Seoul National University, South Korea*; Junghwan Moon, *Seoul National University, South Korea*; Byungjo Kim, *Seoul National University, South Korea*; Maenghyo Cho, *Seoul National University, South Korea*;

Shape-memory polymers (SMPs) are smart materials that respond to external stimuli, such as heat, light, moisture, and so on. The segmented polyurethane copolymer is one of thermos-responsive SMP having urethane linkage which is synthesized with a polyol (soft-segment) and an isocyanate (hard-segment). The dual-segment system consisting of a netpoint and a switching-segment is a necessary condition for SMPs. Here, the hard-segment domains cluster and act as a netpoint for stabilizing the network. The soft-segment domains form crystalline at room temperature and become flexible again at high temperature. This transition serves as a switch for the shape-memory effect. Conventional all-atom (AA) molecular dynamics (MD) simulation can cover the atomistic structure and shape-memory properties. But it takes a considerable amount of calculation time to calculate the vad der waals and the coulombic interaction energy between several atom pairs. So, there are limitations on increasing time scale and length scale and observing meso-scale phenomena, such as polymer crystallization and phase separation. To overcome these limitations, we have developed a coarse-grained (CG) MD simulation model of shape-memory polyurethane copolymer. CG skill is to treat multiple atoms as a single bead to reduce degrees of freedom. AA MD is conducted to derive bonded- and nonbonded-bead potential of the CG model. The bonded potentials composed of bond stretch and angle bend were derived from multi-centered Gaussian function. The nonbonded potentials were derived from the iterative Boltzmann inversion (IBI) methods to match the structural property ; Radial Distribution Function (RDF) and the thermodynamic property ; density. [1] We varied the copolymer composition of shape-memory polyurethane. As a result we could observe aggregation of hard-segment domain and crystallinity of soft-segment domain. And we confirmed the stress-strain curve to investigate the mechanical property under uniaxial loading. Finally, we defined two shape-memory properties, shape-fixity ratio and shape-recovery ratio domain with different hard-segment contents. [2] We expect this study provides an insight to design the segmented polyurethane copolymer to control the shape-memory performance. Acknowledgements This work was supported by a grant from the National Research Foundation of Korea (NRF) funded by the Korea government (MSIP) (Grant No. 2012R1A3A2048841). References [1] V. Agrawal, G. Arya, and J. Oswald, Simultaneous Iterative Boltzmann Inversion for Coarse-Graining of Polyurea, Macromolecules, 47 (2014), 3378-3389. [2] J. Moon, J. Choi, M. Cho, Programmed shape-dependence of shape memory effect of oriented polystyrene : A molecular dynamics study, Polymer, 102 (2016), 1-9, Elsevier.

15th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification in First-Principles Predictions of Lattice Thermal Conductivity

Author(s): *Holden Parks, *Carnegie Mellon University*; Venkat Viswanathan, *Carnegie Mellon University*; Alan McGaughey, *Carnegie Mellon University*;

Density functional theory (DFT) is an ab-initio method that has been successfully used to predict the thermal properties, such as the phonon dispersion and thermal conductivity, of a variety of insulating and semiconducting materials. DFT-based calculations are attractive because, unlike calculations based on empirical potentials, they are free from fitting parameters. A DFT calculation is made computationally tractable by describing the complicated exchange-correlation (XC) electron interactions with an effective potential, called an XC functional. There is no a priori method of choosing an XC functional, so that choosing any single XC functional introduces uncertainty in any quantity derived from that calculation. We present a robust method for quantifying uncertainty in lattice thermal conductivity and harmonic vibrational properties from DFT-based calculations using the BEEF-vdW XC functional. The procedure involves manually displacing atoms in an equilibrium structure and using the energies of these perturbed structures to determine harmonic and anharmonic force constants. Rather than generate a single energy for each perturbed lattice, BEEF-vdW generates an ensemble of energy values as a computationally efficient post-processing step by perturbing the XC functional parameters and solving for the energy of the system non-self consistently. Thus, each perturbed lattice yields an ensemble of energy values. This collection of energy ensembles are then used to determine an ensemble of force constants, which are used as input to a harmonic lattice dynamics calculation. This procedure results in an ensemble of thermal conductivity predictions whose spread can be used to quantify the uncertainty. Ensemble predictions for thermal conductivity are presented for silicon and compared to results predicted using the PBE, RPBE, LDA, and PBEsol XC functionals.

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Title: Finite Temperature Atomic Level Stress Calculation in Crystalline Solids

Author(s): *Ranganathan Parthasarathy, *Adjunct Professor, Tennessee State University*; Anil Misra, *Professor, University of Kansas*; Lizhi Ouyang, *Professor, Tennessee State University*;

Continuum measures computed from atomistic simulations are useful to study the finite temperature thermomechanical, optical, and electrical properties of nanocrystals. Their development requires (a) the connection between the continuum deformation field and the lattice positions of the crystal both in terms of average positions and thermal vibration, and (b) equivalence of free energy between discrete and continuum descriptions. Even for a homogeneously deforming single crystal, we show that the evolution in thermal fluctuations of atoms is non-affine and contributes significantly to the continuum stress, particularly at high temperatures (1). Localizable work conjugate stresses termed “Static Stress” and “Vibration Stress” (2) have been derived for (a) first order deformation gradients corresponding to atomic equilibrium positions and for (b) vibration tensors corresponding to second moments of atomic position, respectively. Although the quantification of entropic contribution to continuum stress using statistical mechanics is well known, this can be done for atomic level stresses per our derivation. Using MD simulation in NVT ensembles for fcc aluminum subjected to [100] uniaxial deformation, the effect of these stress measures on the mechanical behavior in the elastic range and in the vicinity of softening has been demonstrated. The derived stress measures at temperatures of 0.7Tm to 0.9 Tm show reversible softening which is similar to that experimentally observed under ultrasonic radiation. The Vibration Stress quantitatively demonstrates vibrational modes to be precursors to deformation-induced phase transition or mechanical instability, as also observed by neutron scattering experiments and ab initio simulations on crystalline solids. Under compression, the Vibration Stress goes through a softening regime prior to the onset of static non-affinity and mechanical instability. Correspondingly, the phonon group velocities also vary in a non-monotonic manner under compression (3). Under tension at ~0.9Tm, the computed stress differs from the first order approximation by almost 40%. As the material approaches softening under tension, the vibration tensor demonstrates localized zones of non-affinity and anisotropy before similar localization is observed in the static atomic displacements. The vibration tensor and vibration stress explore the local potential landscape at individual atomic sites, and have been used to analyze atomic level residual stress and strain fields in the vicinity of defects. 1 R. Parthasarathy, Mech. Res. Commun. 92, 101 (2018). 2 R. Parthasarathy, A. Misra, and L. Ouyang, J. Phys. Condens. Matter 30, 265901 (2018). 3 R. Parthasarathy, A. Misra, S. Aryal, and L. Ouyang, Contin. Mech. Thermodyn. 30, 1027 (2018).

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Title: Discontinuous Projection Method for Large, Accurate Electronic Structure Calculations in Real Space

Author(s): *John Pask, *LLNL*;

For decades, the planewave (PW) pseudopotential method has been the method of choice for large, accurate Kohn-Sham calculations of condensed matter systems, in ab initio molecular dynamics simulations in particular. However, due to its reliance on a Fourier basis, the method has proven difficult to parallelize at scale, thus limiting length and time scales accessible. In this talk, we discuss new developments aimed at increasing the scales accessible substantially, while retaining the fundamental simplicity, systematic convergence, and generality instrumental to the PW method's success in practice. The key idea is to release the constraint of continuity in the basis set, and with the freedom so obtained, employ a basis of local Kohn-Sham eigenfunctions to solve the global Kohn-Sham problem. In so doing, the basis obtained is highly efficient, requiring just a few tens of basis functions per atom to attain chemical accuracy, while simultaneously strictly local, orthonormal, and systematically improvable. We show how this basis can be employed to accelerate current state-of-the-art real-space methods substantially by reducing the dimension of the real-space Hamiltonian by up to three orders of magnitude. Results for metallic and insulating systems of up to 27,000 atoms using up to 38,000 processors demonstrate the scalability of the methodology in a discontinuous Galerkin formulation. Proceeding via projection of the real-space Hamiltonian instead promises to reach larger scales still. This work was performed, in part, under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Support for this work was provided through the Scientific Discovery through Advanced Computing (SciDAC) program funded by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences.

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Title: Supermodeling of a Tumor with Isogeometric Analysis Solvers

Author(s): *Maciej Paszynski, *AGH University of Science and Technology, Krakow, Poland*; Leszek Siwik, *AGH University of Science and Technology, Krakow, Poland*; Marcin Los, *AGH University of Science and Technology, Krakow, Poland*; Witold Dzwinel, *AGH University of Science and Technology, Krakow, Poland*; Adrian Klusek, *AGH University of Science and Technology, Krakow, Poland*;

In this presentation, we show that it is possible to obtain reliable prognoses about cancer dynamics by creating the supermodel of cancer, which consists of several coupled instances of a generic cancer model, developed with isogeometric analysis [1,2]. Its integration with real data can be achieved by employing a prediction/correction learning scheme focused on fitting several values of coupling coefficients between sub-models, instead of matching scores of tumor model parameters as it is in the classical data adaptation techniques. We show that the isogeometric analysis is a proper tool to develop a generic computer model of cancer, which can be used as a computational framework for developing high-quality supermodels. The details of the supermodeling algorithm are the following. The progression of the tumor growth model is controlled by 21 parameters. We first perform the sensitivity analysis of the tumor growth model, where we identify four most sensitive parameters, namely, tumor cell proliferation and survival time, and threshold oxygen concentration for tumor cells to multiply or die. We set up three different models using different parameters, resulting in different tumor growth evolutions. Next, we construct a supermodel as a linear combination of the models. We run the three models, and every K steps we correct the resulting fields, e.g. b(1)=C_{12}(b(1)-b(2))+C_{1,3}(b(1)-b(3)), where b(i) is the tumor cell density from model i. Next, we correct the fields by referring to the measurements b_meas e.g. b(1)=C_{1,meas}(b_meas-b(1)). Finally, we compute the average field, b=(b(1)+b(2)+b(3))/3, and we correct the coupling constants c_{i,j}=const*integral(b_meas-b)(b(i)-b(j)). Thus, by using the supermodeling approach we can simulate the reality by a linear combination of different models, even if the resulting field is not possible to approximate well by using any of the single models. This approach is similar to the one already used for climate supermodeling [3]. Acknowledgment. This work has been supported by National Science Centre, Poland, grant no. 2017/26/M/ST1/00281 [1] Marcin Los, Maciej Paszynski, Adrian Klusek, Witold Dzwinel, Application of fast isogeometric L2 projection solver for tumor growth simulations Computer Methods in Applied Mechanics and Engineering 316 (2017) 1257-1269 [2] Marcin Los, Adrian Klusek, Muhammad Amber Hassaan, Keshav Pingali, Witold Dzwinel, Maciej Paszynski, Parallel fast isogeometric L2 projection solver with GALOIS system for 3D tumor growth simulations, Computer Methods in Applied Mechanics and Engineering, 343, (2019) 1-22 [3] Frank M. Selten, Francine J. Schevenhoven, Gregory S. Duane, Simulating climate with a synchronization-based supermodel, Chaos 27, 126903 (2017)

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Solution of Inverse Problems Using Adversarial Learning

Author(s): *Dhruv Patel, *Aerospace and Mechanical Engineering, University of Southern California*;
Assad A Oberai, *Aerospace and Mechanical Engineering, University of Southern California*;

The solution of an inverse problem involves using a measured field to infer the field of interest, where the two are connected through a well-defined forward operator. For example, the measured field might be the temperature of a solid and the field to be inferred might be the spatial variation of its thermal conductivity. Most inverse problems are ill-posed, and their solution requires additional information about the inferred field. In this context we consider the scenario where the additional information is in the form of numerous independent samples of the inferred field. We note that it is typically difficult to translate this information into a prior when viewed from point of view of Bayesian inference, or into a regularizer when viewed from minimization-based/deterministic viewpoint of the inverse problem. We address this issue by borrowing concepts from Generative Adversarial Networks (GANs), a class of popular unsupervised machine learning algorithms based on two-player minimax game. In particular, for the components of the inferred field that are strongly informed by the measurement, we rely on the forward operator, and for the other components we rely on a GAN. The generator with the GAN is trained to produce inferred fields that are “realistic” in a sense that is made precise by the samples of the inferred field available to us. In this talk, we describe this hybrid approach of solving inverse problems that is driven in part by physics and in part by algorithms trained purely on data. We also demonstrate the effectiveness of this approach on some canonical linear inverse problems.

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Title: Probabilistic Failure Forecast Method Using a Stochastic Differential Equation Approach to Volcanic Eruption Forecasts

Author(s): *Abani Patra, *University at Buffalo, SUNY*; Andrea Bevilacqua, *INGV, Pisa, Italy*; E. Bruce Pitman, *University at Buffalo, SUNY*;

We present a doubly stochastic method for performing material failure theory based forecasts of volcanic eruptions. The method enhances the well known Failure Forecast Method equation of Voight and coworkers. In particular, we incorporate a stochastic noise term in the original equation, and systematically characterize the uncertainty. The model is a stochastic differential equation with mean reverting paths, where the traditional ordinary differential equation defines the mean solution. Our implementation allows the model to make excursions from the classical solutions, by including uncertainty in the estimation. The doubly stochastic formulation provides a complete posterior probability distribution, allowing users to determine a worst case scenario with a specified level of confidence. We validate the new method on historical datasets of precursory signals, across a wide range of possible values of convexity in the solutions and amounts of scattering in the observations. The results show the increased forecasting skill of the doubly stochastic formulation of the equations.

15th U.S. National Congress on Computational Mechanics
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Title: A Quasi-interpolation Method Based on LR B-splines

Author(s): *Francesco Patrizi, *SINTEF*; Carla Manni, *University of Rome "Tor Vergata"*; Hendrik Speleers, *University of Rome "Tor Vergata"*; Francesca Pelosi, *University of Rome "Tor Vergata"*;

In order to break down the tensor structure of standard B-splines, Locally Refinable (LR) B-splines have been introduced in [1] by extending the concept of knot insertion of the 1D B-splines to local insertion of (d-1)-dimensional boxes for the dD case. Like standard tensor-product B-splines, LR B-splines have local supports, are nonnegative and, using weights in (0,1), they form a partition of unity. However, a full description of their linear independence is still an open problem. LR B-splines are defined over mesh instances, called LR-meshes. These are built as a sequence of local insertions starting from a coarse tensor mesh. In [2] there is provided a way of generating LR-meshes over which the corresponding LR B-splines are locally linearly independent. These meshes have a hierarchical structure, and the procedure requires an a priori knowledge of the subregions of the domain where the mesh should be finer. On the other hand, a quick and light construction of quasi-interpolation schemes based on Truncated Hierarchical (TH) B-splines has been developed in [3]. It is actually also applicable in the general setting where the basis functions have local supports, are nonnegative, form a partition of unity and are locally linearly independent. Moreover, it is proved that such a quasi-interpolant is actually a projector on the space spanned by the basis functions under some not-so-restrictive hypotheses on the given data set. In this talk we combine the above results to get a quasi-interpolant based on LR B-splines. We provide some numerical examples, and make comparisons with THB-splines and tensor-product B-splines. [1] Tor Dokken, Tom Lyche, and Kjell Fredrik Pettersen. "Polynomial splines over locally refined box-partitions." Computer Aided Geometric Design 30.3 (2013): 331-356. [2] Andrea Bressan and Bert Jüttler. "A hierarchical construction of LR meshes in 2D." Computer Aided Geometric Design 37 (2015): 9-24. [3] Hendrik Speleers and Carla Manni. "Effortless quasi-interpolation in hierarchical spaces." Numerische Mathematik 132.1 (2016): 155-184.

15th U.S. National Congress on Computational Mechanics
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Title: Adaptive Local Refinement Based on LR NURBS and Its Application to a Dynamic Phase Field Model for Brittle Shell Structures

Author(s): *Karsten Paul, *RWTH Aachen University*; Christopher Zimmermann, *RWTH Aachen University*; Kranthi K. Mandadapu, *University of California at Berkeley*; Thomas J.R. Hughes, *The University of Texas at Austin*; Chad M. Landis, *The University of Texas at Austin*; Roger A. Sauer, *RWTH Aachen University*;

There is a demand for short development cycles in engineering applications which necessitates the use of efficient computational methods. The reliable prediction of fracture resembles one challenge during the design of today's engineering structures. Within the last years, phase field methods to model fracture have gained popularity. In these, the discontinuity at a crack is smeared so that discontinuities in the solution or geometry are avoided and no ad hoc criteria are necessary to model crack evolution. In the present work, the partial differential equation (PDE) describing the phase field evolution is derived and formulated on a two-dimensional deforming manifold. The latter is used to describe thin shells in a Kirchhoff-Love framework [2]. The coupled system includes two fourth-order nonlinear PDEs which requires at least global C1-continuity in the solution. In isogeometric analysis (IGA) splines are used to represent the solution and thus, it can be of user-defined smoothness. The presented fracture model requires a highly resolved mesh in the transition zone between the different phases which necessitates a local refinement strategy. Since the tensor-product mesh structure in standard IGA is not suitable for local refinement, LR NURBS [3] are employed. For these, parameter spaces are locally represented to enable the local insertion and modification of mesh lines. The LR mesh is adaptively refined based on the current phase field values and it is kept coarse at regions of no damage. Next to the spatial refinement, a time integration scheme [1] with adaptive time stepping is established which allows for large time steps in cases of no crack propagation. The coupled system is solved in a monolithic approach and typical benchmark problems are investigated to prove the established formulation. [1] Borden, M. J., Verhoosel, C. V., Scott, M. A., Hughes, T. J. R., and Landis, C. M., Comput. Methods Appl. Mech. Eng., 217-220:77–95 (2012) [2] Duong, T. X., Roohbakhshan, F., and Sauer, R. A., Comput. Methods Appl. Mech. Eng., 316:43–83 (2017) [3] Zimmermann, C. and Sauer, R. A., Comp. Mech., 60:1011-1031 (2017)

15th U.S. National Congress on Computational Mechanics
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Title: Stress Constrained Topology Optimization: To Aggregate or Not to Aggregate?

Author(s): *Glaucio Paulino, *Georgia Institute of Technology*; Fernando V. da Senhora, *Georgia Institute of Technology*; Oliver Giraldo-Londono, *Georgia Institute of Technology*; Ivan F. M. Menezes, *PUC-Rio*;

We present a methodology for solving topology optimization problems with local stress constraints. The issue of constraint aggregation is briefly discussed, and an approach avoiding aggregation is presented. Our approach is based on the Augmented Lagrangian method. To improve robustness of the aforementioned method, the penalty and objective function terms are modified such that the former reduces mesh-dependency and the later helps to drive the solution towards black and white (0/1). The objective function is tailored to solve mass minimization problems with local stress constraints. In addition, a variation of the vanishing constraint is used because it leads to results that outperform those obtained using relaxed stress constraints. Although maintaining the local nature of stress requires a large number of stress constraints, the formulation presented here requires only one adjoint vector whose cost of evaluation is similar to that of finding the global displacement vector. Several 2D and 3D topology optimization problems, each with a large number of stress constraints, are solved to demonstrate the robustness of the proposed approach.

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Title: B-spline Based Neuron Reconstruction Using Level Set Method

Author(s): *Aishwarya Pawar, *Carnegie Mellon University*; Jessica Zhang, *Carnegie Mellon University*;

Due to vast diversity in the morphology of neurons in the human body, there has been an increase in the interest to reconstruct neuron morphology from images [1]. The poor quality of the neuronal images and the thin branch-like structure of neurons makes the process of automatic reconstruction of neuron morphology very challenging. There are two methods to reconstruct neuron geometry from images, namely the centerline based methods and the boundary extraction methods. In centerline based methods, the irregularities of the neurite surface are not considered. In boundary based methods, segmentation is carried out to evaluate the accurate representation of the neuron geometry. We propose a novel boundary-extraction based reconstruction algorithm that captures the neuron morphology using higher order splines. Unlike the current methods which represent boundaries as piecewise constant functions, we provide a more accurate and smooth representation of the neuron geometry. In the level set segmentation framework, the implicit level set function defining the contour is defined using C2 continuous hierarchical splines [2]. Using adaptive local refinement finer details of the neuron geometry is captured using hierarchical splines. The improvement in the obtained reconstruction result is shown for 2D neuronal images as compared to other methods. Keywords: neuron morphology, image reconstruction, adaptive refinement, level set framework, hierarchical B-splines [1] K. M. Kim, K. Son and G. T. R. Palmore. Neuron image analyzer: Automated and accurate extraction of neuronal data from low quality images. Scientific reports, 5, 17062, 2015. [2] A. Pawar, Y. Zhang, Y. Jia, X. Wei, T. Rabczuk, C. L. Chan, C. Anitescu. Adaptive FEM-based Nonrigid Image Registration Using Truncated Hierarchical B-splines. A Special Issue of FEF 2015 in Computers and Mathematics with Applications, 72:2028-2040, 2016.

15th U.S. National Congress on Computational Mechanics
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Title: Reliability-based and Robust Design Optimization of Microvascular Materials for Active Cooling Applications

Author(s): *Reza Pejman, *Drexel University*; Vahid Keshavarzzadeh, *University of Utah*; Ahmad R Najafi, *Drexel University*;

We present a systematic approach for topology/shape optimization of microvascular materials under uncertainty. The emphasis of this presentation is placed on the efficient approach which combines the topology/shape optimization scheme with non-intrusive polynomial chaos expansion (PCE) method to produce a reliable/robust network design of microvascular materials. We develop a novel hybrid topology/shape optimization scheme for microvascular materials which simultaneously can perform the topological change as well as the shape optimization. In this study, Interface-enriched Generalized Finite Element Method (IGFEM) is used wherein the design geometry is projected onto a stationary mesh. This method eliminates the mesh distortion present in conventional Lagrangian shape optimization methods, as well as the essence of remeshing. In addition, very efficient simplified thermal and hydraulic models are implemented to obtain the thermal response of microvascular composites. Having an efficient model with small computational cost facilitate solving of much more complicated optimization problems such as optimization under uncertainty. The non-intrusiveness of this method allows almost any source of uncertainty to be included virtually in the design optimization process. In the current study, we have introduced uncertainty on loads, material properties, and geometry to address the variability on the working conditions and manufacturing process. Response metrics such as p-norm temperature and pressure drop are characterized as PCE of the underlying uncertain parameters, enabling precise and efficient estimation of statistical moments, failure probabilities and their sensitivities. The sensitivity analysis of the statistical moments and failure probability are conducted by means of PCE in which the necessary gradients on quadrature points are obtained via the adjoint method. A smooth approximation of the indicator function is introduced to facilitate the sensitivity analysis of failure probabilities. Different sets of application problems have been solved to demonstrate the advantages of using the suggested scheme rather than deterministic optimization method for microvascular materials. The comparison of results shows that as opposed to the optimum configurations obtained by Reliability-based and Robust design optimization, the deterministic designs violate the probabilistic constraints and hence represent non-optimal designs in presence of uncertainty.

15th U.S. National Congress on Computational Mechanics
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Title: A Mesoscale-Based Statistical Mechanics Framework for Modeling, Homogenization, and Uncertainty Quantification of Sand and Other Geomaterials

Author(s): *Gerald Pekmezi, *The University of Alabama at Birmingham*; David Littlefield, *The University of Alabama at Birmingham*;

In recent years, renewed research effort has been directed toward characterizing soils in transient applications. The main approach favored towards that end, has been to use one of many “cap” models derived from Mohr-Coulomb failure theory. In addition to a friction-based yielding stress like Mohr-Coulomb, typically such models incorporate a pressure cap. More advanced three-phase models also take into account the great difference in soil response with degree of saturation through “effective” stress. Effective stress isolates the stress in the solid skeleton of the material, from the bulk behavior. One such model, the Hybrid Elastic Plastic (HEP) model has been used extensively to model soils subjected to energetic, highly-transient phenomena using hydrocodes, a class of explicit computational packages geared toward such phenomena. Geomaterials such as soils, differ from other common engineering materials like metals, polymers, and many composites, in that the fundamental evolution of the underlying structure may reasonably be considered to occur at a higher scale, i.e. at the mesoscale rather than the microscale. This offers a somewhat unique opportunity to be able to characterize the underlying structural evolution of the material, and use that characterization to inform a general constitutive framework to model the behavior of a wide spectrum of soils under a range of pressures and distortional transient loading conditions. In the current work, experimental and laboratory data of a poorly graded sand previously modeled using the HEP model, is used to explore the internal evolution of the sand by carrying out particle-based simulations of the behavior at the mesoscale. These simulations are used to conduct a homogenization study of the granular subdomain. This is done in order to 1) identify the threshold at which the transition from discrete mesoscale to the Representative Volume Element (RVE) occurs, and 2) to quantify the uncertainty associated with discretization below that threshold. Additionally, the mesoscale results are used to formulate an effective stress model that matches the behavior observed in the particle-based simulations. This new effective stress model is then compared with the predictions of the sand behavior from the HEP model.

15th U.S. National Congress on Computational Mechanics
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Title: Multi-fidelity Modeling of Stochastic Processes Using Entropy-regularized GANs

Author(s): Yibo Yang, *University of Pennsylvania*; *Paris Perdikaris, *University of Pennsylvania*;

We present a probabilistic deep learning methodology that enables the construction of predictive data-driven surrogates for stochastic systems. Leveraging recent advances in variational inference with implicit distributions, we put forth a statistical inference framework that enables the end-to-end training of surrogate models on paired input-output observations that may be stochastic in nature, originate from different information sources of variable fidelity, or be corrupted by complex noise processes. The resulting surrogates can accommodate high-dimensional inputs and outputs and are able to return predictions with quantified uncertainty. The effectiveness our approach is demonstrated through a series of canonical studies, including the regression of noisy data, multi-fidelity modeling of stochastic processes, and uncertainty propagation in high-dimensional dynamical systems.

15th U.S. National Congress on Computational Mechanics
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Title: Achieving Efficient and Effective Multi-material Topology Optimization

Author(s): *Anderson Pereira, *Pontifical Catholic University of Rio de Janeiro*; Emily Sanders, *Georgia Institute of Technology*; Miguel Aguilo, *Sandia National Laboratories*; Glaucio Paulino, *Georgia Institute of Technology*;

We present a Matlab implementation of topology optimization for compliance minimization on unstructured polygonal finite element meshes that efficiently accommodates many materials and many volume constraints. Leveraging the modular structure of the educational code, PolyTop, we extend it to the multi-material version, PolyMat, with only a few modifications. First, a design variable for each candidate material is defined in each finite element. Next, we couple a Discrete Material Optimization interpolation with the existing penalization and introduce a new parameter such that we can employ continuation and smoothly transition from a convex problem without any penalization to a non-convex problem in which material mixing and intermediate densities are penalized. Mixing that remains due to the density filter operation is eliminated via continuation on the filter radius. To accommodate flexibility in the volume constraint definition, the constraint function is modified to compute multiple volume constraints and the design variable update is modified in accordance with the Zhang-Paulino-Ramos Jr. (ZPR) update scheme, which updates the design variables associated with each constraint independently. The formulation allows for volume constraints controlling any subset of the design variables, i.e., they can be defined globally or locally for any subset of the candidate materials. Borrowing ideas for mesh generation on complex domains from PolyMesher, we determine which design variables are associated with each local constraint of arbitrary geometry. A number of examples are presented to demonstrate the many material capability, the flexibility of the volume constraint definition, the ease with which we can accommodate passive regions, and how we may use local constraints to break symmetries or achieve graded geometries.

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Title: Extrapolation of Welding Simulations via Dynamic Modes for the Estimation of POD Modes

Author(s): *Pablo Pereira Alvarez, *EDF R&D*; David Ryckelynck, *Mines ParisTech*; Sofiane Hendili, *EDF R&D*; Josselin Delmas, *EDF R&D*; Vincent Robin, *EDF R&D*;

In welding, highly localized transient heat cause nonuniform thermal expansion and contraction, and thus result in plastic deformation in the weld and surrounding areas. Then, residual stress and distortion are permanently produced in the welded structures. Stresses are known to promote fracture and fatigue, and no experimental device gives access to the in-situ three dimensional distribution of stresses. Hence, prediction of residual stresses and distortion, are extremely important during the optimization of the welding process. Due to the complexity of the physical processes involved in welding, Finite Element Analysis play an indispensable role in the numerical simulation of welding. When considering mobile heat sources, numerical simulation have a computational complexity that is nonlinearly growing with respect to the length of the passes involved in the process. In many occasions, the Finite Elements simulations are not feasible in reasonable times. Recently, projection based model order reduction have been proposed to speed-up welding simulations [1]. A reduced basis of empirical modes is extracted from offline simulations before setting the reduced equations for online predictions. A common way to perform such an extraction of the reduced basis is the POD method. We propose a prediction step in order to extrapolate finite element predictions from a pass to an other, in order to obtain a reduced order model for passes that have not been simulated yet. Two methods to calculate extrapolated simulations are presented and then they will be combined to improve their performance. A first extrapolation method uses a dynamic mode decomposition (DMD) [2] of the plastic strain. Here the DMD describes the underlying physical mechanisms captured in the data sequence. We assume that these underlying physical mechanisms can be extended from a set of first passes to the remainder of passes. The second extrapolation method is the Physical Fields Shift Method. In this approach, physical transformations in the neighbourhood of the heat source are assumed to be almost steady state transformation in a moving frame. The extrapolated plastic strain is introduced in a linear model that predicts the displacement and stress which are used to create a reduced order model. References: [1] Zhang, Y., Combescure, A., & Gravouil, A. Efficient hyper reduced-order model (HROM) for parametric studies of the 3D thermo-elasto-plastic calculation. Finite Elements in Analysis and Design, 102, 37-51. (2015). [2] Schmid, Peter J. Dynamic mode decomposition of numerical and experimental data. Journal of fluid mechanics, 656:5–28, (2010).

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Title: Kirigami for Viral Capsids with Negative Gauss Curvature: Construction, Maturation, and Buckling Transition of a Two-tailed Archaeal Virus

Author(s): *Luigi Perotti, *University of Central Florida*; Sanjay Dharmavaram, *Bucknell University*;

The construction method proposed by Caspar and Klug (CK) in 1962 [1] allows to classify and characterize many spherical viruses. In the CK construction, five-fold defects are placed in a hexagonal lattice at specific locations according to two numbers, h and k, that determine the capsid size and T number. Although powerful, the original CK construction is limited to viral capsids with positive Gauss curvature. In recent years the archaeal viruses have attracted the attention of several researchers for the variety of their shapes and their ability to thrive in extreme conditions. Here, we present an extension of the original CK method to construct the Acidianus two-tailed virus (ATV), an archaeal virus with regions of negative Gauss curvature [2]. In order to extend the CK construction to the ATV, we assume that its shell is composed of pentamers and hexamers, as in the original CK construction, and heptamers, necessary to introduce the negative Gauss curvature in the regions where the tails connect to the virus central body. We codify the construction of ATV-like shapes using the technique of Kirigami, an extension of Origami where cutting is allowed. As in the original CK construction, we maintain an icosahedral central body - determined by the h and k lattice numbers - and introduce additional lattice constants to determine the tails' length and place seven-fold type defects (heptamers) in the hexagonal lattice. We use the presented Kirigami technique to build continuum models of the two tailed viruses in their immature state. Using thin shell elasticity theory and finite element discretization, we simulate the tails' growth as a function of a modified Föppl-von Kármán number and measures of asphericity. We observe the existence of a buckling transition as in the maturation of some spherical viruses. We conclude by investigating if a similar buckling transition is possible as a result of changes in the capsomers reference configuration, not elastic properties, as previously presented in [3] for the HK97 bacteriophage. [1] D. Caspar, A. Klug, in Cold Spring Harbor Symposia on Quantitative Biology, Vol. 27 (1962). [2] L.E. Perotti, K. Zhang, J. Rudnick, R.F. Bruinsma, Physical Review E, accepted for publication [3] L.E. Perotti, A. Aggarwal, J. Rudnick, R.F. Bruinsma, W.S. Klug, Journal of the Mechanics and Physics of Solids 77, 86 (2015).

15th U.S. National Congress on Computational Mechanics
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Title: High-Order Partitioned Solvers and Fully Discrete Adjoints for Multiphysics Problems

Author(s): *Per-Olof Persson, *University of California, Berkeley*; Daniel Huang, *Stanford University*; Matthew Zahr, *University of Notre Dame*;

We present our recent work on high-order accurate partitioned time-integrators for general coupled multiphysics problems. Using implicit-explicit Runge-Kutta schemes, we can automatically derive various partitioned schemes with different stability properties. We apply these solvers to relevant multiphysics problems, including 2-field and 3-field fluid-structure interaction problems, with applications in aeroelasticity. We obtain high-order spatial accuracy by using a discontinuous Galerkin method for the flow problem and a standard continuous Galerkin finite element method for the structures. In addition, we define quantities of interest for an optimizer, and derive the fully discrete adjoint equations of our numerical scheme to compute exact gradients. These systems can also be solved efficiently in a partitioned way and one stage at a time. We demonstrate our methods on model problems in multiphysics PDE-constrained optimization such as optimal energy extraction. References: 1) D. Z. Huang, P.-O. Persson and M. Zahr, "High-order, linearly stable, partitioned solvers for general multiphysics problems based on implicit-explicit Runge-Kutta schemes." Comput. Methods Appl. Mech. Engrg., Vol. 346, pp. 674-706, 2019. 2) D. Z. Huang, P.-O. Persson and M. Zahr, "A high-order partitioned solver for general multiphysics problems and its applications in optimization." Proc. of the 2019 AIAA Aerospace Sciences Meeting, January 2019.

15th U.S. National Congress on Computational Mechanics
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Title: An Integrated Optimization Approach for Additive Manufacturing of Aerospace Parts

Author(s): *Vignesh Perumal, *Drexel University*; Ahmad Najafi, *Drexel University*; Antonios Kontsos, *Drexel University*;

Weight reduction while maintaining mechanical performance is an important objective of optimization methods used in relation to Additive Manufacturing (AM) of metallic aerospace parts. In this context, lattices provide a way of reducing the non-critical mass while maintaining the desired performance. For example, a functionally graded lattice has been shown to have the lowest strain energy for a given loading envelope compared to other lattice configurations [1]. In this talk, a two-step approach is presented to achieve the objective of AM material optimization. The first step involves optimizing the design domain using topology optimization (TO) to minimize compliance. Then, in the second step, the non-critical, bulky sections of the optimized domain are populated with lattices of uniformly sized unit cells. A lattice and skin optimization (LSO) is run on the members and the enclosing skin of the resulting structure. This results in a functionally graded lattice with non-uniform thickness in regions of higher compliance. Convergence to the optimum solution is attained by solving the optimization problem in an iterative manner. Computational results are shown for a number of selected geometries related to aerospace material applications. The presented results were verified by finite element analysis in static and dynamic analyses. In addition, a select number of optimized geometries was printed to evaluate their performance compared to the corresponding solid ones and assess the potential of the proposed method. [1] A. Panesar, M. Abdi, D. Hickman, and I. Ashcroft, "Strategies for functionally graded lattice structures derived using topology optimisation for Additive Manufacturing," Additive Manufacturing, vol. 19, pp. 81-94, 2018.

15th U.S. National Congress on Computational Mechanics
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Title: Adaptive Multilevel Solvers for the Discontinuous Petrov-Galerkin Method with an Emphasis on High-frequency Wave Propagation Problems

Author(s): Leszek Demkowicz, *ICES, The University of Texas at Austin*; *Socratis Petrides, *ICES, The University of Texas at Austin*;

The work focuses on the development of fast and efficient solution schemes for the simulation of challenging problems in wave propagation phenomena. In particular, emphasis is given in high frequency acoustic and electromagnetic problems which are characterized by localized solutions in problems like ultrasonic testing, laser scanning and modeling of optical laser amplifiers. In wave simulations, the computational cost of any numerical method, is directly related to the frequency. In the high-frequency regime very fine meshes have to be used in order to satisfy the Nyquist criterion and overcome the pollution effect. This often leads to prohibitively expensive problems. Numerical methods based on standard Galerkin discretizations, lack of pre-asymptotic discrete stability and therefore adaptive mesh refinement strategies are usually inefficient. Additionally, the indefinite nature of the wave operator makes state of the art preconditioning techniques, such as multigrid, unreliable. A promising alternative approach is followed within the framework of the discontinuous Petrov-Galerkin (DPG) method. The DPG method offers numerous advantages for our problems of interest: mesh and frequency independent discrete stability even in the pre-asymptotic region, and a built-in local error indicator that can be used to drive adaptive refinements. Combining these two properties together, reliable adaptive refinement strategies are possible which can be initiated from very coarse meshes. The DPG method can be viewed as a minimum residual method, and therefore it always delivers symmetric (Hermitian) positive definite stiffness matrix. This is a desirable advantage when it comes to the design of iterative solution algorithms. Conjugate Gradient based solvers can be employed which can be accelerated by domain decomposition (one- or multi- level) preconditioners for symmetric positive definite systems. Driven by the aforementioned properties of the DPG method, an adaptive multigrid preconditioning technology is developed that is applicable for a wide range of boundary value problems. Unlike standard multigrid techniques, our preconditioner involves trace spaces defined on the mesh skeleton, and it is suitable for adaptive hp-meshes. Integration of the iterative solver within the DPG adaptive procedure turns out to be crucial in the simulation of high frequency wave problems. A collection of numerical experiments for the solution of linear acoustics and Maxwell equations demonstrate the efficiency of this technology, where under certain circumstances uniform convergence with respect to the mesh size, the polynomial order and the frequency can be achieved. The construction is complemented with theoretical estimates for the condition number in the one-level setting.

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Title: Reconstruction of Local Contractility of the Heart Based on Visible Kinematics

Author(s): *Simone Pezzuto, *CCMC, Università della Svizzera italiana*;

The in-vivo quantification of the mechanical function of the heart is a major issue in clinical cardiology. Local contractility of the tissue, that is the ability of the myocardium to pump blood, is indeed clinically relevant for therapeutic planning (e.g., lead placement in cardiac resynchronization therapy) and outcome prediction (reverse remodeling). Current imaging techniques, however, only provide an indirect assessment of contractility. Abnormal regional wall motion (or strain), obtained from echocardiography, cardiac MRI or even electroanatomic mapping [1], has been associated to a loss of contractility. Nonetheless, regions with low contractility may still move, due to the dynamic of the surrounding tissue. Additionally, absence of wall motion is not necessarily associated with absence of contractility. From a mathematical perspective, we can predict the displacement of the myocardium on the basis of the equations the stress balance due to external forces, passive stress and local contraction of the tissue. It is therefore, tempting to address the above problem of measure indirectly the contractility by means of an inverse procedure, that is reconstructing the contractility field by minimizing the mismatch between simulated and measured displacement. To this aim, we have been inspired by the recent literature on this subject [2] and applied an adjoint-based approach to solve the PDE-constrained parameter identification problem. In this work, however, we have also considered Total Variation (TV) regularization and compared it to standard Tikhonov regularizations for the scar identification problem. We found that TV performs very well in this context, yielding an accurate reconstruction of the contractile region even when observation is limited to the boundary of the domain (e.g., known kinematics of the endocardium only). We also show that the standard zeroth-order Tikhonov regularization may lead to non-physiological reconstruction of the contractility in the presence of fibers non-tangent to the boundary. While this may sound uncommon in realistic heart geometries, this observation sheds some light on the poor stability of the reconstruction near the boundaries. We conclude the presentation with an application of clinical interest reconstructing the contractility of the whole cardiac muscle from endocardial displacement, using data obtained from catheter-based mapping. References: [1] Maffessanti, F. et al. (2018). Integrated Assessment of Left Ventricular Electrical Activation and Myocardial Strain Mapping in Heart Failure Patients. JACC: Clinical Electrophysiology, 4(1), 138-146. [2] Balaban, G. et al. (2018). In vivo estimation of elastic heterogeneity in an infarcted human heart. Biomechanics and Modeling in Mechanobiology, 17(5),1317–1329.

15th U.S. National Congress on Computational Mechanics
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Title: Computational Investigation of Magnetoactive Elastomers for Tunable Vibrational Metamaterials

Author(s): *Connor Pierce, *University of Illinois Urbana-Champaign*; Carson Willey, *United States Air Force Research Laboratory, UES Inc.*; Vincent Chen, *United States Air Force Research Laboratory, UES Inc.*; James Hardin, *United States Air Force Research Laboratory, UES Inc.*; John Berrigan, *United States Air Force Research Laboratory*; Abigail Juhl, *United States Air Force Research Laboratory*; Kathryn Matlack, *University of Illinois Urbana-Champaign*;

Vibrational metamaterials control the propagation of elastic waves in novel ways through careful design of their geometry. Of special interest is the potential to exhibit band gaps, or frequency ranges where elastic waves cannot propagate. Such behavior promises to enable highly effective control of structural vibrations. Recently, we fabricated a lattice-based metastructure from a magnetoactive elastomer (MAE) to enable active control over the band gap frequency. MAEs are composite materials consisting of elastomers having embedded magnetically permeable particles and have been shown to change stiffness in the presence of a magnetic field. [1] We found that application of a magnetic field caused an increase in the band gap frequency of our metastructure because of this stiffening effect. To the best of our knowledge, this application of magnetoactive elastomers is unprecedented, and the behavior of such metastructures is largely unexplored. We present the results of a computational study of these metastructures using frequency-sweep and Floquet-Bloch eigenfrequency finite element analyses. We study how the coupled magnetomechanical response of the MAE can be used to control the band gap frequency. In addition, we numerically study how the “shape” of the magnetic field used to actuate the metastructure can be varied to spatially control the elastic wave propagation in the metamaterial. [1] M. R. Jolly, J. D. Carlson, B. C. Munoz, and T. A. Bullions, “The Magnetoviscoelastic Response of Elastomer Composites Consisting of Ferrous Particles Embedded in a Polymer Matrix,” J. Intell. Mater. Syst. Struct., vol. 7, pp. 613–622, 1996.

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Title: Regarding the In Vivo Relevance of Compression/Impact Tests on Unconfined Cylindrical Plugs of Cartilage – A Numerical Study

Author(s): Vukasin Strbac, *University of Connecticut, Storrs, CT*; *David M. Pierce, *University of Connecticut, Storrs, CT*;

Researchers in cartilage biomechanics routinely harvest osteochondral explants from load-bearing regions of the femoral condyles, and results from ex vivo mechanical tests performed on such explants (e.g. unconfined uniaxial compression or impact with a steel platen) form the basis for conclusions about the biomechanics and mechanobiology of cartilage in vivo. Although ex vivo experiments represent a well-established model for mechanical testing of cartilage, concerns remain about the relevance of such tests to conditions in vivo [1]. We used numerical models of patient-specific, intact joints to mimic in vivo conditions and examined (1) the in vivo relevance of uniaxial compression tests on unconfined cylindrical explants (plugs) of cartilage, and (2) the minimum diameter of plug required for the mechanical state of the main (center) axis to reproduce the mechanical conditions in vivo. To compare the through-thickness mechanics of cartilage in intact full joints versus cartilage plugs, we applied corresponding loads for mechanical impacts and compressions using two finite element models: (1) an unconfined in vitro model for plugs, and (2) an intact full-joint model. With these numerical models, we compared first/third principal stresses/strains and fluid pressures though the cartilage thickness of plugs and of intact full joints. We applied physiological loads to full-joint models and extracted distributions in stresses and strains through the thickness from load-bearing regions in the femoral cartilage. Then, by assuming we had extracted cylindrical explants from load-bearing regions within the same joint, we kept the thickness and though-thickness material parameters identical and loaded plugs of varying diameters with matching displacement profiles. Thus, we extracted the same through-thickness mechanical responses of the plugs as a function of plug diameter. Our numerical results show that cylindrical explants of cartilage tested ex vivo reproduce the through-thickness distributions of mechanical responses (e.g. stresses, strains) present during normal loading of an intact full joint, and that under unconfined compression ~10 mm diameter specimens provide results most similar to intact full joints. This study indicates (1) this ex vivo testing protocol can produce results meaningful to mechanical conditions in vivo, and (2) using large diameter explants and normalized mechanical measures (stress, stress rate, and energy density) from the center of the explants (to avoid edge effects) increases model fidelity. [1] M. Nickien, A. Heuijerjans, K. Ito, C.C. van Donkelaar, Comparison between in vitro and in vivo cartilage overloading studies based on a systematic literature review, J. Orthop. Res., 36:2076–2086, 2018.

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Title: Advancements in Isogeometric Analysis of Thin-Walled Structures in LS-DYNA

Author(s): *Marco Simone Pigazzini, *Livermore Software Technology Corporation*; Attila Nagy, *Livermore Software Technology Corporation*; Liping Li, *Livermore Software Technology Corporation*; Stefan Hartmann, *Dynamore*; David Benson, *Livermore Software Technology Corporation*;

The use of isogeometric analysis is rapidly expanding due to combined efforts of structural analysts, scientists and developers. An area of both academic and industrial interest is the development of formulations and technologies for the numerical analysis of thin-walled components. These structures are represented and discretized by means of smooth bivariate spline-based approximations, e.g., (non-uniform rational) B-splines surfaces. In this talk we present some of the recent developments in LS-DYNA aimed at extending the capabilities of isogeometric structural analysis of (multi-layer) shell models. The range of applicability of these additions, which enable the users to further exploit the superior approximation properties of IGA, is illustrated through selected examples.

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Title: A Multiscale Approach to Equivalent Modelling of Rough Contact

Author(s): *Rodrigo Pinto Carvalho, *Institute of Science and Innovation in Mechanical and Industrial Engineering*; António Manuel Couto Carneiro, *Institute of Science and Innovation in Mechanical and Industrial Engineering*; Francisco Manuel Andrade Pires, *Institute of Science and Innovation in Mechanical and Industrial Engineering*; Thiago Doca, *Faculty of Technology, University of Brasilia*;

Keywords: Rough contact; Contact homogenisation; Multiscale modelling. Abstract. In virtually every engineering and biological system, it is by way of contact that bodies interact, coming in touch and interchanging energy. However, although the classical Hertzian contact theory assumes the contacting surfaces to be smooth, under certain magnification all surfaces are rough. This fact has a substantial impact on the physics of contact interaction, with one of the most studied observations being that, for most materials, the real contact area is only a small fraction of the apparent contact area. Among others, the pioneering work by Greenwood and Williamson [1] has been the cornerstone for the so-called asperity-based rough contact models, in which the classical Hertzian solution is extended by including the statistics of the surface roughness. This approach has been extended in order to incorporate many different aspects of rough contact and many analytical models are available in the literature. The focus of this work is placed on a well-known result from contact mechanics: if there is no friction or adhesion between two rough surfaces and the surface slope is small, the elastic contact between two rough surfaces can be mapped to the contact between an equivalent single rough surface and a rigid flat [2]. Therefore, in this contribution, this equivalent modelling technique is ascertained by employing a multiscale homogenisation approach. More specifically, by virtue of the Finite Element Method and dual mortar contact modelling combined with a contact homogenisation framework [3], the validity of this assumption is analysed, specially under circumstances where some of its assumptions are dropped. References Greenwood, J. A. and Williamson, J. P., 1966. Contact of nominally flat surfaces. Proc. R. Soc. Lond. A Math, 295, 300-319. K. L. Johnson, 1985. Contact Mechanics. Cambridge, New York. Stupkiewicz, S, 2007. Micromechanics of Contact and Interphase Layers. Springer, Verlag Berlin Heidelberg.

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Title: CutFEM Approach for Analysing the Stability of Phase Boundaries

Author(s): *Mikhail Poluektov, *University of Warwick*; Alexander Morozov, *Technical University of Berlin; Institute for Problems in Mechanical Engineering of Russian Academy of Sciences*; Alexander B. Freidin, *Institute for Problems in Mechanical Engineering of Russian Academy of Sciences; Peter the Great St. Petersburg Polytechnic University*; Wolfgang H. Müller, *Technical University of Berlin*; Lukasz Figiel, *University of Warwick*;

The analysis of the stability and the kinetics of phase boundaries has a long history in continuum mechanics. More recently there has been an emergence of interest in mechanochemical processes, focusing on describing the influence of mechanical stresses on the kinetics of localised chemical reactions that take place at a surface inside a solid body [1]. In both cases, the interface (phase boundary or chemical reaction front) can be at an equilibrium state, the configurational stability of which depends on the stress conditions. For materials with complex rheology undergoing large deformations, the analysis of the stability must be performed computationally. When the standard Finite-Element Method (FEM) is applied to problems with moving interfaces, the geometry should be remeshed each time the interface moves. Such technique requires using an extremely fine mesh for achieving a sufficient accuracy and additional computational resources for performing remeshing. Furthermore, the automation of the remeshing process can be a non-trivial task. An alternative way of treating such problems is a computational method that allows the interface to cut through the elements and to move independently of the mesh, the so-called CutFEM approach [2]. In this talk, a generalisation of CutFEM to large deformations and arbitrary constitutive behaviour of materials is presented [3]. In the proposed method, the interface conditions (e.g. the force equilibrium and the displacement continuity for mechanics) are enforced weakly by using a Nitsche-like approach. To address the ill-conditionality of the problem related to the interface partitioning the elements into highly unequal spatial fractions, an inter-element stabilisation is added. The total energy functional is formulated, from which the weak form of the problem is derived. It is demonstrated that the proposed implementation of the method has the same convergence rate with respect to the mesh size as the standard FEM. The method is used to simulate the kinetics of phase boundaries and chemical reaction fronts in hyperelastic bodies undergoing large transformation strains. An approach to an equilibrium configuration is modelled and several case studies of configurationally stable and unstable interfaces are considered. To benchmark the method, a comparison with the standard FEM with remeshing for capturing the interface movement is performed for small strains. Acknowledgements: M.P., L.F. acknowledge financial support from EU Horizon 2020 project 685716; A.M., A.F., W.M. acknowledge financial support from DFG/RFFI grants MU1752/47-1 and 17-51-12055. References [1] Int.J.Eng.Sci. (2014) 83:57-75 doi.org/10.1016/j.ijengsci.2014.03.008 [2] GAMM-Mitt. (2005) 28(2):183-206 doi.org/10.1002/gamm.201490018 [3] Comput.Mech. (2018) online doi.org/10.1007/s00466-018-1628-z

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Title: PFEM-FEM Coupling for Fluid-structure Interaction Problems Involving Free Surfaces, Large Solid Deformations, and Strong Added Mass Effects

Author(s): Marco-Lucio Cerquaglia, *ULiège*; Romain Boman, *ULiège*; Luc Papeleux, *ULiège*; *Jean-Philippe Ponthot, *ULiège*;

The present work focuses on the solution of fluid-structure interaction problems involving free surfaces and deformable structures. Free-surface flows are often encountered in reality, but the numerical solution of such problems remains a challenge, especially when the flow interacts with some flexible structure. The Particle Finite Element Method (PFEM) is nowadays a well-established Lagrangian method for the study of free-surface flows [1, 2]. The key feature of this method is the continuous remeshing of the computational domain through an efficient Delaunay triangulation, based on which the equations are solved using classical Finite Elements. In this work, the PFEM is coupled to Metafor, an in-house non-linear Finite Element solver, through a fully partitioned approach. The main advantages of using a partitioned approach are that independent formulations can be employed for the fluid and the solid domains, and that the capabilities of already existing codes can be exploited at their best. In particular, in the problems proposed in this work, the solid structures can undergo very large deformations, and complex material laws, including plasticity for instance, can be easily taken into account. However, the staggered solution of the fluid and solid parts can induce numerical instabilities known as added mass effects. These instabilities becomes more and more important as the solid-to-fluid density ratio reduces. To circumvent the appearance of such instabilities while preserving a fully partitioned approach, the Interface Quasi-Newton Inverse Least Square (IQN-ILS) [3] strategy is employed in this work and compared to more standard approaches, like the Block Gauss-Seidel iterations with Aitken relaxation. To assess the robustness and the efficiency of the technique developed in this work many examples, involving very different density ratios, are proposed. Results are compared to those available in the literature, whenever possible. REFERENCES [1] S.R. Idelsohn, E. Oñate, F. Del Pin, “The particle finite element method. A powerful tool to solve incompressible flows with free-surfaces and breaking waves”, Int. J. Numer. Meth. Engng, 61, 964-989 (2004). [2] M.L. Cerquaglia, G. Deliége, R. Boman, V. Terrapon, J.-P. Ponthot, “Free-slip boundary conditions for simulating free-surface incompressible flows through the particle finite element method”, Int. J. Numer. Meth. Engng, 110(10) 921-946 (2017). [3] J. Degroote, K.-J. Bathe, J. Vierendeels,” Performance of a new partitioned procedure versus a monolithic procedure in fluid-structure interaction”, Computers & Structures, 87(11-12), 793-801(2009)

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Title: Physics-Informed Deep Learning Model for Predicting Ballistic Coefficients of Explosively Driven Fragments*

Author(s): *Kevin Potter, *Sandia National Laboratories*; Peter D. Yeh, *Sandia National Laboratories*; Cari Martinez, *Sandia National Laboratories*; Matthew D. Smith, *Sandia National Laboratories*; Charles Snider, *Sandia National Laboratories*; John Korbin, *Sandia National Laboratories*; Stephen Attaway, *Sandia National Laboratories*;

Deep Learning models have the potential for accelerated predictions of physical phenomenon with an acceptable accuracy loss as alternatives to reduced-order models. In this work, we use a Deep Learning network to perform fast and accurate lift and drag predictions of explosively driven fragments traveling at hypersonic velocities. Specifically, we employed a conditional generative adversarial network (cGAN) to predict the total force on arbitrary shapes fixed in an external supersonic flow. The loss function of the generator was modified with additional loss terms based on the physics of the problem as well as the calculated forces. We then heavily penalizing generated solutions that violated certain physical constraints. We trained our physics-informed network with a large set of flow fields from high fidelity aerodynamics simulations and show that drag and torque were accurately predicted to within 2% average error. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. *Funding from the DOE is gratefully acknowledged.

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Title: Non-invasive Quantification of In-Vivo Aortic Valve Strains

Author(s): Bruno Rego, *University of Texas at Austin*; *Samuel Potter, *University of Texas at Austin*; Alison Pouch, *University of Pennsylvania*; Robert Gorman, *University of Pennsylvania*; Michael Sacks, *University of Texas at Austin*;

The potential clinical benefit of patient-specific biomechanical models of cardiovascular disease remains an unrealized goal, often due to difficulties in non-invasively acquiring necessary kinematic data. This is particularly true in assessing bicuspid aortic valve (BAV) disease. There is thus a need for simulation techniques that can directly integrate individualized BAV geometry and deformation data from in-vivo imaging modalities. Towards this goal, we have extended an approach developed for human mitral valve (MV) to determine tri-leaflet aortic valve (TAV) and BAV leaflet deformations based on clinically obtained in-vivo imaging data. Imaging data was collected on a patient-specific basis for individuals with TAV and for those with BAV. To segment the acquired images, a closed Non-uniform Rational B-Spline (NURBS) curve was fit to the leaflet boundaries and converted into an open NURBS surface. The surface was matched to the segmented image data by least squares error minimization between the surface and segmented data points. In areas of data sparsity, Sobolev regularization was used to stabilize the least squares fit. To acquire diastolic deformation fields across the entire valve leaflet surface non-invasively, we utilized a previously validated image-based strain estimation method developed by our group, which yields local strain information directly from clinical-quality in-vivo images. An essential feature of our approach is that it does not rely on physical markers or assumptions of material point correspondence to extract surface deformations. Instead, we exploited the fact that the gross subject-specific closed-state geometry of the leaflets can be precisely acquired from diastolic scans, and developed a finite-element-based method to enforce this closed shape during simulation of AV closure from the open configuration. This method was able to capture the complex, heterogenous leaflet deformation field of the aortic valve. Resulting strain fields also corresponded well with results of structural simulations based on population-averaged fiber structural data and in-vivo measurements from previous studies. Based on the observed spatial resolution of the observed resultant strain field, this approach is sufficiently sensitive to capture the effects of patient-specific heterogeneity in the in-plane deformations of both TAV as well as BAV leaflets. This study is an essential step toward patient-specific assessment of BAV based on correlating leaflet deformation and disease progression, as it provides a means for assessing patient-specific strain patterns.

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Title: Deflated Assembly Free Elastoplastic Analysis for Additive Manufacturing Simulation

Author(s): *Bhagyashree Prabhune, *University of Wisconsin, Madison*; Krishnan Suresh, *University of Wisconsin, Madison*;

Additive manufacturing (AM) has revolutionized engineering by making it possible to create complex topologies with ease. However, residual distortion is one of the primary challenges, especially in metal AM. Reliable prediction of residual distortion is important to ensure the quality of the manufactured part. Finite element analysis (FEA) is the most popular simulation method today for predicting residual distortion. However, FEA is computationally expensive, taking several days to simulate even small parts. The computational bottleneck in commercial FEA software can typically be traced to extensive and expensive memory access. The present work focuses on developing a strategy for a limited-memory deflated assembly-free elastoplastic FEA where the stiffness matrix is not assembled. This implementation is particularly well suited for large-scale problems and can be easily implemented with multi-core architectures. Using mesh congruency and assembly-free approach, enormous reduction in memory access is achieved has in elastic analysis [1], resulting in significantly reduced computational cost. This work extends this method to elastoplastic analysis in a computationally efficient manner. Elastoplasticity makes assembly-free implementation challenging compared to elastic analysis since the elemental stiffness matrix in the plastic state depends on the stress state of the element reducing the mesh congruency. Further, the nonlinearity introduces the concept of assembly-free tangent matrix. The impact of assembly-free deflation is explored in this context. [1] Yadav, P., Suresh, K., “Large Scale Finite Element Analysis via Assembly Free Deflated Conjugate Gradient,” Journal of Computing and Information Science in Engineering, Volume 14, Number 4, December 2014.

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Title: Embedded Multilevel Monte Carlo for Uncertainty Quantification in Complex Random Domains

Author(s): Santiago Badia, *Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE), Esteve Terradas 5, 08860, Castelldefels, Spain.*; Jerrad Hampton, *Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE), Esteve Terradas 5, 08860, Castelldefels, Spain.*; *Javier Principe, *Centre Internacional de Mètodes Numèrics en Enginyeria (CIMNE), Esteve Terradas 5, 08860, Castelldefels, Spain.*;

Uncertainty quantification requires the solution of a stochastic partial differential equation (PDE) with random data, e.g. material properties, boundary and/or initial conditions and the geometry of the domain. In real situations, geometry is hardly known exactly and surfaces are rarely smooth when looking at sufficiently small scale. This uncertainty can have a strong impact on the solution of a PDE. There are several methods for solving stochastic PDE such as stochastic Galerkin or stochastic collocation but most of them suffer the so-called "curse of dimensionality", a dramatic increase of computational cost with the number of stochastic variables. Besides, some of these methods are intrusive: a code that can be used to solve a deterministic problem needs to be modified to solve a stochastic one. In contrast, the Monte Carlo method does not present these drawbacks but statistical and approximation requirements make it prohibitively expensive. To address this difficulty the Multilevel Monte Carlo (MLMC) method exploits a hierarchy of meshes to compute expectations on each level with a decreasing number of samples (in the finer meshes), thus reducing the computational cost by orders of magnitude. It has been successfully applied to stochastic PDE with random material properties and/or initial and boundary data. There are three approaches to deal with geometric uncertainty. The first one is based on domain mappings to transform a problem in a random domain into a stochastic problem in a deterministic domain. Since it requires the construction of a global smooth mapping, its application is restricted to simple geometries. The second one is based on introducing perturbations (e.g. a Taylor expansion using shape derivatives) to a nominal domain. As any perturbation method, some restrictions on the perturbation size need to be assumed, reducing its applicability. In this work we follow the third approach, exploiting the generality of embedded methods, as proposed in [1]. We discuss how to exploit unfitted finite element techniques in the context of the MLMC method to perform uncertainty quantification when complex geometries with random boundaries are considered. The traditional ill-posedness of these techniques is cured using aggregation techniques for conforming methods [2]. [1] C. Canuto and T. Kozubek. A fictitious domain approach to the numerical solution of PDEs in stochastic domains. Numerische Mathematik, 107(2):257–293, 2007. [2] S. Badia and F. Verdugo and A. F. Mart??n. The aggregated unfitted finite element method for elliptic problems. Computer Methods in Applied Mechanics and Engineering, 336, 533–553, 2018.

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Title: On Flat-Top PU, A-Posteriori Error Estimators and Adaptivity for the GFEM

Author(s): *Sergio Persival Proenca, *University of Sao Paulo, Brazil*; Rafael Lins, *Aeronautics Technological Institute, Brazil*; Murilo Bento, *University of Sao Paulo, Brazil*; Caio Ramos, *University of Sao Paulo*;

The analysis of complex problems including non-linear effects at different scales, time dependent responses and multi-physics coupled phenomena requires the development of robust formulations in the field of numerical methods. The Generalized Finite Element Method (GFEM) is the alternative explored in this investigation. The methodology adopted is aimed at the development of an efficient and stable formulation, in this sense presenting optimal order of convergence and conditioning comparable to the conventional Finite Element Method (FEM). Such aspects can be essentially contemplated by guaranteeing the linear independence of the shape functions, typically generated by enrichment of the partition of unit. Basically the alternative hereby adopted to achieve the objectives of efficiency and overall stability is the use of appropriate bases for the generation of the shape functions. In particular, flat-top partitions of unit are employed for constructing the set of enriched shape functions. Low-order 2D flat-top partitions of unit using triangular and quadrilateral elements are considered. On the other hand, a posteriori error estimates are explored to carry out the control over the accuracy of the resulting numerical solution. A fairly accurate and low computational cost estimate was recently proposed, consisting of a new version of Zienkiewicz-Zhu's classical recovery-based methodology (ZZ). This version, referenced by the acronym ZZ-BD, differs from the classical one by the use of a local weighted projection for the calculation of the recovered stress field over element patches—the set of elements sharing a node. Such projection leads to a block-diagonal system of equations for the recovered stresses. In addition, original adaptive procedures that explore the ZZ-BD estimator as an indicator of the regions where solution improvement is necessary are presented. The applications considered for testing the formulation include static and time-dependent analyzes of problems with singularities, typically situations where a robust GFEM formulation should have clear advantages over the conventional FEM formulation. R. M. Lins, M. D. C. Ferreira, S. P. B. Proenca, and C. A. Duarte, “An a-posteriori error estimator for linear elastic fracture mechanics using the stable generalized/extended finite element method,” Comput. Mech., vol. 56, no. 6, pp. 947–965, 2015. M. A., Schweitzer, “Variational mass lumping in the partition of unity method”. SIAM Journal on Scientific Computing, v. 35(2), p. A1073-A1097, 2013. Q. Zhang, U. Banerjee, I. Babuška, “Strongly Stable Generalized Finite Element Method (SSGFEM) for a non-smooth interface problem”. Comput. Methods Appl. Mech. Engrg, vol. 344, pp. 538–568, 2019.

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Title: Computer Model of the Human Heart

Author(s): *Charles Puelz, *Courant Institute, NYU*; Margaret Anne Smith, *UNC Chapel Hill*; Simone Rossi, *UNC Chapel Hill*; David Wells, *UNC Chapel Hill*; Boyce Griffith, *UNC Chapel Hill*;

In this talk we describe the development of a computer model of the human heart, which includes all four chambers, valves, and some of the great vessels. The numerical approximation of cardiac mechanics and blood flow is handled by the immersed boundary finite element method. In this approach, the solid displacements and forces are approximated in Lagrangian form on a moving finite element mesh, and the fluid is approximated on a fixed Cartesian grid. The heart geometry is derived from patient computed tomography data, and the tissue is assumed to be hyperelastic. The elastic response of the heart myocardium and valves depend on vector fields. In the myocardium, these vector fields roughly align with the orientation of the myocytes, and in the valves these vector fields align with preferential directions of strain from experiments. In particular, the parameters in the stress functions for the valves are chosen to match experimental stress-strain data from the literature. Our results include a full cardiac cycle with both atrial and ventricular contraction. Realistic boundary conditions are imposed on heart to simulate diastolic filling and the afterload experience during contraction.

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Title: Further Investigation into Stable, Unbiased Mortar Contact Approaches

Author(s): *Michael Puso, *Lawrence Livermore Nat'l Laboratory*; Jerome Solberg, *Lawrence Livermore Nat'l Laboratory*;

Mortar contact approaches have primarily been formulated as single pass algorithms and are thus inherently biased. Although this bias is typically not detrimental to the accuracy of the results, it does make it difficult to treat self-contact problems and problems where contact surfaces are automatically generated. An unbiased, mortar contact and mesh tying approach based on Lagrange multipliers is proposed in this presentation and its performance is compared to other competing methods. The approach is based on a stabilization scheme for the Lagrange multiplier fields and is shown to be suitable for linear and higher order mortar discretizations. Strategies for choosing suitable stabilization will be investigated along with different solution procedures for computing the Lagrange multipliers. Results will focus on the accuracy and robustness of the proposed approach with an additional focus on self-contact problems.

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Title: Multiscale Mechanics of Non-collagenous Interfaces in Collagen

Author(s): Yang Wang, *University of Texas at Dallas*; Reza Morsali, *University of Texas at Dallas*; Zhengwei Dai, *Jiaxin University, China*; Majid Minary-Jolandan, *University of Texas at Dallas*; *Dong Qian, *University of Texas at Dallas*;

Bone is a composite material with hierarchical structures. At the lowest hierarchical level of molecular scale, tropocollagen molecules self-assemble into super-twisted collagen microfibrils through hydrogen bonding and covalent crosslinking, and are impregnated with biominerals. The interfibrillar interface constitutes primarily of noncollagenous proteins such osteocalcin (OC) and osteopontin (OPN). While a great deal of research work has been devoted to the mechanics of collagens, the role of collagen interfibrillar interface remains a subject that has been largely unexplored. In this talk, we present a study of the noncollagenous OC/OPN interface and its impact on the mechanical properties of the collagen employing a multiscale computational approach. We first investigate the stress-strain responses and the associated deformation mechanisms when the interfaces are subjected to different types of loading conditions. Our study reveals the important collaborative effects between the OC and OPN proteins, which are supported by the deformation and energy landscape derived from the simulation. Continuum models are then established to elucidate the fundamental mechanisms and the key effects of the hidden length.

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Title: Optimal Experimental Design Based on the Generalized Mean Objective Cost of Uncertainty with Application to Computational Shape Memory Alloy Design

Author(s): Shahin Boluki, *Texas A&M University*; *Xiaoning Qian, *Texas A&M University*; Edward Dougherty, *Texas A&M University*;

An intrinsically robust Bayesian (IBR) operator minimizes the expected cost relative to a prior distribution over an uncertainty class of models. The mean objective cost of uncertainty (MOCU) is the expected increase in cost from using an IBR operator instead of an optimal operator for each system. Optimal experimental design (OED) chooses an experiment yielding maximum decrease in MOCU, thereby minimizing pertinent uncertainty [1]. Design can be implemented sequentially. The generalized definition assumes an uncertainty class, prior distribution, action space, and cost function [2]. For each model in the uncertainty class, an optimal action minimizes the cost. An IBR action minimizes the expected cost. MOCU is the expected performance loss over the uncertainty class from using an IBR action. Given an experiment space and an experiment in that space, we consider the prior conditioned on the experiment, that is, the posterior distribution relative to the experiment. Relative to the conditional uncertainty class, we define IBR actions and the conditional (remaining) MOCU. Taking the expectation over the outcomes of the experiment gives the expected remaining MOCU, which is minimized by an optimal experiment. Generalized-MOCU-based OED fits within Lindley's paradigm for Bayesian experimental design. The Knowledge Gradient and Efficient Global Optimization are special cases. We consider OED for computational shape memory alloy (SMA) design with desired stress-strain profiles for a particular dopant at a given concentration utilizing time-dependent Ginzburg-Landau (TDGL) theory [3]. The goal is to find an optimal dopant and concentration to minimize the simulated energy dissipation, with the least number of times running the TDGL model (least number of experiments). A surrogate model is trained based on fitting some initial data generated from the TDGL model. It approximately predicts the dissipation energy for a specified dopant and concentration, and it is used as the cost function for experimental design. The TDGL model acts as the actual underlying system, and the surrogate model is the model of the actual system. Sequential MOCU-based OED reduces to the OED in [3]. [1] Dehghannasiri, R., et al., “Optimal Experimental Design for Gene Regulatory Networks in the Presence of Uncertainty,” IEEE/ACM Transactions Computational Biology and Bioinformatics, 14(4), 2015. [2] Boluki, S., et al., “Experimental Design via Generalized Mean Objective Cost of Uncertainty, IEEE Access, 7(1), 2019. [3] Dehghannasiri, R., et al., “Optimal Experimental Design for Materials Discovery,” Computational Materials Science, 129, 2017.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Patient-specific Modeling of Bicuspid Aortic Valve Dynamics

Author(s): *Tongran Qin, *Georgia Institute of Technology*; Andres Caballero, *Georgia Institute of Technology*; Wenbin Mao, *Georgia Institute of Technology*; Wei Sun, *Georgia Institute of Technology*;

Introduction: Bicuspid aortic valve (BAV) is one of the most common congenital cardiac malformation. A better fundamental understanding of BAV biomechanics has many clinical implications, such as BAV calcification and BAV related ascending aortic aneurysm formation. However, patient-specific modeling of BAV dynamics are still limited. In this study, a fluid-structure interaction (FSI) analysis was performed to investigate BAV leaflets FSI with the aortic root for type 0 and type 1 BAV patients. Materials and Methods: The patient-specific 3D geometries of the BAV leaflets, aortic root, and calcifications were reconstructed from CT images. Firstly, FE modeling was performed for the BAV leaflets (with and without calcification) to analyze in vivo valve closure, where only the leaflets were simulated. The displacement of the leaflet-sinus attachment curve between the mid-systole and mid-diastole phases was prescribed, and the patient-specific transvalvular pressure was applied to simulate BAV closure. Secondly, FSI modeling based on the combination of smoothed particle hydrodynamics (SPH) and nonlinear FE formulation was performed. Pressure boundary conditions were applied at the left ventricle outflow tract inlet and aortic outlet. The unpressurized (stress-free) geometries were obtained using the generalized pre-stressing algorithm based on the geometries from the mid-systole phase, and are selected as the starting point of the simulation. Two cardiac cycles were conducted where the results from the second cycle were analyzed. The human valve leaflet and aortic root material properties were obtained from in vitro biaxial testing, and the mechanical responses were modeled with a modified Holzapfel-Gasser-Ogden material model. Results and Discussion: The model was validated by comparing mid-diastolic BAV leaflets geometries with the CT images, and the hemodynamic parameters with the clinical Echo measurement. The FE results show that peak stresses were near the calcification and the raphe. It was found that both the properties of calcification and the setting of fused leaflet fiber orientation affect the valve closure geometries. The FSI modeling results were able to show the effect of the hemodynamic force on the mechanical response of BAV, and the effect of stress-free geometry. Conclusions: We performed patient-specific FSI modeling for both type 0 and type 1 BAV patients. We were able to predict valve deformation and fluid dynamics, as well as the strain and stress distribution of patient-specific BAVs. This study provides useful insights for BAV biomechanics, and can be used to improve our understanding of BAV associated disease progression and treatment.

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Title: Phase Field Simulations of Co-Precipitation in AM Processed 625 and 718 Alloys during Post-Process Anneal

Author(s): *Bala Radhakrishnan, *Oak Ridge National Laboratory*; Sarma Gorti, *Oak Ridge National Laboratory*; Ranadip Acharya, *United Technologies Research Center*; Vijay Jagdale, *United Technologies Research Center*; Lyle Levine, *National Institute of Standards and Technology*; John Turner, *Oak Ridge National Laboratory*;

The microstructure in components made by additive manufacturing (AM) typically consists of columnar or equiaxed dendrites with solute microsegregation that depends on local solidification conditions. The laser powder bed fusion (LPBF) AM process has extensively been used to produce components in alloy 625 and 718. Available experimental evidence suggests that the LPBF microstructure in these alloys does not contain any precipitates, but significant microsegregation of alloying elements, especially Nb, exist. In addition to the solute segregation, the as-processed microstructures show definite evidence for increased dislocation content. Post-processing heat treatment is required in order to (1) reduce the residual stress in alloy 625, and (2) to induce precipitation hardening in alloy 718, required for meeting target properties in the AM component. Recent characterization evidence in LPBF 625 alloy after stress-relief anneal (1143K, 1 hr.) indicate co-precipitation of gamma" and delta phases [1], while in LPBF 718 samples thermally cycled to 1150K with heating and cooling rates ranging from 1 K/s to 0.01 K/s, both gamma' and gamma" formation was reported, although no metallographic evidence was provided for the co-precipitation of the delta phase [2]. Theoretical analysis of co-precipitation in alloys 625 and 718 has largely been conducted using a phenomenological approach based on classical nucleation theory and spherical growth rate [2,3]. Phase field simulations are capable of capturing both the kinetic and morphological aspects of multiple phase evolution, as well as providing spatial distributions of the phases in the microstructure required for rigorous, location-dependent structure-property calculations in the AM component. The current phase field simulations will include the effects of initial dislocation density, solute segregation, elastic strain, and alloy thermodynamics on the co-precipitation of phases in LPBF 625 and 718 alloys during post-process anneal to capture potential differences in the co-precipitation in the two alloys under identical heat treatment conditions. The simulations will be compared against experiments in alloy 625 from the ongoing NIST AM-Bench effort, and in alloy 718 from ongoing AM effort at UTRC. Research is sponsored by the Exascale Computing Project and the HPC for Manufacturing (HPC4Mfg) program at the Oak Ridge National Laboratory under contract DE-AC05-00OR22725, and HPC4Mfg program at UTRC. Phase field simulations will utilize resources of the Oak Ridge Leadership Computing Facility. 1. Lass, E.A. et al., Metall. Trans. A, 48 (2017) 5547-5558 2. Foster, S.J. et al., Metall. Trans. A, 49 (2018) 5775-5798 3. Lass, E.A. et al., Scripta Mater. 154 (2018) 83-86

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Title: Uncertainty Quantification by a Spline Dimensional Decomposition

Author(s): *Sharif Rahman, *The University of Iowa*; Ramin Jahanbin, *The University of Iowa*;

This study debuts a spline dimensional decomposition (SDD) of a square-integrable random variable comprising hierarchically ordered measure-consistent orthonormal basis splines (B-splines) in independent random variables. A dimensionwise decomposition of a spline space into orthogonal subspaces, each spanned by a reduced set of measure-consistent orthonormal B-splines, results in SDD. Using the modulus of smoothness, the SDD approximation is shown to converge in mean-square to the correct limit. Analytical formulae are proposed to calculate the second-moment properties of a truncated SDD approximation for a general output random variable in terms of the expansion coefficients involved. Numerical results indicate that a low-degree SDD approximation with an adequate mesh size generates a significantly more accurate estimate of the output variances than a high-order approximation from polynomial dimensional decomposition.

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Title: Nonlinear Vibration of Thin Circular Plate Under Moving Point Load

Author(s): *Amit Kumar Rai, *Indian Institute of Technology Kanpur, Kanpur - 208016, India*; Shakti Singh Gupta, *Indian Institute of Technology Kanpur, Kanpur - 208016, India*;

Moving load problems are found in several engineering discipline e.g. bridges, rails, percussion or string musical instruments or machining of a disc. A few representative studies in the line of our research are as follows. Mote [1] studied the resonances in a circular annular plate subjected to moving point loads. Fryba [2] in his book presented the linear dynamic response of a uniform rectangular plate subjected to moving point loads. Very recently, dynamic response of a geometrically nonlinear and elastic rectangular plate under a moving mass has been studied by Rofooei et al [3]. Here, nonlinear response of a thin circular plate under moving point load subjected to clamped and simply supported boundary conditions is studied. The plate material is assumed to be homogeneous, isotropic and linearly elastic. von Karman strain-displacement relations are used to include the geometric nonlinearity. The coupled nonlinear partial differential equations of motion in all principle directions of the plate are derived by using Hamilton's principle and solved through Galerkin's method employing appropriate eigenfunctions. Thus obtained non-linear coupled ordinary differential equations are solved using Runge-Kutta method. Time and frequency response of the plate under circularly, radially and spirally moving point loads are computed. It is found that the amplitude of the transverse deflection computed from the nonlinear model is less compared to that from linear model. The amplitude of deflection verses frequency of rotation of load curve exhibits the hardening nonlinearity. References: [1] Mote, C. D. 1970. "Stability of circular plates subjected to moving loads." Journal of The Franklin Institute, 290: 329-344. [2] L. Fryba, "Vibration of solids and structures under moving loads", Noordhoff International, Groningen, the Netherlands, 1972. [3] Rofooei, F., Enshaeian, A. and Nikkhoo, A. 2017. "Dynamic response of geometrically nonlinear, elastic rectangular plates under a moving mass loading by inclusion of all inertial components." Journal of Sound and Vibration, 394: 497-514.

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Title: A Variational Method Avoiding Locking a-priori on the Theory Level

Author(s): Simon Bieber, *University of Stuttgart*; Bastian Oesterle, *University of Stuttgart*; Manfred Bichoff, *University of Stuttgart*; *Ekkehard Ramm, *University of Stuttgart*;

Since some time the group of the authors follows the objective designing formulations for thin-walled structures that are intrinsically free from geometrical locking, when using equal-order interpolation for all involved fields. In other words, the formulations ought to avoid locking on the theory level, i.e. prior to discretization. In previous studies, we derived primal displacement-based concepts for Reissner-Mindlin and 3D shells from the virtual work principle, a priori free from transverse shear locking and curvature thickness locking. The key idea follows a reparametrization of primal parameters in the sense of a hierarchical formulation, introducing either hierarchic rotations or displacements [1], [2]. A corresponding extension avoiding membrane locking is still a matter of research. Since membrane locking is a crucial challenge for curved structures, the present contribution addresses a novel variational method [3]; in addition to the standard formulation, further displacement-like primal variables are introduced, however in the context of a mixed formulation. The approach was inspired by the Discrete Strain Gap (DSG) method; in fact, the additional degrees of freedom in this Mixed Displacement (MD) method can be interpreted as the strain gaps of the DSG method. The method is theoretically related to the above-mentioned hierarchical displacement formulation. Equal-order interpolation for all involved fields adjusts the functions spaces so that all geometrical locking phenomena, including membrane locking, are automatically avoided. Furthermore, the method is independent of the underlying discretization, no matter whether standard finite elements, isogeometric finite elements based on NURBS, or meshless methods are used. A further consequence of the balanced function spaces in the MD approach is that similar to the hierarchical displacement formulation a coarse mesh accuracy and high quality stresses/stress resultants being free from oscillations are obtained. The promising behavior of the MD variational method is demonstrated by several numerical examples for geometrically linear and nonlinear problems of thin-walled structures. References: [1] Echter R, Oesterle B, Bischoff M. A hierarchic family of isogeometric shell finite elements. Comput Methods Appl Mech Eng. 2013; 254: 170-180. [2] Oesterle B, Ramm E, Bischoff M. A shear deformable, rotation-free isogeometric shell formulation. Comput Methods Appl Mech Eng. 2016; 307: 235-255. [3] Bieber S, Oesterle B, Ramm E, Bischoff M. A variational method to avoid locking— independent of the discretization scheme. Int J Numer Methods Eng. 2018; 114(8), 801- 827.

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Title: Co-designed Image-based Experimental and Computational Investigation of Damage in Particulate Composites

Author(s): *Katherine Ramos, *University of Notre Dame*; Sangmin Lee, *University of Notre Dame*; Karel Matouš, *University of Notre Dame*;

Understanding the mechanical behavior that arises from the heterogeneity at different length scales of natural and synthetic heterogeneous materials has been a long-standing endeavor. Moreover, the optimization of material design has long been determined through costly and timely experimentation and empirical correlations between processing conditions and desired performance. Therefore, a predictive multi-disciplinary approach in material design which challenges this traditional approach is essential. One that exploits the use of experimental data at multiple length scales and its ability to guide computations (i.e., data-driven design). In this work, we develop such a framework and present an image-based (data-driven) co-designed experimental and computational framework to advance predictive multi-scale modeling. An image-based modeling concept alongside complex three-dimensional imaging techniques is used to understand the influence of microstructure and local damage phenomenon on the effective mechanical response of rubber-glass bead composites. The experimental framework encompasses utilizing the X-ray micro-computed tomography imaging technique to obtain a detailed characterization and statistical analysis of the evolution of structural features upon uniaxial compression loading. A rich analysis is performed on various experimental studies offering an understanding of the complex phenomena attributing to the material's response to loading including the mechanical and morphological response of non-linear viscoelastic materials. The nondestructive, three-dimensional image-based analysis protocol (which provides high fidelity of sample testing and data assessment) is leveraged in the development of representative computational domains. Representative unit cells (RUCs) respecting the characteristic length scales, as determined through analysis of statistical correlation functions, enable the ability to perform complex computations on relatively smaller domains all the while conserving the statistical characteristics of the original microstructure. By properly representing the microstructure (i.e., through the creating of RUCs) and calibrating relevant physical models accurate numerical predictions are realized. In addition to the fundamental understanding, the experimental testbed will serve as validation data sets for the multi-scale modeling approach. In particular, the analysis is used in the development of a novel damage model with split deviatoric and volumetric responses for Finite Element Analysis. This analysis and co-designed framework yield new insight into these composite materials required for the optimal material design. Moreover, independent components (i.e., statistics based modeling, computational homogenization, and finite element analysis) are bridged into one seamlessly co-designed framework essential in advancing predictive materials modeling capabilities.

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Title: Numerical Simulation of Fatigue Crack Propagation Behaviour of Plate Specimen Level Under Cyclic Bending Load

Author(s): R. Suresh Kumar, *Indira Gandhi Centre for Atomic Research, Kalpakkam, India*; *B. N. Rao, *Indian Institute of Technology Madras, Chennai, India*; K. Velusamy, *Indira Gandhi Centre for Atomic Research, Kalpakkam, India*;

Development of accurate numerical methods to predict the Fatigue Crack Growth (FCG) behaviour of prototype components can ensure fast and economic demonstration on structural integrity. The validation of the prediction with the experimental results can confirm the accuracy of the numerical prediction. The accuracy also depends upon the governing crack growth law used in the numerical simulation. In this paper, one of the typical plate specimen test data available in the literature has been used to validate numerical crack growth results. The Fatigue Crack Growth (FCG) simulation is performed as per Paris crack growth behaviour (da/dN = C ?Km) as well as Foreman's crack growth behaviour {da/dN = C?Km/ [(KC/Kmax)- 1]} where C & m are the FCG material parameters, ?K is the range of stress intensification factor, KC fracture toughness and Kmax is the maximum stress intensification factor. FCG simulation for the plate specimen has been performed using the FRANC3D software. FRANC3D software has the potential to simulate 3D FCG analysis in companion with the general-purpose Finite Element (FE) solvers. It can deploy the sub-modelling concept such that FCG simulation becomes computationally efficient. The direction of crack propagation is determined based on the ‘Kink angle’ measurement at the base of the crack front. The SIF is computed based on M-integral concept at mid-side nodes along the crack front using the maximum tensile stress. The sub modelling concept deployed in the FRANC3D helped the cracked portion of the component geometry to be meshed as fine as possible in a computationally efficient manner. It also takes care of the mesh connectivity of the local fine mesh with the coarse global mesh. Higher mesh density is provided in the case of shallow cracks. Also, a pattern of elements with controlled mesh size and shapes are placed around the crack front for the accurate estimation of SIF. The results of the FCG behaviour estimated as per Paris’ and Foreman's law is presented in this paper. The role of identification of an appropriate crack growth law for accurate prediction and its comparison is presented in this paper.

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Title: Multiscale Computational Modeling of Bio-Inspired Impact-Resistant Composites

Author(s): *Chengping Rao, *Northeastern University*; Yang (Emily) Liu, *Northeastern University*;

The hierarchical structure of the bio-inspired composites can be designed and optimized to exemplify the material's fracture toughness and impact resistance. In this study, we focus on the Bouligand structure in the dactyl club of the smashing mantis shrimp, which is capable of withstanding repetitive high-energy impact from its prey without catastrophic material failure. The Bouligand structure is characterized by a helicoidal arrangement of strong fibers in a weak matrix, an architecture which has high impact resistance and energy absorbance. It is crucial to understand the fundamental resistance mechanism of such an advanced material, in order to inspire and improve the design of the next generation of impact-resistant composites for protection systems such helmets and body armors. To this end, a bottom-up multiscale computational approach is proposed, which explicitly models the hierarchical Bouligand microstructure at the microscale, for predicting the macroscopic mechanical behaviors of bio-inspired composites under high-speed impact loads. The effect of the microstructural arrangements, such as the fiber volume fraction, interlayer spacing and the layer-to-layer pitch angle, on the nonlinear behavior and fracture mechanism of the helicoidal composite is investigated through multiscale analysis. The proposed multiscale modeling framework can be used to aid the design and optimization of the helicoidal bio-inspired composites for lighter, tougher and stronger materials that won't fail under extreme loading conditions.

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Title: Finite Element Modeling and Flow Visualization of Polyurethane Foaming and Curing in a Complex Mold

Author(s): *Rekha Rao, *Sandia National Laboratories*; Christine Roberts, *Sandia National Laboratories*; Melissa Soehnel, *Sandia National Laboratories*; Kevin Long, *Sandia National Laboratories*; James Tinsley, *Honeywell Federal Manufacturing & Technologies*;

Polyurethane structural foams are used as supports in a wide range of industries from furniture to refrigeration. Accurate models of the foam filling process and resulting physical properties, from thermal conductivity to density and modulus, can be useful for designing both the molds and the foaming process. Here a validation study is undertaken to compare the results of the computational modeling of foam filling and curing, which is then compared to a flow visualization study of foam filling a clear mold. This presentation uses a computational fluid dynamic model of a moderate density PMDI structural foam, PMDI-10, which was developed in a recent paper [1]. The model is a coupled finite element discretization of the homogenized continuum foaming and polymerization model with a level set method to capture the location of the free surface over time. The foam cures and foams simultaneously, making it very sensitive to processing parameters such as temperature, orientation, and foam injection location. Various mold tilt angles and temperatures are evaluated to determine the best process variable to minimize defects. Metrics are developed to evaluate the efficacy of the filling process such as deviation from constant density and maximum void content. The experiment and models match well, giving confidence in the numerical predictions. Extensions of the model to include more bubble-scale information and improved interface capturing methods will also be discussed. [1] Rao, Rekha, et al. "Density predictions using a finite element/level set model of polyurethane foam expansion and polymerization." Computers & Fluids 175 (2018): 20-35. *Sandia National Laboratories is a multi mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Title: The 3D Partitioned Element Method

Author(s): *Mark Rashid, *University of California, Davis*; Brian Giffin, *Lawrence Livermore National Laboratory*;

The partitioned element method (PEM) is a polyhedral finite element method for second-order elliptic BVPs that is tolerant of essentially arbitrary polyhedral element shape. The PEM relies on a partition of each polyhedral element into quadrature cells, which are themselves polyhedra. The cells serve to define both the element's quadrature rule, as well as its shape functions. Specifically, the shape functions are piecewise-linear on the complex of cells, while the quadrature rule assigns one sampling point to the centroid of each cell. The (in general discontinuous) piecewise-linear shape functions are governed by a quadratic minimum problem that seeks to optimize some combination of continuity, smoothness, and conformity with boundary values. It bears mentioning that this quadratic minimum problem is not simply equivalent to minimization of the mean-square gradient, as this leads to pathologies if the element is non-convex. These ideas are applied first on each face of the element, in order to establish the boundary variation of the shape functions; and then on the element's volume. The end result is a mapping of the element's nodal values to the linear-function coefficients for each cell. The quality of the shape functions is closely tied to the choice of geometric partitioning method. A few possibilities will be discussed. An attractive feature of the PEM is that not every vertex of the polyhedral element need be a shape-function-bearing node. This allows for a measure of control over the total DoF in the problem, independent of the geometric complexity of the problem domain. However, separate, slightly different shape functions must be generated for the test functions and for the trial solutions in order to realize both linear approximability and quadrature consistency. The overall method is therefore in the class of Petrov-Galerkin methods. Other aspects of the PEM formulation to be discussed include mitigation of volumetric locking, approximation error, and computational geometry as it relates to the partitioning of the element.

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Title: Imaging-based Modeling of Right Ventricular Mechanics

Author(s): Sotirios Kakaletsis, *University of Texas at Austin*; Kiernan Akers, *University of Texas at Austin*; Marcin Malinowski, *Spectrum Health*; Tomasz Jazwiec, *Spectrum Health*; Tomasz Timek, *Spectrum Health*; *Manuel Rausch, *University of Texas at Austin*;

The orchestrated action of left and right ventricle ensure life-long and continuous blood supply even to the farthest corners of our bodies. Although, anatomically arranged like parallel pumps, hemodynamically they function as serial pumps. Hence, dysfunction of one ultimately renders the whole system broken. In the past, most clinical research has focused on the left ventricle. Recently, research focus has shifted toward the right heart. This shift has occurred as it is becoming clearer that knowledge about the left heart cannot be simply extrapolated to the right heart. Despite increased efforts to understand the right ventricle, relatively little is known about right ventricular function. Being a pump, an important first step toward a more complete picture of its functioning is to quantify the force-producing unit, the right ventricular myocardium. Toward this end, our goal is to determine right ventricular wall-stress across the entire ventricle. Because there are no direct means to determine wall stress, we combine an invasive imaging modality in sheep, microstructural imaging, mechanical testing, and computational modeling to access this information. Specifically, we implant 14 sonomicrometry crystals across the right ventricular ovine epicardium. After weaning the animals from bypass, we wait until hemodynamic data are stabilized and record those crystal coordinates in the beating ovine heart from several complete cardiac cycles. From these coordinates, we can then create coarse, manually triangulated meshes of the epicardium throughout the cardiac cycle. Combining a triangular subdivision algorithm with an iterative optimization scheme, we can smoothen these surfaces and thus achieve realistic, epicardial surfaces representations. Next, we explant those hearts from the sheep and image them using a diffusion tensor imaging protocol from which we can derive myocardial fiber orientations and thickness maps. Subsequently, we isolate cuboid myocardium samples from those same hearts and test them in our custom-built triaxial shear devices to derive myocardial material properties. We combine these data to build a model of the right ventricular free wall of each ovine subject with subject-specific geometry, microstructural architecture, material properties, and hemodynamic boundary conditions. To derive full wall-stress maps from these data, we solve the arising boundary value problem using the open source, nonlinear finite element software FEBio. We will present above approach and resulting wall-stress maps from five healthy sheep and discuss our findings. Specifically, we will elucidate the importance of anisotropic and heterogeneous stresses as they relate to pumping efficiency and their contribution to a healthy cardiovascular system.

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Title: The Role of Heat Conduction on Hot-spot Formation in Energetic Materials

Author(s): *Babak Ravaji, *Texas A&M University*; Justin Wilkerson, *Texas A&M University*;

Understanding and mitigating the formation of hot-spots in energetic materials, e.g. polymer-bonded explosives (PBX), is vital to improving their overall safety. Accidental hot-spot formation can occur when heat generated via plastic dissipation overwhelms the rate of thermal conduction. It is commonly assumed that under dynamic loading conditions, e.g. strain rates in excess of 100% per millisecond, that thermal conductivity is too slow to be effective, i.e. adiabatic. As such, it has become common place to carry out computational simulations of such high strain-rate deformation assuming adiabatic conditions. Here, we carry out mesoscale (explicitly resolving the microstructure in PBX) finite element calculations with and without adiabatic assumptions. The effect of loading rate is studied in detail to elucidate the effect of competing timescales of loading rate versus thermal transport timescales. These calculations enable us to map out the regimes where the adiabatic assumption is appropriate and regimes where it can introduce non-trivial inaccuracies, i.e. over-predictions of hot-spot temperatures. Moreover, we find that strong thermal gradients can be produced by microstructural features (e.g. pores, cracks, and corners of crystals), which enhance the rate of thermal transport away from the hot-spots. Lastly, for situations where thermal conduction plays a fairly significant factor on hot-spot formation, we study the implications for the design of PBX with reduced sensitivity to accidental ignition. In particular, we find that enhancing the thermal conductivity of the binder phase, e.g. through the incorporation of nanoparticles with ultrahigh conductivities, can result in the generation of cooler hot-spots and hence improved sensitivity.

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Title: Role of Mechanical Factors in Wrinkling and Aging of Skin

Author(s): Poorya Chavoshnejad, *Binghamton University*; *Mir Jalil Razavi, *Binghamton University*;

The skin is the largest organ of the body which contains the internal organs and muscles. Primarily, skin acts as a barrier to the environment and secondly, controls inward and outward passage of water. Nowadays, skin research is a fully interdisciplinary research area which integrates multiple scientific, engineering, and clinical studies. One of the most important specifications of the skin is wrinkling, a natural part of aging. Wrinkling is a morphological pattern on the skin surface which increases by the aging. As the appearance of skin wrinkles, especially facial skin, is a sign of aging, therefore people tend to give much attention to the prevention of wrinkles. Hence, understanding the mechanics of wrinkling is vital because it is key to have a healthy skin and its associated juvenescent appearance. Despite the extensive studies on the surface instabilities conducted in the last decade, most of the theoretical models associated with skin wrinkling are restricted to idealized conditions. Therefore, there is a lack of understanding and absence of a theoretical-computational framework to explain the wrinkling and aging of the skin. The goal of this study is to propose an integrated theoretical-computational method to investigate the mechanics of wrinkling and aging of the skin. The skin is modeled with a soft structure having different layers with various thicknesses and material properties. Analytical interpretation provides preliminary insight into the critical compressive strain to start wrinkling while the advanced computational model with surface microrelief (a network of furrows and ridges small patterns on the surface of the skin) offers clues for skin’s post-wrinkling morphology. Especially, tissue geometry, material properties, and microrelief pattern are explored as the most determinant parameters to control the wrinkling of a compressed skin model. Results show that when the compressive strain is applied gradually, small wrinkles appear on the surface of the model to form primary lines. Interestingly, edges of the connected cells of microrelief create routes for the formation of the small wrinkles. In higher strain level, the depth of some valleys increases to form larger wrinkles. Similar to the real skin, the patterns of wrinkles are not completely identical, and also their lines are not straight. Results also show that number and type of large wrinkles are controlled by the geometry and mechanical property of the layers. According to the stiffness ratio of the layers, different wrinkle patterns are observed.

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Title: Hierarchical Construction of Predictive Models for Incompressible Fluid Flows Using Turbulence Models of Different Fidelity Levels

Author(s): *Mani Razi, *University of Utah*; Robert Kirby, *University of Utah*; Akil Narayan, *University of Utah*;

A novel approach for taking advantage of available computational fluid dynamics (CFD) methods with variable degrees of accuracy in the surrogate model construction for incompressible flows is developed. In the context of CFD, there is a set of computational models that is used for modeling turbulent incompressible flows. These models often provide estimation of the same set of parameters in response to variations of the same set of input parameters and therefore can be used for multi-fidelity predictive model construction. However, they are different with regards to their computational efficiency as well as their level of accuracy. Among them, relatively inexpensive computational methods with low accuracy are coined low-fidelity models. On the contrary, accurate but computationally expensive models are defined as high-fidelity models. The proposed approach provides a low-rank approximation to high-fidelity models by leveraging the correlation between high- and low-fidelity models. For this purpose, the low-fidelity CFD models data is obtained on a set of uniformly sampled points in the designated parameter space. Based on these data, an optimal kernel function is selected in a data-driven optimization process. The analysis of the resultant Gramian matrix which is constructed based on the selected kernel function provides a near-optimal sampling strategy for high-fidelity data acquisition. Finally, the multi-fidelity surrogate model is determined using both high- and low-fidelity data. The novelty of the proposed approach is in leveraging fast low-fidelity CFD simulations in the construction of high-fidelity CFD models. The benchmark test problems studied in this work involves the use of standard first and second order turbulence models for modeling incompressible fluid flows. Hence, the fidelity parameter in this context is discrete and is a model indicator. The set of the models considered in this work includes Spalart-Allmaras, k-epsilon, Reynolds Stress Models, implicit LES (high-order finite element model), and LES. Here, these models provide the estimation of the same set of flow parameters but with different levels of accuracy. In this work, we assume that the low- and high-fidelity models share a common set of tunable parameters. The results for the application of the proposed approach on benchmark test problems indicate both computational efficiency and high accuracy of the resultant multi-fidelity predictive models for estimation of quantities of interest.

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Title: Advanced Isogeometric Modeling and Applications with a Focus on Shells and Laminates

Author(s): *Alessandro Reali, *University of Pavia*; Alessia Patton, *University of Pavia*; John-Eric Dufour, *University of Texas at Arlington*; Pablo Antolin, *EPFL*;

Isogeometric Analysis (IGA) is a recent simulation framework originally proposed by Hughes and coworkers (2005) with the aim of bridging the Computational Mechanics and Computer Aided Design. Thanks to the high-regularity properties of its basis functions, IGA has shown a better accuracy per degree-of-freedom and an enhanced robustness with respect to standard finite elements in a number of applications ranging from solids and structures to fluids and fluid-structure interaction. The lecture focuses on some recent advances on modeling and applications of shell structures allowed by the unique IGA features, with special attention to an accurate and inexpensive simulation technique for laminates. An overview of other interesting applications will be presented as well.

15th U.S. National Congress on Computational Mechanics
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Title: Automatic Block Decomposition of General 3D Domains Using Cross Fields

Author(s): *Maxence Reberol, *UCLouvain*; Jean-François Remacle, *UCLouvain*;

We propose an approach to decompose 3D models into blocks suitable for hexahedral meshing. The internal surfaces of the decomposition are built by clustering large numbers of cross field streamlines. The input cross field defines three directions at each vertex of a tetrahedral mesh. The streamlines are traced with an explicit scheme, using the closest directions at each step of the propagation. The streamline tracing and the clustering stages rely on geometric criteria, so it is critical for our approach to have a high-resolution 3D cross field with a correct topology (i.e. hex-meshable). However, current state-of-the-art cross field generation methods produce fields with various flaws that prevent a direct application of our approach. Notably, the cross fields (a) have wrong topology (not hex-meshable), (b) are not smooth enough (mesh imprinting) and (c) the computation do not converge with mesh refinement (as gradient tends to infinity at singularities). We discuss these issues and propose various strategies to correct or accommodate them. We show applications of our approach to various non-trivial 3D models, where we are able to successfully build the block decomposition. From this decomposition, it is straightforward to produce high-quality block-structured hexahedral meshes.

15th U.S. National Congress on Computational Mechanics
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Title: On Nonlocal and Non-Classical Mechanics and Computational Approaches

Author(s): *J.N. Reddy, *Texas A&M University*;

Structural continuum theories require a proper treatment of the kinematic, kinetic, and constitutive issues accounting for possible sources of non-local and non-classical continuum mechanics concepts [1] and solving associated boundary value problems. There is a wide range of theories, from higher gradient to truly nonlocal. These include, for example, strain gradient theories [2, 3], couple stress theories, Eringen's stress gradient theories, and micropolar theories (the micropolar theory of elasticity includes an independent microrotation), and thermodynamically consistent structural theories. A salient feature of the micropolar models is that, unlike classical or couple-stress models, they allow antisymmetric shear deformation to emerge at locations where detailed 2-D and 3-D deformations cannot be reduced to mid-surface deformations by considering only symmetric shear behavior. In this lecture, an overview of recent research on strain gradient, stress gradient, couple stress, micropolar, and thermodynamically consistent theories in developing the governing equations beams, plates, and sandwich structures and computational approaches will be discussed [4]. In addition, a graph-based finite element framework (GraFEA) suitable for the study of damage in brittle materials will be discussed [5]. Acknowledgements: The author is pleased to acknowledge the collaboration on non-local and non-classical mechanics with Karan Surana (KU), Arun Srinivasa (TAMU), and and Debasish Roy (IISc). References 1. K. S. Surana, R. Shanbhag, and J.N. Reddy, "Necessity of Balance of Moments of Moments Balance law in Non-Classical Continuum Theories for Solid Continua," Meccanica, 53(11-12), 2939-2972, Sep. 2018. 2. A.R. Srinivasa and J.N. Reddy, "A model for a constrained, finitely deforming, elastic solid with rotation gradient dependent strain energy, and its specialization to von Karman plates and beams," Journal of Physics and Mechanics of Solids, 61(3), 873-885, Mar 2013. 3. A.R. Srinivasa and J.N. Reddy, "An overview of theories of continuum mechanics with nonlocal elastic response and a general framework for conservative and dissipative systems," Applied Mechanics Reviews, 69, 10.1115/1.4036723, May 2017. 4. A.T. Karttunen, J.N. Reddy, and J. Romanoff, Composite Structures, 185, 656-664, 2018. 5. Parisa Khodabakhshi, A.R. Srinivasa, and J.N. Reddy, "A Nonlocal Fracture Criterion and its Effect on Mesh Dependency of GraFEA," Int. J. Solids & Structures, in print.

15th U.S. National Congress on Computational Mechanics
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Title: Computational Assessment of Mitral Valve Remodeling Using In-Vivo Imaging Data

Author(s): *Bruno Rego, *University of Texas at Austin*; Amir Khalighi, *University of Texas at Austin*; Eric Lai, *University of Pennsylvania*; Robert Gorman, *University of Pennsylvania*; Joseph Gorman, *University of Pennsylvania*; Michael Sacks, *University of Texas at Austin*;

Each year, more than 40,000 people in the United States undergo mitral valve (MV) repair surgery to treat mitral regurgitation caused by myocardial infarction (MI). Unfortunately, long-term efficacy of repair procedures remains a challenge, with 30% of patients experiencing recurrence of regurgitation. Although continual strain-driven remodeling of the MV is believed to be a major cause of repair failure, the effects of MI and repair surgery on MV deformation patterns are not well understood. The goal of the present study was thus to quantify the effects of MI on MV geometry and strains, to facilitate functional assessment and surgical planning. MI was induced in eight adult Dorset sheep, and real-time three-dimensional echocardiographic (rt-3DE) scans were collected pre?MI, immediately post?MI, 4 weeks post?MI, and 8 weeks post?MI. The acquired images were segmented to extract open-state and closed-state MV geometries. A previously validated image-based morphing pipeline was used to register corresponding open- and closed-state scans and infer local directional strains across the leaflet surface at both diastole and systole. Analysis of rt-3DE images showed that the MV annulus is substantially dilated and flattened post-MI, consistent with previous findings. Moreover, both leaflets were severely tethered post-MI, causing them to exhibit greater tenting in closure. These MI-induced effects propagated throughout both leaflets to yield substantial changes in strain patterns. Following MI, diastolic stretches in both circumferential and radial directions changed substantially, though with significant regional heterogeneity, and mostly stabilized by t = 4 wk. In systole, when referenced to the pre-MI diastolic configuration, directional stretches remained largely unchanged over much of the leaflet, suggesting that the MV's post-MI remodeling is driven mostly by alterations in diastole. These findings are highly relevant to the design of MV repair devices and the optimization of surgical strategies. While current MV repair endeavors largely seek to return the valve to its pre?diseased state, our results suggest that this approach may not be favorable, and that an effort to place the MV in an alternative homeostatic state may lead to decreased repair failure. Moreover, repair strategies to relieve leaflet strains could curb adverse leaflet remodeling and thus improve long-term outcomes. Our computational method for leaflet strain estimation will thus serve as a platform for in-silico studies that aim to improve MV repair by identifying a repair state that leads to favorable remodeling in the MV leaflet tissues.

15th U.S. National Congress on Computational Mechanics
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Title: Simultaneous Spatial and Temporal Coarse-graining: from Particle Dynamics to Continuum Elastodynamics

Author(s): *Celia Reina, *University of Pennsylvania*;

In this talk, we propose a systematic spatio-temporal coarse-graining strategy that bridges particle dynamics and continuum elastodynamics. The upscaling procedure will recover classical thermodynamic relations in generalized coordinates, leading to generalized notions of entropy and temperature, and it will also provide extremely simplifi ed explanations of fundamental, yet not necessarily tangible, thermodynamic concepts and relations. The multiscale scheme will be demonstrated for various examples with different levels of complexity, and the continuum predictions will be compared with molecular dynamic simulations.

15th U.S. National Congress on Computational Mechanics
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Title: GMSH 4.x

Author(s): *Jean-Francois Remacle, *Universite catholique de Louvain*;

Gmsh is one of the most widely used mesh generator in the world. Gmsh started in 2006 and has encountered major evolutions since version 1.0. In this presentation, we will present some of the new features of GMHS4.x. More specifically, we will discuss 1) GMSH's hex and quad meshing capabilities based on frame field computations. 2) GMSH's new developper API 3) GMSH's new boundary layer meshing capabilities. A timeline that details futher developments will finally be presented.

15th U.S. National Congress on Computational Mechanics
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Title: An Alternative Computational Approach to Evaluate the Directional Behavior of Periodic Media

Author(s): *David Restrepo, *The University of Texas at San Antonio*; Camilo Valencia, *Universidad EAFIT*; Juan David Gomez, *Universidad EAFIT*; Pablo Zavattieri, *Purdue University*;

One of the most relevant problems in the dynamic analysis of periodic media is the determination of the directional behavior of the material. As a result, the preferred propagation directions, which are a function of the material structure, are identified. In the typical analysis method, one computes the material dispersion surfaces which result after solving a generalized eigenvalue problem corresponding to the imposition of the so-called Bloch periodic boundary conditions upon the unit cell. The preferred propagation directions are identified from the shapes appearing in the iso-frequency contour plots of the gradients over the first two modes of the dispersion surfaces. As a complement, it is also frequent to use a polar histogram of these gradients. This approach has a conceptual inconvenience. First, in the dispersion relations, the wave types and modes are usually mixed. For instance, it may be the case that information from several wave types originated at different Brillouin zones appear in the first mode. Similarly, since the approach is based on the first two modes the analysis might erroneously eliminate directional behavior associated to the high frequency regime. In this work we present an alternative approach to conduct directional analysis of periodic media where we consider the first N modes from the generalized eigenvalue problem. We compute the magnitude and directional distribution of a single vector field V computed after considering the N modes simultaneously. The results are then presented as a combination of phase velocity and a vector count held over V. Since we take information from several modes, as opposed to single mode biased methods, we obtain more representative descriptions of the directional response valid in the low and high frequency regime. Our presentation is organized as follows: - Description of the classical approach for directional analysis focusing on its two major drawbacks. - Detailed description of the proposed approach using N modes and a vector field. - Applications showing the validity and versatility of the proposed approach.

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Title: A C0-Continuous Mixed Finite Element Formulation for Gradient Elasticity at Finite Strains

Author(s): *Johannes Riesselmann, *Ruhr-University Bochum*; Jonas Ketteler, *WWU University Muenster*; Daniel Balzani, *Ruhr-University Bochum*; Mira Schedensack, *WWU University Muenster*;

Although classical elasticity formulations are well established and employed in a broad spectrum of numerical applications, these formulations have limitations when it comes to specific problems. For example, if the body of interest has e.g. sharp corners, the occurrence of non-phyisical stress singularities is possible and can lead to a pathological mesh dependency of corresponding finite-element simulations. The gradient elasticity approach can represent a remedy in these cases. Through enrichment of the formulation by second-order gradients, the smoothness of the corresponding solution is increased and the before-mentioned singularities are avoided. Another field of application is the modeling of very small structures, in which the microstructure has an influence on the constitutive behavior. These so called size-effects can not be described with the material bulk moduli of classical elasticity formulations. Gradient elasticity formulations in contrast can capture the size effects through additional constitutive parameters imposed through the gradient enrichment. However, despite these advantages over classical formulations, the research of formulations has yet to overcome challenges in the development of practical finite element formulations. Namely, due to the appearance of higher order gradients, a straightforward discretization requires C1-continuity, for which a retaining compatibility with standard software as well as the meshing of arbitrary structures are known difficulties. Another common approach is to use mixed formulations instead, in which next to the displacements, displacement gradients are introduced as solution variables. Consequently, a relaxation of continuity requirement to C0 is obtained, yet, at the downside of a relatively high computational cost. In this contribution a new formulation is proposed, in which the displacements are not part of the problem anymore, but only the displacement gradients, leading to a reduced number of variables, while holding on to the advantage of requiring only C0-continuity. Corresponding discretizations are proposed and numerically evaluated in the large strain framework. Numerical results are compared to adaptations of existing mixed formulations.

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Title: A Discontinuous Galerkin Method For The Solution Of Black-Oil In Heterogeneous Media

Author(s): *Beatrice Riviere, *Rice University*; Loic Cappanera, *Rice University*;

Black-oil model is a popular model of three-phase flows in petroleum engineering. The co-existing phases are liquid, vapor, and aqueous. A classical model assumes that the aqueous phase is made entirely of the water component and that gas and oil components can transfer between the liquid and vapor phases. In this work, we present a discretization of a formulation of black-oil model that is based on the discontinuous Galerkin (DG) method. The unknowns are the liquid phase pressure, the aqueous phase saturation and the total mass fraction of gas. The proposed algorithm is sequential implicit and uses recently developed techniques for DG methods to make the simulations robust in three-dimensional heterogeneous media. These techniques include weighted averages, projection of phase velocity into an H(div)-conforming space, the use of upwind fluxes and the use of sub-iterative scheme for higher accuracy. The choice of primary variables yields an algorithm that easily handles the appearance and disappearance of phases. Numerical results show the convergence and robustness of the numerical method for several three-dimensional porous media. Gravity effects are also investigated.

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Title: Accelerative Jacobian Free Techniques for Mechanical Metamaterial Homogenization

Author(s): *Corbin Robeck, *Thornton Tomasetti - Weidlinger Applied Science*; Jeffrey Cipolla, *Thornton Tomasetti - Weidlinger Applied Science*;

An increasingly important use of functionally graded metamaterials is for the generation of acoustic cloaks. For an acoustic cloak to be effective it must have very specific waveguide properties dictated by transformation acoustics cloaking theory. For the Norris elastic version of the theory, these waveguide properties translate into very specific elastic tensor and density properties for the functionally graded microstructure. To achieve the required material properties for the entire microstructure, each unit cell within the microstructure must be homogenized to ensure the cell’s parameter combinations yield the correct elastic stiffness tensor and density. The static homogenization process that yields the elastic tensor for a unit cell requires solving many costly high dimensional finite element problems for each new microstructure cell of interest. Therefore, any acceleration of the domain space search and subsequent homogenization solution represents significant cost savings. In practice, the high dimensional finite element homogenization problem is almost always solved using an iterative solution of large system matrices to find a static solution. Even using advanced solutions methods, this approach puts significant demands on computational memory and processing power. This work presents a method of accelerating mechanical metamaterial homogenization using a special finite element formulation called the Jacobian Free Newton Krylov (JFNK) method. The JFNK method appears popular in computer science but its adoption in solid mechanics, especially statics, has been rare. The approaches investigated in the work avoid the formation of a system level matrix completely thus allowing the procedure to take full advantage of explicit solution strategies to solve a traditionally implicit problem (statics). In the work presented, the preconditioned conjugate gradient algorithm is coupled with the explicit JFNK procedure to solve the finite element based static equations. Full scale finite element examples were chosen to show the method’s comparison to traditional implicit methods as well as it’s ability to handle a range of standard element types and problem setups. Strategies for preconditioning the system when no system level matrix exists are discussed as well as JFNK's application to corresponding problems in other metamaterial applications. Finally, the implementation’s ability to transfer to high performance computing applications (supercomputing clusters and GPU accelerators) is analyzed.

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Title: Computational Challenges in Reverse Time Migration Uncertainty Quantification

Author(s): *Fernando Rochinha, *Universidade Federal do Rio de Janeiro*; Alvaro Coutinho, *Universidade Federal do Rio de Janeiro*; José Alves, *Universidade Federal do Rio de Janeiro*; Marta Mattoso, *Universidade Federal do Rio de Janeiro*; Carlos Barbosa, *Universidade Federal do Rio de Janeiro*; Romulo Silva, *Universidade Federal do Rio de Janeiro*; Bruno Silva, *Universidade Federal do Rio de Janeiro*; Charlan Dellon, *Universidade Federal do Rio de Janeiro*; Henrique Costa, *Universidade Federal do Rio de Janeiro*; Rodolfo Freitas, *Universidade Federal do Rio de Janeiro*; Gabriel Guerra, *Universidade Federal do Rio de Janeiro*;

Reverse Time Migration (RTM) is considered, by many, a workhorse for seismic imaging in the Oil&Gas industry. In the present work, we assess the presence of uncertainties and how they affect the reliability of the produced images. We particularly emphasize the role of high-performance computing and identify the main bottlenecks of an Uncertainty Quantification (UQ) analysis in such a context. To assess the final impact of uncertainties in the process of building a seismic image, we designed a workflow formed by three axles connected by a high-performance layer responsible for moving data and managing provenance between them. The first axle is dedicated to obtaining a velocity subsurface model conciliating measured signals on the surface and expert knowledge. The scarcity of noisy measurements along with human subjective intervention leads to significant sources of uncertainties. We employ a Bayesian travel time tomography formulation to accommodate such aspects of the velocity model, leading to a set of realizations of a random spatial field, what serve as inputs for the second axle. We employ an Eikonal solver in the tomography to make it computationally feasible within the workflow, what constitutes another uncertainty source due to the limited physics involved. To carry out a consistent probabilistic analysis, the number of realizations tend to be large, and each one of them is supposed to be highly defined to capture the variability of the spatial field. The second axle migrates the input velocity by solving twice (direct and reverse time) an acoustic wave equation, that requires very fine computational grids, and, consequently, very time-consuming. To perform the UQ analysis, we employ a Monte Carlo (MC) algorithm, solving the two-way acoustic migration for each sample of the velocity field. The third axle provides automatic computational tools for supporting the geologists to pick up important features within the images. The biggest computational challenge in that final step of the proposed workflow relies on how to handle a significant number of samples generate in the previous axle by the MC analysis. In the end, we present some examples to illustrate the performance and challenges of the workflow.

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Title: Second-Order Homogenization of Polycrystalline Materials

Author(s): *Igor A. Rodrigues Lopes, *Faculty of Engineering of the University of Porto*; Miguel Vieira de Carvalho, *Faculty of Engineering of the University of Porto*; Daniel de Bortoli, *Institute of Science and Innovation in Mechanical and Industrial Engineering*; Francisco M. Andrade Pires, *Faculty of Engineering of the University of Porto*;

Keywords: Multi-scale modeling, Heterogeneous materials, Second-order homogenization, Finite strain, Finite element method. Multi-scale analyses are of utmost importance in order to understand the micro-scale mechanisms that influence the macroscopic material behavior. Materials that are heterogeneous at a certain spatial scale may be modeled by a Representative Volume Element (RVE), where phenomena arising at the micro-scale due to a macro-scale loading may be analyzed in detail, accounting for the effect of material heterogeneities. The coupled finite element analysis of the material behavior (FE2) is usually performed with a first-order homogenization scheme, where only the linear part of the macroscopic loading is considered. This formulation implicitly assumes the uniformity of the macroscopic fields applied to each RVE based on the concept of separation of scales, which might not be appropriate in regions of high gradients at the macro-scale. However, with a second-order homogenization approach, the deformation prescribed to the RVE also includes the second gradient of the macro-scale displacement [1,2,3], enabling more adequate modeling of regions with higher gradients. The formulation and finite element implementation of a second-order homogenization-based multi-scale model based on the Method of Multi-Scale Virtual Power was developed and is presented in this contribution. This model is employed to assess the behavior of polycrystalline materials at both micro and macro-scales. References: [1] V.G. Kouznetsova, M.G.D. Geers and W.A.M. Brekelmans, Multi-scale constitutive modelling of heterogeneous materials with a gradient-enhanced computational homogenization scheme. Int. J. Numer. Meth. Eng., Vol. 54, pp. 1235-1260, 2002. [2] D.J. Luscher, D.L. McDowell and C.A. Bronkhorst, A second gradient theoretical framework for hierarchical multiscale modeling of materials. Int. J. Plast., Vol. 26, pp. 1248-1275, 2010. [3] P.J. Blanco, P.J. Sánchez, E.A. de Souza Neto and R.A. Feijóo, The method of multiscale virtual power for the derivation of a second order mechanical model. Mechanics of Materials, Vol. 99, pp. 53–67, 2016.

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Title: A Hybridizable Discontinuous Galerkin Phase-Field Model: Adaptivity and Continuous-Discontinuous Transition

Author(s): Alba Muixí, *UPC-BarcelonaTech*; Sonia Fernández-Méndez, *UPC-BarcelonaTech*; *Antonio Rodríguez-Ferran, *UPC-BarcelonaTech*;

Phase-field models of fracture are very demanding on the spatial discretization: very fine meshes are required to capture the narrow damage bands typical of small length scale parameters [1]. We present an adaptive phase-field model that addresses this issue. The key ingredient of our proposal is that it is based on the Hybridizable Discontinuous Galerkin (HDG) discretization technique [2], rather than the standard Finite Element (FE) method. Among all DG methods, we choose HDG because it involves less degrees of freedom. HDG has a computational efficiency close to standard continuous FE and better convergence properties. The most attractive feature of HDG for our purposes is that approximation functions are discontinuous across elements, and inter-element continuity of the displacement and damage fields is imposed weakly. This means that two adjacent elements may have very different size h and/or shape functions of very different degree p, and this is handled in a natural manner by the formulation. As a result, a coarse background mesh can be adaptively refined where needed as the cracks propagate, with no need of a smooth transition of size h or degree p. We illustrate our adaptive phase-field model, both for h- and p-adaptivity, with various numerical examples. This adaptive phase-field model takes care of the continuous regime. We envisage a continuous- discontinuous approach [3], in which sharp cracks (i.e. displacement jumps) are inserted when dictated by a transition criterion. Once this discontinuous regime is activated, a fine spatial discretization is only needed in the diffuse crack tip (i.e. the neighbourhood of the sharp crack tip), so the mesh may be de- refined in the wake of the crack tip. References [1] Ambati, M., Gerasimov, T., and De Lorenzis, L. A review on phase-field models of brittle fracture and a new fast hybrid formulation, Comput Mech (2015) 55:383–405. [2] Cockburn, B., Gopalakrishnan, J., and Lazarov, R. Unified hybridization of discontinuous Galerkin, mixed and continuous Galerkin methods for second order elliptic problems, SIAM J Numer Anal (2009) 47:1319–1365. [3] Geelen, R.J.M., Liu, Y., Dolbow, J.E. and Rodri?guez-Ferran, A. An optimization-based phase-field method for continuous-discontinuous crack propagation, Int J Numer Methods Eng (2018) 116(1):1-20.

15th U.S. National Congress on Computational Mechanics
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Title: Reliability and Scalability of Entropy Stable Methods for Computational Fluid Dynamics

Author(s): *Diego Mauricio Rojas Blanco, *KAUST*; Lisandro Dalcin, *KAUST*; Stefano Zampini, *KAUST*; Matteo Parsani, *KAUST*;

Modern computational resources are increasingly complex systems that require a significant investment to set up and operate. This financial effort implies algorithms must be up to the task regarding reliability and smart use of computing time. There has been increasing interest in the development of reliable and scalable computational fluid dynamics tools since a significant part of the computing time in these systems is used in the analysis of fluid flow problems for industrial and environmental applications. Entropy stable methods have gained attention in recent years as a tool to address this problem. They provide nonlinear stability proofs in the semidiscrete level, which addresses the concern for reliable implementations. In addition, they open the door to high order methods improving the scalability and economic use of computing resources. In this work, a comparison between conventional Discontinuous Collocation (DC) and entropy stable DC (SSDC) applied to the solution of the compressible Navier Stokes equations is presented. The simulations were performed on canonical problems for subsonic and supersonic flow. The superior reliability of the entropy stable implementation was evident in high order cases, and therefore better performance was obtained. These results suggest the great potential of entropy stable methods applied to the analysis of complex engineering problems.

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Title: Estimation of Modeling Errors in Local Quantities of Interest in the Elastostatic Analysis of Heterogeneous Solids

Author(s): *Albert Romkes, *SD School of Mines & Technology*; Justin King, *SD School of Mines & Technology*;

We consider the analysis of the mechanics of multiphase composite materials. Such materials generally exhibit very complex microstructure with highly oscillatory material properties. It is prohibitive to resolve all the features of the microstructure in a computational process. Classical approaches have therefore focused on methods of homogenization, generally based on the assumption that the microstructure of the media is periodic or on techniques for determining effective properties of representative volume elements. These averaged material models cannot account for local micromechanical effects that are critical factors in determining the behavior and service life of structural components. To resolve this issue, Oden et al. developed the Goal-Oriented Adaptive Modeling (GOAM) method. It represents a systematic approach for adaptive multi-scale modeling of heterogeneous materials based on control of the modeling error in a local quantity of interest (i.e. goal) of the material response that is specified by the user. The basic idea is to start with an initial analysis based on homogenized properties that are obtained via the classical averaging techniques. The homogeneous surrogate model is then enhanced in an iterative process of including the material microstructure in a local area surrounding the quantity of interest that increases in size with every iteration step. A critical element in the GOAM method is the ability to accurately estimate the modeling error. Currently, this is established by providing a residual-based a posteriori error estimator. It involves solving for a global influence function, related to the quantity of interest, and subsequently computing global integrals of governing residual functionals. In the case of multiphase composite materials, this estimation process can be computationally prohibitive, again due to the complexity of the microstructure. Hence, we propose a new technique for local, goal-oriented estimation of the modeling error that resolves this computational issue. It is based on a local variational approach and therefore requires computing a local influence function and local residual integrals at low computational cost. We introduce this new approach for the multi-scale analysis of linear elastostatics problems of multiphase composites and the investigation of linear local quantities of interest of the material response.

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Title: The Influence of Constitutively Assumed Anterior Cruciate Ligament Shear Properties on Simulated Whole-knee Biomechanics

Author(s): *Ryan Rosario, *University of Michigan*; Ellen Arruda, *University of Michigan*; Rhima Coleman, *University of Michigan*;

Finite element (FE) models of the knee are used to study anterior cruciate ligament (ACL) injury and repair. When constructing whole-knee FE models, ACL material models are commonly fit tension data along the ligament fiber direction (longitudinal) and occasionally tension data orthogonal to the fiber direction (transverse). There has been no study to date where an ACL material model also fit shear data. By not fitting shear data, researchers assume the nature of the shear response of the ACL. This assumed stress-strain shear behavior can vary by orders of magnitude depending on the choice of material model. In this study, three material models were used to describe the ACL: the transversely isotropic freely-jointed eight-chain model (FJC), the Holzapfel-Gasser-Ogden model (HGO), and the Weiss model. These models were fit to longitudinal and transverse tension data. Due to the nature of the constitutive equations, the FJC model had a tunable shear response while maintaining high quality-of-fit to longitudinal and transverse data. This allowed us to have two fits for the FJC model, one stiffer in shear (stiff FJC) and one more compliant in shear (compliant FJC). These ACL material models were then inputted into a validated whole-knee model [1]. Muscle forces and a 134 N anterior tibial drawer force were applied. Decreasing the shear stiffness of the ACL resulted in increased shear strain in the ACL, increased anterior tibial displacement, increased average contact pressure in femoral and lateral tibial cartilage, and changes in the shape of the contact zone for articular cartilage. Results from this study were then compared to previous findings from Wan et al., where longitudinal behavior was held constant while transverse behavior varied [2]. This comparison suggested that fitting longitudinal and shear behavior, rather than fitting longitudinal and transverse behavior, would result in a more accurate prediction of knee biomechanics. This hypothesis was confirmed through additional simulations where longitudinal and shear behavior were held constant while transverse behavior varied. Taken together, this suggests that material models for the ACL should be well-fit to shear data in addition to longitudinal and transverse data to best predict the in vivo response of the human knee to applied loads References: [1] Marchi B.C., et al., (2017). Biomech Model Mechanobiol. [2] Wan C., et al., (2013). J Biomed. Eng.

15th U.S. National Congress on Computational Mechanics
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Title: A New Perspective in the Geometric Modeling of Defects in Solids

Author(s): *Debasish Roy, *Indian Institute of Science*;

We discusses a geometric approach to the modeling of defects in solid continua. A Weyl geometric setting for large thermo-mechanical deformation of solid continua with metrical defects is considered. We assume the geometry of the reference and deformed configurations to be of the Weyl type. This assumption introduces a new set of degree of freedom called the Weyl one-form, which determines the ratios of length between vectors form different tangent spaces. The Weyl one-form prevents the metric from being compatible with the Weyl connection, this incompatibility is used to characterize metrical defects in the body. When a body with metrical defect is subjected to temperature change, it introduce additional incompatibilities in the body, which also interacts with the defects. This interaction is modeled using the Weyl transform, which keeps the Weyl connection invariant, while changing the non-metricy of the configuration. The problem of relating incompatible strain with the stress is resolved by taking recourse to the Doyle-Ericksen formula, which is understood as relationship between the intrinsic geometry of the body and the stresses developed in it. Thus, the Cauchy stress is assumed conjugate to the deformed Weyl transformed metric tensor. The temperature evolution equation, coupling the temperature, deformation and Weyl one-form are established using the first law of thermodynamics. Using the geometric model, we establish conditions for a thermo-mechanical deformation to be stress-free, specific stress-free deformations are also computed for simple prescribed defect distribution and temperature change. The second part of the talk is about modeling defects via Riemannian geometry, emphasizing the role of curvature. Classical continuum mechanics assumes reference and deformed configurations as flat Riemannian. This is relaxed by assuming the metric tensor an independent field. The free-energy of the deformed configuration is taken as a function of the curvature tensor, which permits us to include the energy contribution due to incompatible strains introduced by the defects. A separate evolution equation for the deformed metric tensor is derived via energy minimization. Based on the Riemannian setting for defects, we also perform numerical studies to determine stress-free configurations generated by growth. A finite element discretization is adopted for the deformation variables and the components of connection. We interpret the above descriptions (both Weyl and Riemannian) for defects as genuine gradient theories, since they incorporate higher order terms in a geometrically consistent manner. We also emphasize that these models are mere prototypes for adopting the connection itself as an independent variable.

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Title: An Interaction Based FE Framework for Large Deformation Adhesive Contacts

Author(s): *Suprateek Roy, *Indian Institute of Science, Bangalore*; Narayan K Sundaram, *Indian Institute of Science, Bangalore*;

The large deformation (LD) contact response of micro and nanoscale bodies, governed by adhesive (van der Waals attraction) and steric repulsive forces, is very important in biological and micro-mechanical systems. Successful FE simulation of LD adhesive contact of arbitrarily shaped bodies presents multiple challenges, including the need to accurately capture short-range adhesive interactions in a computationally efficient manner. Moreover, the quasi-static adhesive contact behavior of soft bodies involves intrinsic instabilities ("jump-to-contact" and "jump-off-contact"). Prior LD FE frameworks for arbitrary geometries include the Coarse-Grained Contact Model (CGCM) [1], which uses volume to volume interactions and is based on modeling the solid as a quasi-continuum, and surface to surface models based on classical continuum FE [2, 3]. Despite these important advances in LD FE for adhesion, several issues remain to be addressed in combining continuum FE and adhesive interactions. For instance, extension of volume to volume models beyond the nanoscale is computationally prohibitive. Moreover, formulations that require modifications to the continuum are cumbersome to incorporate. Surface to surface models, while computationally more efficient, often include subtle approximations to the interactions. Lastly, the interaction parameters (e.g. Lennard-Jones sigma and epsilon) used to demonstrate these frameworks are often based on computational convenience, and it is not clear that these are physically representative in many cases. In this work, we present a volume-volume interaction-based FE model with an underlying classical continuum base to simulate the quasi-static microscale adhesive contact behavior of soft bodies. Our framework incorporates an algorithm to accelerate the interaction calculations, automatically handles instabilities associated with adhesive contact attachment and detachment, and scales up to simulate interactions of microscale bodies. Our formulation is also designed to handle a spectrum of different interaction force laws. Validation in the small deformation limit against classical adhesive contact models (JKR, DMT, Maugis) is ongoing. After validation and optimization, we expect our algorithm to allow exploration of a wide variety of adhesive interaction problems of biological interest. References: [1] Sauer RA, (2006) An atomic interaction based continuum model for computational multiscale contact mechanics (Ph. D. thesis), University of California, Berkeley. [2] Fan H, Ren B, Li S, (2015) An adhesive contact mechanics formulation based on atomistically induced surface traction, Journal of Computational Physics, 302, 420-438. [3] Fan H, Li S, (2016) A three-dimensional surface stress tensor formulation for simulation of adhesive contact in finite deformation, International Journal for Numerical Methods in Engineering, 107(3), 252-270.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Reduced Order Methods for PDEs: State of the Art and Perspectives with Applications in Industry, Medicine and Environmental Sciences

Author(s): *Gianluigi Rozza, *SISSA, Int. School for Advanced Studies, Trieste*;

We provide the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs), and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD). Efficient parameterisations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments in CFD include: a better use of stable high fidelity methods, considering also spectral element method and finite volume discretisations, to enhance the quality of the reduced model too; more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, as well as the dimension of online systems; the improvements of the certification of accuracy based on residual based error bounds and of the stability factors, as well as the the guarantee of the stability of the approximation with proper space enrichments. For nonlinear systems, also the investigation on bifurcations of parametric solutions are crucial and they may be obtained thanks to a reduced eigenvalue analysis of the linearised operator. All the previous aspects are very important in CFD problems to focus in real time on complex parametric industrial, environmental and biomedical flow problems, or even in a control flow setting. Model flow problems will focus on few benchmark, as well as on simple fluid-structure interaction problems. Further examples of applications will be delivered concerning shape optimisation applied to industrial problems. This is a joint work within ERC AROMA-CFD group at SISSA mathLab. [1] G. Stabile and G. Rozza : Finite volume POD-Galerkin stabilised reduced order methods for the parametrised incompressible Navier-Stokes equations, Computers & Fluids, 2018. [2] M. W. Hess, A. Alla, A. Quaini, G. Rozza and M. Gunzburger: A Localized Reduced-Order Modeling Approach for PDEs with Bifurcating Solutions, ArXiv e-prints, 2018. [3] M. Strazzullo, F. Ballarin, R. Mosetti, and G. Rozza: Model Reduction for Parametrised Optimal Control Problems in Environmental Marine Sciences and Engineering, SIAM Jour- nal on Scienti c Computing, 40(4) (2018), pp. B1055-B1079. [4] S. Hijazi, S. Ali, G. Stabile, F. Ballarin, G. Rozza: The E ort of Increasing Reynolds Number in Projection-Based Reduced Order Methods: from Laminar to Turbulent Flows, ArXiv e-prints, 2018.

15th U.S. National Congress on Computational Mechanics
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Title: Necking Phenomena in Biological Membranes – Modeling Instabilities Using Kirchhoff-Love Shell Kinematics

Author(s): *Shiva Rudraraju, *University of Wisconsin-Madison*; Ritvik Vasan, *University of California, San Diego*; Padmini Rangamani, *University of California, San Diego*; Krishna Garikipati, *University of Michigan, Ann Arbor*;

Numerical treatment of Kirchhoff-Love thin shell kinematics is elegant and straightforward in the framework of curvilinear coordinates and local basis. However, the continuity requirements of such formulations and the differential geometric treatment inherent to the kinematics of surfaces have limited its widespread adoption and application. Isogeometric analysis, given its C^n continuity and exact geometric representation properties, is an ideal framework for developing thin shell formulations. In this work, we present an isogeometric analysis based, finite-strain Kirchhoff-Love shell implementation and its application to a variety of problems involving biological membranes. One specific problem of interest is the necking of membranes and tubules. The formation and constriction of membrane necks as a precursor to membrane fission is a fundamental step for a variety of biological processes including endocytosis, cytokinesis, etc. Using the thin shell framework described above, we model the deformational response and instabilities in various membrane geometries, study the suitability of Helfrich like material models, and determine the boundary conditions needed to induce preferred deformation modes. Interesting insights into asymmetric modes that lower necking energy barrier will be presented. Further, extensions of this framework to problems involving mechano-chemistry on membranes will also be discussed.

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Title: Mesoscale Modeling and Simulation of Microstructure Evolution Driven by Strong Anisotropic Grain Boundary Energy and Mobility

Author(s): *Brandon Runnels, *University of Colorado Colorado Springs*;

Nanocrystalline materials have exceptional mechanical properties. Because of their small microstructural lengthscale, their macroscopic properties are dramatically influenced by grain boundaries (GBs). GBs, the least understood of all material defects, elude simplicit characterization due to complexity of their behavior over the five degree of freedom orientation space. In this work, the effects of anisotropic boundary energy and orientation-dependent boundary motion are quantified, with applications to grain boundary engineering. An analytic model for grain boundary energy is presented that accurately captures GB energy, for boundaries with arbitrary character, with a minimal set of parameters. The model is extended to account for microscale faceting by implementing a faceting relaxation construction, which is used to validate against experimental observation. Microstructure evolution is effectively modeled using the phase field method, but grain boundary energy anisotropy and orientation dependence induce complexity in constructing the Allen Cahn equation. Furthermore, determining an accurate estimate of free energy for grain boundaries with arbitrary orientation is challenging due to the large space of grain boundary configurations and relatively sparse knowledge of energy data. As such, even rudimentary simulations with orientation dependence are restricted to certain cases with well-known boundary energy. In this work we develop an algorithm for constructing the Allen-Cahn equation for grain boundary migration including an orientation-dependent, nonconvex, anisotropic boundary energy. The energy minimizing morphology for boundaries with nonconvex energy is faceted, but lacks a lengthscale, resulting in unstable solutions in phase field gradient flow. It is therefore necessary to include a second-order regularization to penalize corners, inducing two lengthscales for (1) facet length and (2) radius of curvature. This is effected by constructing a penalization based on the second two principal curvatures of the order parameter, leaving the first unpenalized to avoid any effect on boundary thickness. To compute the variational derivative of this complex free energy, we simplify by transforming into the eigenbasis of the Hessian. This reduces the computation of principal curvatures to second derivatives with respect to the second and third principal axes, which preserves computational efficiency.The model is implemented in real-space, with MPI and OpenMP parallelization and adaptive mesh refinement to increase performance. To incorporate realistic boundary behavior, the lattice-matching model is used to calculate boundary energy for arbitrary orientations, on-the-fly. Simulations are conducted for grain boundary faceting, spherical inclusions, and randomized microstructure evolution in a real-space implementation using adaptive mesh refinement. It is shown that the phase field model accurately converges towards the theoretically-predicted minimum energy morphology for multiple energy functionals, that facet lengthscales are induced and controlled by the second order term, and experimentally observed microstructure is reproduced.

15th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization for Brittle Fracture Resistance

Author(s): *Jonathan Russ, *Columbia University*; Haim Waisman, *Columbia University*;

Structural topology optimization in the context of material degradation and fracture has been gaining considerable interest in recent years. In light of this, we will present some recent work in which the phase field method for fracture is employed in order to increase the fracture resistance of a structure comprised of a quasi-brittle material in a density-based topology optimization setting. The phase-field approximation of the fracture surface energy is utilized in the optimization problem definition and analytical sensitivities are computed for the path-dependent problem. Numerical examples highlighting the effectiveness of the proposed approach will be presented and some more recent results will also be discussed.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Multiscale Modeling of Mesoscopic Defects in Laser-welded Structures Using Hybrid-Hyperreduction

Author(s): *David Ryckelynck, *MINES ParisTech, PSL Research University*; Laurent Lacourt, *CEA*; François Willot, *MINES ParisTech, PSL Research University*; Samuel Forest, *MINES ParisTech, PSL Research University*; Sylvain Flouriot, *CEA*; Victor de Rancourt, *CEA*;

Laser welding is frequently used as an assembly process in complex systems. This process results in change in the microstructure, residual stresses, sharp crack-like notches due to partial penetration, defects formation in the fusion zone. Hence, predicting the mechanical behavior of the resulting welded joint is a challenge. More- over, non-destructive testing (NDT) techniques such as X-Ray computed tomography (XCT) are nowadays able to detect, locate and give the shape of the defects [1]. The present work aims at developping a tool and new numerical methodologies at the inteface beetween NDT and mechanical modeling. It has been divided into four main parts: (i) defect characterization and meshing through image analysis, (ii) statistic modeling of defects populations, (iii) mechanical simulations of defective parts and (iv) development of model-order reduction techniques to accelerate the resolution. First, the image analysis method will be presented. From XCT images, the defects are localized and their morphology is characterized. Several classes of defects are then created based on morphological indicators. Further analysis of these data provides a numerical tool able to generate realistic configurations of defects. The impact of the defects on the mechanical reliability of the welded part must then be quantified. The developped strategy relies on model order reduction methods and particularly the hyper-reduction method [2]. Under the assumption of separate scales, two reduced basis are built independently. The first one gathers the physics at the macroscopic scale. No defects are introduced to built it. Then, a second reduced basis is built on the fly and renders the fluctuations due to the defects. These fluctuations are localized around the defect. In the cases when the assumption of separate scales fails, methods have been developped to improve the prediction. ?[1] J. D. Madison and L. K. Aagesen [2012]: “Quantitative characterization of porosity in laser welds of stainless steel”, Scripta Materialia 67, 783-786 ?[2] D. Ryckelynck, K. Lampoh and S. Quilici [2016]: “Hyper-reduced predictions for lifetime assessment of elasto-plastic structures”, Meccanica 51, 309-317

15th U.S. National Congress on Computational Mechanics
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Title: A Mathematical Model for the Post-implant Collagen Maturation Behavior of Engineered Tissues

Author(s): *Michael Sacks, *University of Texas at Austin*;

The principle driver of this work is to elucidate the long term in vivo remodeling processes in engineered cardiovascular tissues using models developed from first principles and based on quantifiable microstructural details. Manifestations of the maturation of collagen fiber network were explicitly modeled. Moreover, it will be shown that the growth and remodeling phenomena observed in the present study are driven by an increase in collagen modulus due the underlying process. To the best of the author's knowledge, this is the first time collagen maturation model of a large artery implant has been developed. The specific key remodeling events are summarized in the following: 1. The conduit maintains its gross dimensions, including length, diameter, and thickness, over the entire remodeling period. Due to the stable conduit geometry and external loading conditions over the entireimplant period of 100 weeks, the conduit is subjected to the same stress state throughout the maturation process. Using the Law of Laplace this is estimated to be Tcc =25 kPa and TLL =12.5 kPa. 2. A rapid, near linear increase in ? c that ceases at about one year. No further changes in collagen modulus occur. 3. A shift towards increased collagen fiber organization, manifested as a parallel increase in average value and reduction in variance of ?s . 4. 0-50 weeks: Maturation of the collagen structure, manifested as increasing modulus and a shift in mean ?s and a reduction in ?s. 15 5. 50-100 weeks: Maturation process appears to be complete, with no further remodeling apparent. The model was able to capture the mechanical behaviors at each time point. Most interestingly, the model was able to faithfully simulate gradual increase in effective collagen fiber mechanical behavior and fiber recruitment. It is interesting to note that this evolution is direct result of the increase in in collagen modulus, which is part of the maturing process. In the present study, a structural model-based formulation for the time evolution of a maturing collagen tissue was formulated and evaluated. The key findings included. 1. Modeling approach was able to account for time evolution of collagen crimp 2. Maintained angular fiber dispersion with an explicit constraint 3. First model known G&R structural model that is based on evolution of material properties (fiber modulus) and not changes in boundary conditions. Current work includes extending the model initial implant phase and studies changes in boundary conditions (e.g. resulting from a change pressure)

15th U.S. National Congress on Computational Mechanics
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Title: A Micromechanical Approach to Design of Multifunctional Random Heterogeneous Materials

Author(s): Fayyaz Nosuhi, *School of Mechanical Engineering, University of Tehran, Tehran, Iran*; Majid Baniassadi, *School of Mechanical Engineering, University of Tehran, Tehran, Iran*; *Masoud Safdari, *Aerospace Engineering Department, University of Illinois, Urbana, IL*;

A novel methodology for the design of multifunctional heterogeneous materials is presented. The method combines flexible stochastic microstructural reconstruction with efficient, fast Fourier transform (FFT) based thermomechanical homogenization. Homogenized thermomechanical properties are evaluated and optimized in a continuous design space rendered by multipoint correlation functions, starting from a parametric microstructural representation for a particular class of multiphase heterogeneous materials. Current work reports on the computational algorithms developed for steps involved. The algorithms utilized for the reconstruction, homogenization and optimization steps are carefully crafted to minimize computational costs associated to iterative design and optimization loops observed in related materials design methodologies such as finite element-based shape and topology optimization techniques. The study also presents the feasibility of the approach for the design of materials in a series of demonstrative case studies. The first case study investigates the applicability of the methodology for both classes of isotropic and anisotropic random heterogeneous materials with varying volume fractions of constituents. The second case study scrutinizes the feasibility of obtaining the desired set of elasticity/thermal properties. Finally, the third case study demonstrates the efficiency and applicability of the method for the design of multifunctional heterogeneous materials. All case studies also report on the advantages and limitations of the proposed methodology.

15th U.S. National Congress on Computational Mechanics
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Title: Bayesian Estimation of Random Field Biases in Pollutant Emissions Using Multiscale Data

Author(s): *Cosmin Safta, *Sandia National Labs*; Ray Bambha, *Sandia National Labs*; Hope Michelsen, *Sandia National Labs*;

Methane is a powerful greenhouse gas, and understanding the relative spatial and temporal contributions from various anthropogenic sources is very important for developing and improving emission models. This effort is challenged by large discrepancies between the sparse set of available measurements and prior methane flux estimates based on inventories of sources. To circumvent some of these challenges we employ a hierarchical Bayesian framework to estimate emission fluxes from atmospheric concentration measurements using a Lagrangian transport model (Weather Research and Forecasting and Stochastic Time-Inverted Lagrangian Transport). We represent the corrections in emission fluxes as random fields and rely on Karhunen-Loeve expansions to efficiently capture spatio-temporal correlations. We augment this representation with point sources to enable detection of localized emission events. We conduct the analysis at regional scales and select the appropriate model parsimony based on model evidence estimates.

15th U.S. National Congress on Computational Mechanics
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Title: Machine Learning in Drug Development: Characterizing the Effect of 30 Drugs on the QT Interval with Gaussian Process Regression, Sensitivity Analysis, and Uncertainty Quantification

Author(s): *Francisco Sahli Costabal, *Stanford University*; Kristen Matsuno, *Stanford University*; Jiang Yao, *Dassault Systemes Simulia Corporation*; Paris Perdikaris, *University of Pennsylvania*; Ellen Kuhl, *Stanford University*;

Prolonged QT intervals are a major risk factor for ventricular arrhythmias and a leading cause of sudden cardiac death. Various drugs are known to trigger QT interval prolongation and increase the proarrhythmic potential. Yet, how precisely the action of drugs on the cellular level translates into QT interval prolongation on the whole organ level remains insufficiently understood. Here we use machine learning techniques characterize the effect of 30 common drugs on the QT interval. We combine information from high fidelity three-dimensional human heart simulations with low fidelity one-dimensional cable simulations to build a surrogate model for the QT interval using multi-fidelity Gaussian process regression. Once trained and cross-validated, we apply our surrogate model to perform sensitivity analysis and uncertainty quantification. Our sensitivity analysis suggests that compounds that block the rapid delayed rectifier potassium current IKr have the greatest prolonging effect of the QT interval, and that blocking the L-type calcium current ICaL and late sodium current INaL shortens the QT interval. Our uncertainty quantification allows us to propagate the experimental variability from individual block-concentration measurements into the QT interval and reveals that QT interval uncertainty is mainly driven by the variability in IKr block. In a final validation, we demonstrate an excellent agreement between our predicted QT interval changes and the changes observed in a randomized clinical trial for the drugs dofetilide, quinidine, ranolazine, and verapamil. We anticipate that both the machine learning methods and the results of this study will have great potential in the efficient development of safer drugs.

15th U.S. National Congress on Computational Mechanics
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Title: A Dynamic High-order Variational Multiscale Method on Unstructured Meshes for Flow Problems

Author(s): Zelu Xu, *Rensselaer Polytechnic Institute*; *Onkar Sahni, *Rensselaer Polytechnic Institute*;

In this talk, we will present a high-order variational multiscale (VMS) method where the stabilization parameter is computed dynamically. The current dynamic procedure takes in the given structure/form of the stabilization parameter with unknown coefficients and computes them in a local fashion resulting in a dynamic VMS method. Thus, a static stabilization parameter with pre-defined coefficients is not needed. A local version of the variational Germano identity (VGI) that is suitable for unstructured meshes and high orders is developed to perform the dynamic computation of the coefficients in the stabilization parameter (e.g., at each interior node in the mesh). The overall dynamic procedure based on the local VGI relies on a sequence of locally coarsened spaces that are constructed from the primary coarse-scale space. To make the current procedure practical, any locally coarser solution is reconstructed from the primary coarse-scale solution, which is done over local patches. Further, pathline averaging is employed to make the local dynamic procedure robust. We apply the new dynamic VMS formulation for advection-dominated flow problems with different basis orders up to p=7. We show that the current dynamic VMS method yields results of better quality as compared to the static counterpart, especially at high orders.

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Title: Arbitrary Lagrangian–Eulerian Finite Element Method for Biological Lipid Membranes

Author(s): *Amaresh Sahu, *UC Berkeley*; Yannick Omar, *UC Berkeley*; Roger Sauer, *RWTH Aachen*; Kranthi Mandadapu, *UC Berkeley*;

We present an arbitrary Lagrangian–Eulerian (ALE) finite element method for arbitrarily curved and deforming lipid membranes. We provide a formalism to determine the equations of motion governing lipid membrane behavior using an irreversible thermodynamic analysis of curved surfaces. We develop an ALE theory by endowing the surface with a mesh whose in-plane velocity is independent of the in-plane material velocity, and which can be specified arbitrarily. The general isoparametric finite element implementation of the theory, based on an arbitrary surface parametrization with curvilinear coordinates, is used to model lipid membranes in several biologically relevant situations. A new physical insight is obtained by applying the ALE developments to cylindrical lipid membrane tubes: though lipid membrane tubes are stable, in the limit of vanishing bending rigidity (the limiting case of a fluid film) we numerically and analytically find tubes to be unstable with respect to long-wavelength perturbations when their length exceeds their circumference.

15th U.S. National Congress on Computational Mechanics
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Title: Numerical Modelling of Thermal Spallation in Concrete: a Meso-Mechanical Approach Based on Embedded Discontinuity FEM

Author(s): *Timo Saksala, *Tampere University of Technology, Finland*;

This work presents a numerical modelling of thermal spallation of concrete. Here thermal spallation refers to fragmentation and ejection of concrete surface material when subjected to rapid external heating. The special application in mind is the drilling or breakage of concrete by a thermal shock, i.e. a short duration high intensity heat flux. For this end, a numerical procedure for modelling the thermal shock induced fracture in concrete material is developed. The concrete fracture model is based on the embedded discontinuity finite element approach. In the present implementation, a displacement discontinuity (crack) is embedded perpendicular to the first principal direction in a linear triangle element upon violation of the Rankine criterion. Concrete is a bi-phase material consisting typically of mortar matrix and rock like aggregates. As the aggregates have a significant effect on the concrete behaviour, a meso-scopic approach is chosen. Accordingly, the aggregates are modelled as shrinked and rotated Voronoi polygons, while the whole skeleton of numerical concrete, i.e. the mortal and aggregates, is meshed with ordinary linear triangle elements. In this approach, the effect of interfacial transition zone can be accounted for by lowering the strength of the elements in a strip around the aggregates. The heating due to mechanical dissipation is neglected as insignificant in comparison to the external heat flux. Thereby, the underlying thermo-mechanical problem becomes uncoupled and the only input from the thermal part to the mechanical part are thermal strains. This problem is solved with explicit time marching using the mass scaling to speed up the solution. A thermal spallation problem of a numerical concrete sample is simulated under axisymmetric conditions as a numerical example. The simulations demonstrate that the present method predicts the salient features of thermal spallation of concrete.

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Title: Alternative hp-enrichment of Test Spaces for the DPG Method. Numerical Assessment and Comparison with h- and p- Enrichment.

Author(s): *Jacob Salazar Solano, *University of Texas at Austin*; Jaime Mora Paz, *University of Texas at Austin*; Leszek Demkowicz, *University of Texas at Austin*;

We propose and investigate the use of an hp-refinement strategy for the enrichment of the local test spaces in the context of Discontinuous Petrov-Galerkin (DPG) with optimal test functions developed by Demkowicz and Gopalkrishnan [1]. Adequate resolution of the optimal test functions is fundamental for finding a solution for a DPG discretization, but also for the adaptive refinement evolution. Resolution improvements have a positive effect in the reliability of the error representation function, which guides the a-posteriori error estimator and ultimately determines the elements to be refined. Optimal test functions resolution is improved through local enrichment of the discrete spaces, which has traditionally been performed by increasing the polynomial degree of the basis functions; this however is not in general effective. By adopting an approach similar to the one used by Niemi et. al. [2], we propose a mixed strategy where an element sub-mesh is introduced for the optimal test functions computation and B-splines are used as basis functions [3]. Given the proved stability of the ideal DPG method, it is natural to study its applicability for singular perturbation problems. We discuss numerical results for the convection-dominated diffusion problem, and compare conditioning and mesh refinement evolution with other enrichment strategies (p-enrichment and h-enrichment). [1] Demkowicz L. and Gopalakrishnan J. A class of discontinuous Petrov-Galerkin methods. II. Optimal test functions. (2011) Numer. Methods Partial Differential Equations 27(1), 70–105 [2] Niemi A. H., Collier N. O., and Calo, V. M. Automatically stable discontinuous Petrov–Galerkin methods for stationary transport problems: Quasi-optimal test space norm. (2013) Computers & Mathematics with Applications, 66(10), 2096–2113. [3] Salazar J., Mora J. and Demkowicz L. Alternative enriched test spaces in the DPG method for singular perturbation problems. (2019) Accepted for publication in Computational Methods in Applied Mathematics

15th U.S. National Congress on Computational Mechanics
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Title: A Stable Generalized/eXtended FEM with Discontinuous Interpolant for Fracture Mechanics

Author(s): *Alfredo Sanchez Rivadeneira, *University of Illinois at Urbana-Champaign*; Carlos Duarte, *University of Illinois at Urbana-Champaign*;

The successful development of an optimally convergent Generalized FEM (GFEM) with conditioning not worse than FEM for fracture mechanics problems has been mostly limited to first-order accurate approximations. Numerical studies with quadratic GFEM approximations are presented, showing errors that are orders of magnitude smaller than the FEM with quarter-point elements, which in general is not the case for first-order GFEM approximations. However, they lead to severely ill-conditioned systems of equations. Enrichment modifications able to address the ill-conditioning of quadratic GFEM approximations while preserving optimal convergence are proposed. An enrichment modification strategy based on a discontinuous finite element interpolant is proposed to control the conditioning of branch function enrichments, while a combination of enrichment shifting by its nodal value and a local finite element mesh modification in the neighborhood of the crack surface is used to address the lack of robustness of Heaviside enrichments. The discontinuous FE interpolant is a generalization of the continuous one used with the Stable GFEM (SGFEM). It is shown that SGFEM spaces based on p-hierarchical FEM enrichments are the same as their GFEM counterparts. This guarantees that both GFEM and SGFEM spaces will lead to the same solution, which is not the case for other classes of second-order spaces. The robustness of the proposed approximation spaces with respect to the position of the mesh relative to the crack is demonstrated numerically.

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Title: Topology Optimization Framework for Frequency-response Design Using a Modified Error in Constitutive Equations Approach

Author(s): *Clay Sanders, *Duke University*; Julian Norato, *University of Connecticut*; Timothy Walsh, *Sandia National Laboratories*; Wilkins Aquino, *Duke University*;

Consideration of vibration and dynamic loading conditions has crucial implications mechanical, aeronautical, and structural engineering applications. Design strategies for dynamic structural behavior can be used to control resonant vibration, reduce sound emission, or minimize vibrational amplitude. However, incorporating dynamics in design optimization schemes introduces significant difficulties, as structural objectives become highly non-convex and gradient-based optimization schemes can converge towards suboptimal designs in local minima. This work presents a topology optimization strategy to improve the robustness of frequency-response topology optimization, both with respect to initial guesses and the considered loading conditions. We adapt the Modified Error in Constitutive Equations (MECE) penalty method, used previously in material identification inverse problems, for the design of structures subject to loading in frequency-domain dynamics. Our proposed framework relies upon relaxation of the optimization problem's partial differential equation (PDE) constraints to "smooth" the objective function. We permit violation of both the constitutive laws relating stresses and strains and the relation between inertial forces and structural displacements, physical laws which would normally be enforced in PDE constraints. Instead, error functionals which measure violation of these assumed physical laws are included in the optimization objective. Minimization of these error terms is weighted against minimization of the structural design objective, allowing for design objectives to be achieved while providing regularization to the objective function to avoid numerical instabilities. We show that relaxation of the PDE constraints improves the convexity of the objective function, alleviating the susceptibility to convergence towards local minima, and that this method can obtain superior designs to direct, gradient-based optimization approaches. The MECE strategy integrates into a density-based topology optimization scheme for void-solid or two-phase material structural design. We highlight the merits of our approach in a variety of design scenarios for direct frequency response design, considering multiple frequency load cases and a variety of structural objectives. We demonstrate that our approach can yield stable structures with highly-specialized vibration behavior. While we focus on examples of structures subject to harmonic vibration, this flexible topology optimization strategy can be applied for design problems subject to other steady state dynamics, such as acoustic structural interaction or acoustic metamaterial design. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525

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Title: An Open-Source Integrated Computational Environment for Multi-Physics/Phase/Scale Simulation, Optimization and Uncertainty Quantification

Author(s): *Anjali Sandip, *University of North Dakota*;

Traditionally, multi-physics simulation software programs lack tools for uncertainty quantification and optimization [1]. More recently, there is a growing body of research that has integrated these tools into multi-physics simulation software programs [2, 3]. Building on this methodology, the study integrated open-source software programs -- DAKOTA for optimization and uncertainty quantification and ELMER for multi-physics/phase/scale simulations. Furthermore, the coupled software was successfully applied to benchmarks. The overarching goal was to develop an open-source integrated computational environment for multi-physics/phase/scale simulation, optimization and uncertainty quantification. The applications of this integrated computational environment span several industries ranging from aerospace and energy to healthcare and manufacturing and can be applied to solve problems that are of great interest to the federal agencies. References [1]. Di Gallo, L., Reux, C., Imbeaux, F., Artaud, J. F., Owsiak, M., Saoutic, B., ... & Duchateau, J. L. (2016). Coupling between a multi-physics workflow engine and an optimization framework. Computer Physics Communications, 200, 76-86. [2]. Witte, I., Stephanopoulos, K., Wray, T., & Agarwal, R. K. (2018). Uncertainty Quantification of Turbulence Model Coefficients in OpenFOAM and Fluent for Mildly Separated Flows. In 2018 Fluid Dynamics Conference (p. 3553). [3]. Elwasif, W. R., Bernholdt, D. E., Pannala, S., Allu, S., & Foley, S. S. (2012, December). Parameter sweep and optimization of loosely coupled simulations using the DAKOTA toolkit. In Computational Science and Engineering (CSE), 2012 IEEE 15th International Conference on (pp. 102-110). IEEE.

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Title: Mechanisms Associated with Temperature Dependence of Grain Boundary Migration in FCC Metals

Author(s): *Ali Sangghaleh, *Brigham Young University*; Ryan Anderson, *Brigham Young University*; Eric Homer, *Brigham Young University*;

Grain boundaries (GBs) in metals are important structural defects that control physical processes in crystal growth, microstructure evolution, corrosion inhibition, and segregation engineering. There has been significant attention focused on the motion of GBs by atomistic simulations. According to the recent simulation results, some GBs demonstrate different migration behaviors at different temperatures and the reason for this is not clear. Therefore, a single analytical model that can rationalize the change in migration behaviors with temperature would be useful. The present work focuses on recent models and mechanisms dealing with motion of GBs in metals. We introduce a non-Arrhenius model that is capable of predicting GB mobility over a large range of temperature and different migration behaviors. This model is based on the conservative motion of GBs via a combined vacancy diffusion and dislocation glide. The applicability of this model will be described and compared with molecular dynamics simulations in nickel bicrystals over temperatures ranging from 100 to 1400 K for various boundaries. Case studies will also be presented for tilt, twist, and mixed GBs. The current work provides insights into the mechanisms for specific GB mobility trends.

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Title: Interactive Planner: Real-time Blood Flow Simulations and Application to Stenting Serial Lesions

Author(s): *Sethuraman Sankaran, *HeartFlow, Inc.*;

Hemodynamic indices are helpful in the assessment of health or disease of a patient. Blood flow simulations can help assess these indices non-invasively. The true power of blood flow simulations lie in the predictive modeling of hemodynamics in response to unknown events (for e.g. progression or regression of lesions), or the outcome of planned procedures (e.g. surgical intervention). For predictive modeling to be realistic and clinically useful, it is imperative that these tools are real-time. We propose a method that enables real-time assessment of changes in hemodynamics in response to changes in the lumen geometry. The method uses a reduced order model parameterized by a full order model using three-dimensional simulations performed at certain pre-set configurations. The pre-set configurations involve exploration of both, the space of lumen geometries and boundary conditions. By construction, the prediction of the reduced order model is identical to the full order model at these pre-set configurations. We achieved a good trade-off between offline simulation time and algorithm accuracy using four full order simulations. We demonstrate that we are able to predict the results of three dimensional simulations for coronary blood flow simulations accurately with a mean absolute error of 0.01 (95% CI: [-0.03, 0.03]), a bias within 0.01 and correlation coefficient of 0.99 on unseen patient data (N = 500). We also demonstrate the performance of the algorithm in predicting hemodynamics post-PCI against invasive data for serial lesions, and demonstrate its use as an interactive planning tool.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Incorporation of Melt Pool Fluid Flow in a Reduced-order Additive Manufacturing Model

Author(s): *Mohammad Javad Sarfi, *Northwestern University*; Gregory Wagner, *Northwestern University*;

It has been widely recognized in the field of additive manufacturing that the fluid flow and heat transfer in the melt pool strongly influence many AM characteristics, e.g. the melt pool shape and dimensions, microstructure, and ultimately mechanical properties of the manufactured part. However, using computationally expensive CFD modeling of the fluid convection in the melt pool is not feasible for simulating practical and industrial additively manufactured parts that do not necessarily have simple geometries and are composed of multiple layers. Furthermore, accounting for the turbulent nature of the molten flow that results in enhanced diffusion and mixing adds up to the complexity and expense of this type of simulations. Therefore, the melt pool fluid flow is often ignored in AM simulations and many resort to solving only the heat conduction equation to speed up the computations. Needless to say that this approach is fraught with inaccuracies due to overprediction of temperature, cooling rates and thermal gradients and adversely affects the prediction of the melt pool shape. Since the velocity field within the melt pool quickly reaches a steady state in a single laser track, it is reasonable to assume that it does not have much variations throughout the build process. The steady velocity field of the molten liquid metal, which is predominantly driven by surface tension forces, is obtained in a fixed frame of reference using our in-house parallel CFD code that is based on Control Volume Finite Element numerical method. Importing the obtained velocity field to a faster parallel code and then solving only the advection-diffusion equation through Petrov-Galerkin FEM to include the convection of heat with the fluid flow results in tremendous improvements in accuracy while maintaining the high speed of the FEM model by obviating the need to repeatedly solve the coupled fluid momentum equations. Efforts have been made to improve the efficiency of this method by importing the velocity field to a coarser FEM mesh than the CFD grid. These include mapping the velocity field into a higher number of Gauss quadrature points in the FEM model and also adopting variational multiscale method in order to resolve the fine-scale phenomena in the coarse mesh.

15th U.S. National Congress on Computational Mechanics
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Title: Bond-based Peridynamic Model Model for Concrete Structures Using Stresses

Author(s): *Nicolas Sau, *Assistant Professor*; Jose Medina, *Assistant Professor*;

Concrete structures subjected to loads that cause the formation and propagation of cracks exhibit a behavior where continuum mechanics is no longer applicable because most conventional models do not consider the discontinuities that appear and propagate as a result of concrete tension failure. In an effort to correct the shortcomings of continuum models, the peridynamic bond-based model was proposed in 2000. One of the shortcomings of the bond-based peridynamic model is that was not able to model materials with Poisson´s ratio different from 1/4 in three dimensions and 1/3 for plane stress problems. To overcome this problem, the state-based peridynamic model was proposed in 2007. The micropolar peridynamic model improves the bond-based peridynamic model by allowing moment densities in addition to force densities to interact among particles inside the material horizon, nevertheless a clear connection between the micropolar peridynamic model and continuum models was not fully established. The stress tensor using the peridynamic theory was first introduced by Silling in 2000, and modified later by Lehoucq in 2008 to include the interaction between two volumes. In this work, it is proposed a framework where the micropolar peridynamic stress is developed, in which relationships between conventional stress strain and the micropolar peridynamic stress-strain tensor for linear elastic materials are obtained. A numerical scheme was developed, in which the stress tensor is analyzed in regions where the displacement field is discontinuous. In this numerical non-linear model, bond failure criterion is modified using conventional failure criteria. Closed form results show convergence with classical linear elastic solutions for small values of the material horizon and numerical results match fairly well with laboratory flexural tests.

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Title: Monolithic Simulation Approaches to Fluid-structure-contact Interaction of Membranes and Shells

Author(s): *Roger Sauer, *AICES, RWTH Aachen University*; Maximilian Harmel, *AICES, RWTH Aachen University*; Michal Rajski, *AICES, RWTH Aachen University*;

Membranes and thin-walled shells have low bending stiffness and are thus easily excited by a surrounding flow field. Large structure deformation can ensue and thus lead to self-contact or contact with neighboring objects. In order to capture flows at high Reynolds numbers, the full Navier-Stokes equations need to be solved. At low Reynolds numbers, Stokes' flow condition can be considered, making the flow equations linear. Boundary integral formulations can then be used to solve the flow. This work presents monolithic simulation approaches for both cases. Curvilinear, isogeometric surface finite elements are used to discretize the structure, contact and boundary integrals, while the generalized-alpha scheme is used for the temporal discretization [1,2]. For Navier-Stokes flow, stabilized Petrov-Galerkin finite elements are used considering a conforming, sharp interface discretization and an arbitrary Lagrangian-Eulerian formulation around the structure [3]. The resulting formulation is very general and admits diverse applications. This is demonstrated by several numerical examples exhibiting strong coupling between fluid and structure. These include balloon inflation, droplet rolling, bubble rising, cavity filling and flag flapping. They span a Reynolds number range from 0.001 to 2000. [1] T.X. Duong, F. Roohbakhshan and R.A. Sauer (2017), A new rotation-free isogeometric thin shell formulation and a corresponding continuity constraint for patch boundaries, Comput. Methods Appl. Mech. Engrg., 316:43-83 [2] M. Harmel and R.A. Sauer (2017), Boundary element and finite element analysis for the efficient simulation of fluid-structure interaction and its application to mold filling processes, Proc. Appl. Math. Mech., 17:513-514 [3] R.A. Sauer and T. Luginsland (2018), A monolithic fluid-structure interaction formulation for solid and liquid membranes including free-surface contact, Comput. Methods Appl. Mech. Engrg., 341:1-31

15th U.S. National Congress on Computational Mechanics
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Title: Stokes Coordinates

Author(s): *Yann Savoye, *Robert Gordon University*;

Cage-based polyhedral structures are reduced subspace deformers enabling non-isometric stretching deformations induced by clothing or muscle bulging. In this paper, we reformulate the cage-based rigging as an incompressible Stokes problem in the vorticity space. In this paper, we describe a method for generating mesh bind weights for control cages built upon the conceptual fluid-cage connection. Inspired by the incompressible flow theory, we introduced a new high-order coordinates system for cage-based rigging called Stokes Coordinates, allowing non-isometric stretching. We borrow the idea from fluid dynamics to express shape deformation as a Stokes problem. In particular, we explored stencil computation and governing field equations for cage weighting functions. The key to our approach is a compact stencil allowing the expression of fluid-inspired high-order coordinates. Thus, our cage-based coordinates are obtained by vorticity transport as the numerical solution of the linearized Stokes equations. Then, we turn the incompressible creeping Newtonian flow into Stokes equations, and we devise a second-order compact approximation with center differencing for solving the vorticity-stream function. To the best of our knowledge, our work is the first to devise a vorticity-stream function formulation as a computational model for cage-based weighting functions. Finally, we demonstrate the effectiveness of our new techniques for a collection of cage-based shapes and applications. Our framework offers three cage-based applications employing our novel coordinates system: interactive cage-based mesh editing, cage-based shape encoding, and cage-based performance capture reuse.

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Title: Computational Modeling of the Biochemical and Biomechanical Degeneration in Alzheimer's Disease

Author(s): *Amelie Schaefer, *Stanford University*; Johannes Weickenmeier, *Stevens Institute of Technology*; Ellen Kuhl, *Stanford University*;

Alzheimer's disease is an irreversible neurodegenerative disorder that manifests itself in the progressive aggregation of misfolded tau protein, neuronal death, and cerebral atrophy. A reliable diagnosis of these changes in the brain is challenging because they typically precede the clinical symptoms of Alzheimer's disease by at least one, if not two, decades. Volumetric magnetic resonance imaging holds promise as a non-invasive biomarker for disease onset and progression by quantifying cerebral atrophy in time and space. Recent studies suggest that the patterns of brain atrophy are closely correlated with the regional distribution of misfolded tau protein; yet, to date, there is no compelling computational model to simulate the interaction of misfolded protein spreading and tissue atrophy. Here we establish a multiphysics model that couples misfolded protein spreading and tissue atrophy to explore the spatio-temporal interplay of biochemical and biomechanical degeneration in Alzheimer's disease. We discretize the coupled bio-chemo-mechanical problem using a nonlinear finite element approach with the misfolded protein concentration and the tissue deformation as primary unknowns. In a systematic parameter study, we probe the role of the individual model parameters and compare our results against cerebral atrophy curves of patients with early onset Alzheimer's disease. A critical link between biochemical and biomechanical degeneration is the atrophy rate, which reflects both natural aging-induced atrophy and accelerated misfolding-induced atrophy. Our simulations reveal that misfolding accelerates natural atrophy by a factor of three to five, and that regions near the hippocampus are most affected by brain tissue loss. Our quantitative model could help improve diagnostic tools, advance early detection, and, ultimately, enable early interventions to delay the onset of cognitive decline in familial or sporadic Alzheimer's disease.

15th U.S. National Congress on Computational Mechanics
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Title: Variational and Multiscale Modeling of Silica Glass

Author(s): *William Schill, *Caltech*;

We develop a critical-state model of fused silica plasticity on the basis of data mined from molecular dynamics (MD) calculations and maximum entropy atomistics (MXE) calculations. The MD data is suggestive of an irreversible densification transition in volumetric compression resulting in permanent, or plastic, densification upon unloading. Moreover, this data exhibits dependence on temperature and the rate of deformation. We show that these characteristic behaviors are well-captured by a critical state model of plasticity, where the densification law for glass takes the place of the classical consolidation law of granular media and the locus of constant volume states denotes the critical-state line. A salient feature of the critical-state line of fused silica, as identified from the MD data, that renders its yield behavior anomalous is that it is strongly non-convex, owing to the existence of two well-differentiated phases at low and high pressures. We argue that this strong non-convexity of yield explains the patterning that is observed in molecular dynamics calculations of amorphous solids deforming in shear. We employ an explicit and exact rank-2 envelope construction to upscale the microscopic critical-state model to the macroscale. Remarkably, owing to the equilibrium constraint the resulting effective macroscopic behavior is still characterized by a non-convex critical-state line. Despite this lack of convexity, the effective macroscopic model is stable against microstructure formation and defines well-posed boundary-value problems. However, owing to the temperature dependence of the model, the macroscopic model is unstable against adiabatic shear localization. Thus, the material adopts small interfacial regions where the shear strain is extremely high. We characterize the shear band size and spacing using matched asymptotics – thereby predicting a yield knockdown factor at the macroscale. We finish by studying continuum mechanics examples of silica glass involving ballistic impact.

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Title: Modelling and Simulation of Fracture at Multiferroic Cohesive Interfaces

Author(s): *Alexander Schlosser, *Institute of Mechanics, University of Kassel*; Andreas Ricoeur, *Institute of Mechanics, University of Kassel*;

The efficiency in converting magnetic into electric energy and vice versa makes magnetoelectric (ME) composites promising candidates for many technical applications. The ferroelectric matrix as well as the magnetostrictive inclusions of particle composites and the layers of laminates are mostly ceramics or other brittle materials, thus being prone to cracking. Independent from the kind of composite, the transmission of stresses via the interfaces between the constituents plays the key role in its functionality. Therefore, the investigation of delamination processes is of great interest for the prediction of durability and coupling factors. In order to investigate delamination processes in ME composites, cohesive elements are being developed and applied in combination with nonlinear ME finite elements described in [1] and [2]. The mechanical behavior of the cohesive zone is classically prescribed by a bilinear traction-separation-law. Magnetic and electric fluxes emanate from evolution laws of magnetic and electric permeabilities, respectively, accounting for micro crack damage in the process zone and electrostatic stresses at the interfaces. Piezoelectric and piezomagnetic properties of the interfaces are taken into account introducing an appropriate thermodynamical potential accounting for the coupling effects. Electric and magnetic properties change during damaging processes, being controlled by damage variables, which in turn are determined by the separation between the boundaries. The cohesive zone approach and associated crack tip opening displacements are related to other electromagnetomechanical fracture quantities such as energy release rates or the J-Integral. Based on simulations influence factors on delamination like the arrangement of the composites, the ME poling processes or loading regimes are investigated, finally with regard to improving ME coupling coefficients. [1] Avakian, A., Gellmann, R., and Ricoeur, A. (2015). Nonlinear modeling and finite element simulation of magnetoelectric coupling and residual stress in multiferroic composites. Acta Mechanica, 226(8), 2789-2806. [2] Avakian, A., and Ricoeur, A. (2016). Constitutive modeling of nonlinear reversible and irreversible ferromagnetic behaviors and application to multiferroic composites. Journal of Intelligent Material Systems and Structures, 27(18), 2536-2554.

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Title: The Shifted Boundary Method for Embedded Domain/Interface Computations: Applications to Sub-Surface Flow

Author(s): *Guglielmo Scovazzi, *Duke University*;

In modern engineering, numerical simulations with complex geometries remain challenging. Numerical techniques such as embedded and immersed boundary methods are gaining popularity since they avoid the burden of conformal mesh generation. However, the proper imposition of the boundary conditions is cumbersome since these methods do not preserve the optimal rate of convergence of the numerical schemes. To circumvent this issue, we propose to use the Shifted Interface Method [1,2,3,4]. The key feature of the proposed approach is to shift the location of the interface to a surrogate interface, for which the interface conditions are appropriately modified and weakly enforced. In this work, the closest point projection on one side of the interface is used to define the surrogate interface, and a Taylor expansion enables to modify in a proper way the interface conditions. This method is shown to be favorable in terms of accuracy, robustness, and computational cost as demonstrated for the imposition of boundary or jump interface conditions. We also show how the shifted boundary method can be combined with front tracking or level-set algorithms, used to describe the motion of interfaces. REFERENCES [1] Main*, G. Scovazzi, “The shifted boundary method for embedded domain computations. Part I: Poisson and Stokes problems,” Journal of Computational Physics, 372, 972-995, 2018. [2] A. Main*, G. Scovazzi, “The shifted boundary method for embedded domain computations. Part II: Advection-diffusion and Navier-Stokes equations,” Journal of Computational Physics, 372, 996-1026, 2018. [3] T. Song*, A. Main*, G. Scovazzi, M. Ricchiuto “The shifted boundary method for hyperbolic systems: Embedded domain computations of linear waves and shallow water flows,” Journal of Computational Physics, 369, 45-79, 2018. [4] O. Colomés*, A. Main*, L. Nouveau*, G. Scovazzi, “The shifted boundary method for free surface flow problems,” Journal of Computational Physics (in preparation).

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Title: Bond-based peridynamics: A tale of two Poisson's ratios

Author(s): *Pablo Seleson, *Oak Ridge National Laboratory*; Jeremy Trageser, *Oak Ridge National Laboratory*;

In this presentation, we discuss the restrictions imposed by bond-based peridynamics, particularly with respect to plane strain and plane stress models. We begin with a review of the derivations in [1] wherein for isotropic materials a Poisson's ratio restriction of 1/4 for plane strain and 1/3 for plane stress is deduced. Next, we show Cauchy's relations are an intrinsic limitation of bond-based peridynamics and specialize this result to plane strain and plane stress models, generalizing the results of [1] and demonstrating the Poisson's ratio restrictions in [1] are simply a consequence of Cauchy's relations. We conclude with a discussion of the validity of peridynamic plane strain and plane stress models formulated from two-dimensional bond-based peridynamic models. Reference: [1] Gerstle, W., Sau, N., Silling, S.: Peridynamic modeling of plain and reinforced concrete structures. In: 18th International Conference on Structural Mechanics in Reactor Technology (SMiRT 18), pp. 54-68 (2005).

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Title: Machine Learning for Sub-Grid Scale Turbulent Combustion Modeling

Author(s): *Andréa Seltz, *CORIA – CNRS, Normandie Universite?, INSA de Rouen, France. SAFRAN Aircraft Engines, France.*; Pascale Domingo, *CORIA – CNRS, Normandie Universite?, INSA de Rouen, France*; Luc Vervisch, *CORIA – CNRS, Normandie Universite?, INSA de Rouen, France*;

The reconstruction of unresolved scalar sources and transport terms from Convolutional Neural Network (CNN) is discussed in the context of sub-grid scale (SGS) modeling of premixed turbulent flames. A Direct Numerical Simulation (DNS) imbedded in a Large Eddy Simulation (LES) of a premixed turbulent jet flame [1] is coupled with machine learning, to propose a self-consistent modeling with tabulated detailed chemistry. First, the statistical properties of the progress variable filtered chemical source and of the unresolved SGS scalar transport by momentum and molecular diffusion are examined in the light of deep learning specific requirements. Mining the DNS database, specific features are observed connecting filtered non-linear chemical sources and the divergence of the unresolved fluxes, respectively, to the burning rates and the divergence of the diffusive fluxes computed from the resolved LES fields. These features suggest that image-type machine learning can be readily applied to dynamically determine two mapping functions from Convolutional Neural Network, so that all unknown terms in the progress variable equation, driving the coupling with the chemical lookup table, are dynamically reconstructed from a neural network. A priori tests are then conducted varying the LES filter size between 0.3 mm and 1.2 mm. The capability of CNN to provide a reliable approximation of the two mapping functions (chemical source and divergence of fluxes) is confirmed for all filter sizes. It is also observed that blurring the data in the training phase, improves reliability with cases not initially learned by the CNN. To extend the prediction to some pollutants, the proposed approach can be complemented by the progress variable SGS variance estimation from CNN recently discussed in [2], then both flame dynamics and emissions are predicted through deep learning. References [1] P. Domingo, L. Vervisch (2017) DNS and approximate deconvolution as a tool to analyse one-dimensional filtered flame sub-grid scale modeling, Combust. Flame, 177: 109-122. [2] Z. Nikolaou, C. Chrysostomou, L. Vervisch, S. Cant, Turbulent premixed flame modelling using convolutional neural networks: application to sub-grid scale scalar variance and filtered reaction rate, submitted.

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Title: Computing the Effective Thermal Conductivity of Anisotropic Porous Media from Micro-computed Tomography Images

Author(s): *Federico Semeraro, *UIUC at NASA Ames Research Center*; Joseph Ferguson, *STC at NASA Ames Research Center*; Francesco Panerai, *University of Illinois at Urbana-Champaign*; Nagi Mansour, *NASA Ames Research Center*;

The design of effective ablative thermal protection systems, used to protect spacecraft during the severe aerothermal conditions of atmospheric entry, requires high-fidelity material response models. In this context, the ability to compute material properties based on grayscale images of its microstructure is instrumental in order to accurately inform the macro-scale response models. These images are obtained through the use of X-ray micro-tomography and they are reconstructed into 3D models, upon which simulations are conducted. One of the main focuses in the prediction of heatshield material response is predicting the effective thermal conductivity of the bulk material, often difficult to determine experimentally. A common assumption for solid conduction is that the thermal conductivity of the various phases is isotropic. Although this assumption may be valid in some cases, there are many materials that have anisotropic properties at the micro-scale, including fiber-based and woven materials. To simulate the isotropic or anisotropic solid conduction, a fully-conservative finite volume scheme based on the Multipoint flux approximation (MPFA) technique [1] has been formulated and implemented into the Porous Microstructure Analysis (PuMA) software [2]. One challenge in modeling the solid conduction of porous materials is determining the constituent thermal conductivities. Experimental and numerical techniques to determine these values have been considered and will be discussed. The simulation tools were verified against several analytical steady-state solutions and compared to previous computational studies. The heat transfer models were then applied to fibrous and woven materials used by NASA as thermal protection systems and the results were compared to experimental data when available. [1] I. Aavatsmark, Multipoint flux approximation methods for quadrilateral grids, in: 9th International forum on reservoir simulation, Abu Dhabi, 2007, pp. 9–13. [2] J. C. Ferguson, F. Panerai, A. Borner, N. N. Mansour, PuMA: the Porous Microstructure Analysis software, SoftwareX 7, 2018, pp. 81 – 87.

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Title: Leaflet Kinematics and Transvalvular Hemodynamics in Normal and Thrombosed Transcatheter Aortic Valves

Author(s): *Jung Hee Seo, *Johns Hopkins University*; Shantanu Bailoor, *Johns Hopkins University*; Hoda Hatoum, *Ohio State University*; Lakshmi Prasad Dasi, *Ohio State University*; Rajat Mittal, *Johns Hopkins University*;

Transcatheter aortic valves (TAVs) are rapidly becoming the dominant option for aortic valve replacement. These valves are however susceptible to a number of complications (“malfunctions”) such as paravalvular leaks, leaflet tears, endocarditis, and most importantly, leaflet thrombosis. Since these conditions are expected to alter the valve motion and transvalvular hemodynamics, valve malfunction can possibly be detected by monitoring the valve kinematics and hemodynamics. In this regard, characterizing the kinematics and hemodynamics of healthy as well as “malfunctioning” valves is particularly important. In the present study, experimental and computational studies are used to investigate the characteristics of the valve leaflet kinematics and transvalvular hemodynamics in normal and thrombosed transcatheter aortic valve (TAV) models. Imaging data from in-vitro experiments are used to characterize the leaflet kinematics in terms of leaflet modal shapes and principal components. Data from the experiments are also employed to parameterize computational fluid-structure interaction (FSI) of TAV function as well as to analyze the simulation data. The simulations allow us to generate a large range of conditions that mimic leaflet thrombosis-induced reduced leaflet motion and the simulation results are analyzed to determine those features of hemodynamics that provide robust detection of leaflet thrombosis.

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Title: Newton Raphson Modification for Fast Convergence of Cohesive Interfaces

Author(s): *Reza Sepasdar, *Virginia Tech*; Maryam Shakiba, *Virginia Tech*;

Cohesive zone models (CZMs) have become popular in the past decade to model interfaces, cohesive contacts, and crack propagation in finite element (FE) simulations due to their simplicity in applications. However, convergence difficulty may arise in a static analysis under certain circumstances, and as a result, undermines the efficiency of CZMs. Different researchers believe that convergence difficulty arises because of either a physical instability due to an unbalanced state of energy or the numerical instabilities due to the presence of multiple solutions. The convergence problem of CZMs has been reported numerously in the literature, and consequently, a few methods have been proposed to address the issue. However, the proposed methods are either expensive or involve altering the CZM's constitutive behavior which affects the accuracy of the analysis. In this work, we explain the reason which induces the convergence problem and propose a new simple modification to the Newton-Raphson iterative method to overcome the issue. It is shown that after the modification is applied, the system of equations will converge to the root quickly. The modification method is independent of the material's constitutive relationship because secant stiffness is used for the material. The developed technique is also applicable to the cases where the material is nonlinear (e.g., when a damage model is used) regardless of the function or shape of the nonlinearity. In the end, the efficiency of the proposed method is presented by a few application examples.

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Title: Improving Convergence of Bayesian Inference

Author(s): Jiacheng Wu, *UC Berkeley*; Jianxun Wang, *Notre Dame*; *Shawn Shadden, *UC Berkeley*;

Data-driven inference methods can be coupled with computational models for solving inverse problems in mechanics (e.g., inferring appropriate parameters, boundary conditions, etc.). Notably, Bayesian inference and approximate Bayesian inference methods such as Kalman filtering variants can be effective but prone to poor convergence or inaccuracies when, e.g., the model system is nonlinear or when there is limited data. This talk will discuss methods to improve convergence in such scenarios. We will first discuss the inclusion of physical constraints based on prior knowledge. Such knowledge can be used to constrain the data-driven estimation or parameter search process for inverse problems to help ensure physically-valid solutions or improve convergence. We will show how this can be formulated as a statistical inference problem, and the relation of such inference formulation to more traditional constrained optimization. We will also discuss a method to improve the convergence of approximate Bayesian inference methods, such as iterative ensemble Kalman filtering, through appropriate perturbation of the covariances by resampling, which can be important in nonlinear problems. Similarly, the relation of the statistical structure of this method will be discussed and compared to a traditional gradient-based viewpoint.

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Title: Topology Optimization of Unit Cells for Additively Manufactured Lattice Structures

Author(s): *Conner Sharpe, *UT Austin*; Carolyn Seepersad, *UT Austin*;

Additive manufacturing enables the fabrication of mechanical metamaterials, such as lattice or honeycomb materials, with highly customized properties, including lightweight stiffness, strength, and energy absorption. However, it also constrains the manufacturability of these metamaterials and introduces anisotropy that is not typically observed in conventionally fabricated materials. In this research, a geometric projection method is utilized to design unit cells for lattice structures. The method reduces the dimensionality of the design problem and facilitates the incorporation of fabrication constraints and anisotropy. The method is coupled with a Bayesian optimization algorithm to eliminate the need for gradient information and expand the types of properties that can be optimized.

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Title: Modeling Multi-Stage Hydraulic Fracturing from a Borehole within a GFEM Framework

Author(s): *Nathan Shauer, *University of Illinois at Urbana-Champaign*; Carlos Armando Duarte, *University of Illinois at Urbana-Champaign*;

Hydraulic Fracturing is the process in which a fracture propagates through the injection of pressurized fluid in its cavity. This process is widely used in the oil and gas industry to increase reservoir permeability which leads to high rates of both injection and production. Hydraulic fractures are often created in a multi-stage process which leads to complex fracture geometries due to interactions and fracture realignment with the preferential propagation direction. The fracture shape, and consequently pressure drop, varies significantly between fracture clusters. As a result, the majority of the gas and oil production comes from only 20 to 30% of the clusters. Computational methods able to predict the near wellbore tortuosity and pressure drop can play a key role in improving the performance of multistage fracturing. This presentation reports on recent advances of an adaptive Generalized Finite Element Method (GFEM) for the simulation of multiple 3-D non-planar hydraulic fracture propagation near a wellbore. This method is particularly appealing for the discretization of the fractures since it does not require the finite element mesh to fit fracture faces. Additionally, analytical asymptotic solutions are used to enrich the fracture fronts, which increases the accuracy of the approximation. Stress intensity factors (SIF) with fluid pressure on fracture faces are extracted using the displacement correlation method. The methodology is verified with analytical solutions and compared with experimental results from the literature. Different wellbore and fracture configurations are investigated to demonstrate the non-intuitive propagation behavior in these near-wellbore conditions and the robustness of the proposed GFEM methodology. Gupta P., Duarte C. Coupled hydromechanical-fracture simulations of nonplanar three-dimensional hydraulic fracture propagation. International Journal for Numerical and Analytical Methods in Geomechanics 2018; 42(1): 143–180.

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Title: Advances in Automated Uncertainty Analysis for Model Calibration and Machine Learning

Author(s): *David Sheen, *Chemical Sciences Division, National Institute of Standards and Technology*;

Machine learning (ML), which in general refers to the calibration of mathematical models using experimental data, has enabled tremendous advances in computational science. For instance, calibrating models against the MNIST digital handwriting database has resulted in important advances in digital character recognition. However, models developed from (ML) are often treated as a black box, where data goes in and predictions come out. Very little concern is given to the uncertainty in the predictions of these models, which is another way of saying that little concern is given to their reliability. This becomes of critical concern when dealing with questions of systems safety and forensics. For instance, the admissibility of evidence generated by ML models is an unresolved question, and the central issue is whether life-and-death decisions can turn on the result of a model that no one understands. Knowing the uncertainty in a model's predictions allows for more robust assessments of the model's performance and can even provide some insight into its underlying behavior. Understanding and appreciation of uncertainty in models would be improved if modeling packages had a more transparent means of estimating uncertainty. Several computational methods have been developed to estimate uncertainty in ML models, including Bayesian uncertainty analysis and bootstrapping. Likewise, these algorithms have been implemented in various computer packages. In this talk, I will discuss existing uncertainty estimation codes, with focus on the strengths of their implementation and potential areas for improvement. I will focus on NIST's MUM-PCE as well as a machine-learning uncertainty package under development at NIST, although the conclusions that I draw will be broadly applicable to most uncertainty analysis packages. In general, although uncertainty analysis codes serve well at implementing the uncertainty analysis algorithms, they are still mostly written for uncertainty experts rather than users of common simulation packages.

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Title: Wavelet Transformation-based Multi-Time Scale (WATMUS) Modeling of Microstructure Informed Plastic Deformation under Cyclic Loading

Author(s): *Jinlei Shen, *Johns Hopkins University*; Somnath Ghosh, *Johns Hopkins University*;

Fatigue analysis for metallic materials typically involves finite element simulations of thousands of cycles, depending on the material and loading condition. Modeling cyclic deformation, especially for large number of cycles, and evolving plasticity-based internal variables using conventional time integration scheme, however, can be computationally expensive. In single time scale simulation, each cycle is discretized into a number of time steps, over which integration is performed. For rate-dependent plasticity model, a high resolution of time steps is typically required for each cycle throughout the loading process, leading to demanding computational efforts. To meet this computational challenge, a novel wavelet transformation-based multi-time scale (WATMUS) was developed [1] to accelerate crystal plasticity finite element simulations for large number of dwell loading cycles. The wavelet decomposition naturally retains the high frequency response through the wavelet basis functions and transforms the low frequency material response into a cycle scale problem undergoing monotonic evolution. In this work, the WATMUS algorithm is extended to implement for macroscopic scale simulations. Specifically, the WATMUS is integrated with a parametrically homogenized continuum plasticity model (PHCM) to perform accelerated simulations under large number of loading cycles, which is important for fatigue life prediction of polycrystalline alloys at specimen level. The WATMUS is also advanced to be capable of adaptively handling the change of loading magnitude at some time during the loading process. The results demonstrate that WATMUS is significantly more efficient than single time scale method without compromising the accuracy. Reference: Chakraborty, Pritam, and Somnath Ghosh. "Accelerating cyclic plasticity simulations using an adaptive wavelet transformation based multitime scaling method." International Journal for Numerical Methods in Engineering 93.13 (2013): 1425-1454.

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Title: Application of Numerical Ductile Fracture Simulation in LBB Evaluation of Pressure Piping

Author(s): *Tao Shen, *Faculty of Mechanical Engineering and Mechanics, Ningbo University, Ningbo 315000, P. R. China*; Chang-Sung Seok, *Department of Mechanical Engineering, Sungkyunkwan University, Republic of Korea*;

The leak-before-break (LBB) concept is widely used to design the pressure piping systems, and the LBB evaluation requires considerable experimental work to obtain the fracture resistance curves of cracked pipes. Numerical ductile fracture simulation of cracked pipe can effectively limit the experimental work. However for practical application of ductile fracture FE simulation in large-scale pressure pipe, the effect of element size on the efficiency and accuracy of simulation should be considered. In this work, the stress modified fracture model is used to simulate the ductile fracture of through-wall cracked pipe. Both the effects of parameters in fracture model and element size are studied. The simulation results are compared to the LBB evaluation results based on the fracture resistance curves of full scale pipes, which shows that the efficiency and accuracy of ductile fracture simulation in LBB evaluation of pressure pipe can meet the design process requirement.

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Title: Parallel Particle-in-Cell Simulations on Unstructured Meshes

Author(s): *Mark Shephard, *Rensselaer Polytechnic Institute*; Eisung Yoon, *Ulsan National Institute of Science and Technology*; Gopakumar Perumpilly, *Rensselaer Polytechnic Institute*; Cameron Smith, *Rensselaer Polytechnic Institute*; Garrett Diamond, *Rensselaer Polytechnic Institute*; Onkar Sahni, *Rensselaer Polytechnic Institute*; William Tobin, *Rensselaer Polytechnic Institute*;

Particle-in-cell (PIC) methods are becoming more commonly applied to resolve fine scale physics in problems in which PDE based methods alone are not sufficient. In these simulations particle motion is dictated by fields that are solved for on the mesh, and the mesh fields are influenced by the values associated with the particles. Thus there is a strong coupling between the particle motion and mesh-based solution processes as the solution steps from an initial state to a final state. In many applications areas with complex geometries and/or highly varying and/or anisotropic fields, there is a desire to employ unstructured meshes for the field solutions. This talk will discuss recent efforts on the development of a set of tools to support massively parallel PIC simulations on fully unstructured meshes. Topics to be covered include: (i) The distributed mesh with full part overlaps that supports particle push operations with no communications while employing a memory efficient method to coordination needed particle migration during the gather/scatter operations executed during the field solve process, (ii) The element based particle data structures that support effective calculations on many core or GPU accelerated computer nodes. (iii) A fast dynamic load balancing procedure to account for changing particle distributions. The unstructured mesh tools for PIC simulations being developed are being used in the development of two fusion plasma physics codes. The first, XCG, is a gyrokinetics code is focused on the accurate modeling of the complex flow physics in the region of tokamak near the wall. The second, GITR, is an impurity transport code that models the interactions of wall materials with the plasma within the tokamak. An overview will be given of how the unstructured mesh tools for PIC simulations are being used within these codes and indicate the results obtained to date.

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Title: A Modeling Exploration of Ultraordnance Impacts on Concrete

Author(s): *Jesse Sherburn, *U.S. Army Engineer Research and Development Center*; Omar Flores, *U.S. Army Engineer Research and Development Center*; Z. Kyle Crosby, *U.S. Army Engineer Research and Development Center*; William Heard, *U.S. Army Engineer Research and Development Center*;

Concrete is the most-produced manmade material in the world and is typically an integral component of US military assets. These assets are designed to resist extreme impulsive loads such as those from blast or penetration. Conventional ordnance produces impacts on the order of 500 to 1,300 m/s [1] which has been studied for many decades involving concrete materials. One area that has received little study is in the area of ultraordnance impacts on concrete in which impact velocities exceed 1,300 m/s. In this regime, material strength becomes less of a factor in the overall impact and penetration process. Computational modeling of concrete materials in this regime has also seen little attention in the literature due to the dearth of relevant experimental data. Some recent work has shown that a number of numerical methods have the ability to model the higher pressures expected in this regime [2]. This study is meant to be an exploration of three different numerical methods' ability to model a sphere impacting a semi-infinite concrete target in the ultraordnance regime. Different methods such as the Eulerian finite volume method using the shock wave code CTH, the meshfree method known as the reproducing kernel particle method (RKPM), and the meshfree conversion method within the EPIC code will be exercised in this study. Multiple constitutive models in CTH, RKPM, and EPIC will be evaluated, and their results compared to each other in anticipation of future planned experiments. [1] Backman, M.E., and Goldsmith, W. 1978. The Mechanics of Penetration of Projectiles into Targets. International Journal of Engineering Science, 16:1-99. [2] Sherburn, J.A., and Heard, W.F. 2018. Modeling of Ultra-High Performance Concrete Flyer Plate Experiments. 13th World Congress on Computational Mechanics, July 22-27, 2018, New York, NY. * Permission to publish was granted by Director, Geotechnical and Structures Laboratory.

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Title: An Optimization-Based Approach for High-Order Accurate Discretization of Conservation Laws with Discontinuous Solutions

Author(s): Matthew Zahr, *University of Notre Dame*; Per-Olof Persson, *University of California, Berkeley*; *Andrew Shi, *University of Notre Dame*;

We introduce a high-order accurate, nonlinearly stable numerical framework for solving steady conservation laws with discontinuous solution features such as shock waves [1]. The method falls into the category of a shock tracking or r-adaptive method and is based on the observation that numerical discretizations such as finite volume or discontinuous Galerkin methods that support discontinuities along element faces can perfectly represent discontinuities and provide appropriate stabilization through approximate Riemann solvers. The difficulty lies in aligning element faces with the unknown discontinuity. The proposed method recasts a discretized conservation law as a PDE-constrained optimization problem whose solution is a (curved) mesh that tracks the discontinuity and the solution of the discrete conservation law on this mesh. The discrete state vector and nodal positions of the high-order mesh are taken as optimization variables. The objective function is a discontinuity indicator that monotonically approaches a minimum as element faces approach the shock surface. The discretized conservation law on a parametrized domain defines the equality constraints for the optimization problem. A full space optimization solver is used to simultaneously converge the state vector and mesh to their optimal values. This ensures the solution of the discrete PDE is never required on meshes that are not aligned with discontinuities and improves nonlinear stability. The method is demonstrated on a number of one- and two-dimensional transonic and supersonic flow problems. In all cases, the framework tracks the discontinuity closely with curved mesh elements and provides accurate solutions on extremely coarse meshes. References: [1] M.J. Zahr and P.-O. Persson. An optimization-based approach for high-order accurate discretization of conservation laws with discontinuous solutions. Journal of Computational Physics, 365:105 – 134, 2018.

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Title: Application of the Generalized Finite Element Method for Computational Fluid Dynamics

Author(s): *Troy Shilt, *The Ohio State University*; Patrick O'Hara, *The Air Force Research Laboratory*; Rohit Deshmukh, *The Ohio State University*; Jack McNamara, *The Ohio State University*;

Despite advances in both computer hardware and numerical solution strategies, high-fidelity fluid simulations remain limited in scope. Thus, there is a continued motivation to improve both computational hardware and methods. Historically, Finite Difference Methods (FDM) and Finite Volume Methods (FVM) were preferred, where high-order schemes, motivated by the challenge to mitigate the computational burden of fine scale analysis, are now ubiquitous. Yet, the continued desire to broaden the scope of application of fine scale CFD analysis has invigorated interest in the Finite Element Method (FEM) as a means to enable multi-scale solution on relatively coarse, unstructured meshes. Application of FEM to fluid dynamics has long standing problems such as spurious oscillations in the advection term of the Navier-Stokes equations, instability in solution of the continuity equation for incompressible flows, capturing sharp gradients due to shocks in compressible flows, and multi-scaling to capture turbulence. The state-of-the-art of FEM for CFD enables analysis of fluid problems that contain these issues. However, we argue that the methods used represent workarounds to the above challenges. As an alternative, we are exploring application of the Generalized Finite Element Method (GFEM), with the goal to establish natural and elegant treatment of problems traditional FEM faces with numerical solutions of fluid dynamics. We will present current results of our work on GFEM applied to the 1D unsteady advection-diffusion equation and the 2D steady Stokes equations. The 1D unsteady advection-diffusion equation addresses the challenge associated with stability in finite-element based approaches arising from the advection term, where we demonstrate that the GFEM approach enables high-order, stable solutions at fewer degrees of freedom than typical FEM approaches. From the 2D steady Stokes equations, stability concerns arising from the continuity equation are also examined. Results demonstrate the ability of a GFEM approach to maintain stability given selection of particular enrichments, and its ease of developing stable, high-order methods when compared to alternative approaches: mixed finite element formulations and stabilized methods.

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Title: Combining In Vitro and In Silico Experiments for Data Driven Multiscale Analysis of Biological Systems

Author(s): *Vickie Shim, *University of Auckland*; Justin Fernandez, *University of Auckland*; Thor Besier, *University of Auckland*; Rod Barrett, *Griffith University*; David Lloyd, *Griffith University*; Mike Dragunow, *University of Auckland*; Shaofan Li, *UC Berkeley*;

Biological systems contain complex processes that involve a variety of spatial and temporal scales. In order to have a holistic understanding of many biological and diseases processes, multi-scale models that capture the relevant properties on all these scales are required. This challenge is being met by forming large consortia. One such example is the Physiome Project, which unites researches from all around the world [1]. The Physiome project demonstrated that multiscale models can deepen our insight on many important disease processes such as cardiac arrhythmia [2] and osteoarthritis [3]. Despite the demonstrated applicability of multi-scale models, however, we still lack important experimental results and computational methods for analyzing them. For example, great successes have been achieved by cellular network models in the past, but multi-cellular organisms and their microenvironments are more than a collection of pathways, and the physics-based models alone may not be able to capture their complexity. The recent development in data driven modelling, especially model reduction methods and surrogate modelling can be promising candidates for filling this need. But what we need is solid experimental data. We have developed a 3D dynamic cell mechanical device capable of applying in vivo like mechanical signals directly to cells [4] and measure their responses. The uniqueness of our approach lies in the close link it has with our model. The macro level models provided quantitative information on the mechanobiological environment of the cells during key daily activities or injurious situations. The cell mechanical device, on the other hand, generate abundant experimental data, from which we can build surrogate models of the cells under various mechanical and biochemical conditions. Then the physics-based macro level models are linked to the surrogate micro level models using our multi-scale framework. Specifically, the input-output coupling between macro level and micro level models is established to simulate the how the macro level stimuli are translated down to cell levels leading to various disease states. In this presentation, I will present the results of our recent works in two different disease processes – tendinopathy and brain concussion. [1] Hunter and Borg. Nat. Rev. Mol. Cell. Biol., (2003) 4(3):237-243 [2] Anuradha et al. European Heart Journal (2015)36 (35):2390-2401 [3] Shim et al. IEEE Trans Biomedical Engineering 58 (2011) 3532-3536 [4] Kim et al. ASME Journal of Biomechanical Engineering (2016) 138 (12) 121003

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Title: Data-driven Shape Functions for Higher-order Beam Finite Element Analysis of Thin-walled Composite Beams

Author(s): *Dongil Shin, *School of Mechanical and Aerospace Engineering, Seoul National University*; Yoon Young Kim, *School of Mechanical and Aerospace Engineering, Seoul National University*;

To analyze the complex behavior occurring in thin-walled beams using a one-dimensional beam analysis, it is critical to define accurately the cross-sectional shape deformation functions, such as warping or distortion. When it comes to composite thin-walled beams, the accurate definition of the functions becomes more critical because anisotropic and laminate effects produce more complicated deformation patterns. The purpose of this study is to analyze composite thin-walled beams by an advanced beam model that utilizes the shape functions identified by a data-driven approach. Here, we suggest a new method to find the shape functions, while the framework for the advanced beam model is based on the higher-order beam theory [1]. Our approach is to extract the shape functions through data processing and subsequent analysis. From the static analysis results of the composite thin-walled beam shell model [2], big data representing cross-sectional deformations were obtained and then the principal component analysis [3], a data-processing technique, was performed to identify the cross-sectional shape deformation functions. After the shape deformation functions were derived by the data-driven approach and the higher-order beam finite elements using the shape functions were formulated with them, static, vibrational and buckling analysis of thin-walled composite beams were conducted for the validation of the developed approach. The apparent advantage of this approach is that the shape functions can be derived without considering the ply orientations or stacking sequences, and also without any specific assumptions on the behavior of sectional deformations required in most existing studies. We demonstrate by numerical examples that the present data-driven results agree well with those obtained by full shell analysis results. It is expected that the proposed method can be critically applied to various problems where the identification of cross-sectional shape deformation functions is critically needed. Reference [1] D. Shin, S. Choi, G.-W. Jang, Y.Y. Kim, Higher-order beam theory for static and vibration analysis of composite thin-walled box beam, Composite Structures, 206 (2018) 140-154. [2] D. Simulia, ABAQUS 6.13 User’s manual, Dassault Systems, Providence, RI, (2013). [3] I. Jolliffe, Principal component analysis, in: International encyclopedia of statistical science, Springer, 2011, pp. 1094-1096.

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Title: Equilibrium Theory for a Lipid Bilayer with a Conforming Cytoskeletal Membrane

Author(s): *Milad Shirani, *Department of Mechanical Engineering, University of California, Berkeley, CA, US.*; David Steigmann, *Department of Mechanical Engineering, University of California, Berkeley, CA, US.*;

In this work, a simple mechanical nonlinear model for lipid bilayers considered as a fluid shell coated with an elastic solid membrane is proposed. To derive the model, it is assumed that the coating, as well as the lipid bilayer, behave as hyperelastic bodies along with their corresponding elastic energies. To enforce the constraints, Lagrange multipliers are introduced and physical interpretations for these multipliers are provided. Afterward variational methods are applied to obtain appropriate balance laws and boundary conditions. A simple problem is solved for the case where the lipid bilayer is coated with an isotropic elastic membrane.

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Title: Untangling High-order Curvilinear Triangular Meshes Via Signed Angles

Author(s): Mike Stees, *University of Kansas*; *Suzanne Shontz, *University of Kansas*;

High-order finite element methods are popular due to the additional accuracy which is obtained by increasing the polynomial degree of the basis functions associated with the mesh elements. To take full advantage of these high-order methods, a high-order mesh that conforms to the domain is required. The most popular approach to generating a high-order mesh is to increase the order of a linear mesh and then project the newly added boundary nodes onto the true boundary of the domain. This curving step has the potential to create tangled or highly distorted elements near the boundaries. As a result, some type of untangling or quality improvement pass is generally required to obtain a valid high-order mesh. In this talk, we will present a reformulation of our method for untangling high-order curvilinear triangular meshes [1]. Our current approach is a node-based optimization method for untangling high-order curvilinear meshes based on the signed angles of curvilinear triangles. For each high-order interior edge-node, the triangles which share the node are identified and the signed angles are computed. Positive angles indicate a valid patch, while negative angles indicate tangling in the patch. An optimization problem is then formulated to solve for the new locations of the high-order interior edge-nodes with the goal of ensuring positive angles. We will present several numerical examples in two dimensions which demonstrate the capabilities of our method for untangling triangular meshes. Future work will include extending the method to three dimensions. REFERENCES [1] M. Stees and S.M. Shontz (2018), An angular approach to untangling high-order curvilinear triangular meshes, Proc. of the 27th International Meshing Roundtable.

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Title: Coupled Thermomechanical Cohesive Element and Study of Material Properties of Nanocomposites

Author(s): *Wenya Shu, *Rice University*; Ilinca Stanciulescu, *Rice University*;

Nanocomposites materials have properties that are significantly improved over those of the base materials in which the nano particles are introduced. As a consequence, they are used in many applications, e.g., as electronic devices, packaging, automotive components, where well controlled thermomechanical properties are sought. In particular, the interface thermal resistance and interfacial debonding are believed to have great impact on the thermal and mechanical behaviors of nanocomposites. However, the effects of imperfect interfaces on the interacting thermal and mechanical properties of nanocomposites are insufficiently understood and require further study. A computational framework for the coupled thermomechanical simulation of interface separation and heat transport in nanocomposite materials will be presented in this talk. The numerical approach adopted is based on the framework of a cohesive zone model (CZM), with fully coupled interactions between load transfer and heat conduction incorporated into the model. The load transfer behavior is described by extending the thermodynamically consistent damage (bilinear) model [1] to account for the thermal degradation of the interface mechanical properties. The crack conductance consists of the conductance of solid-solid bond, air and contact and is coupled to the cohesive zone damage and interface contact pressure. Numerical examples are presented to demonstrate the predictive capabilities of the interface element. The element is then used to numerically study the thermomechanical properties of nanocomposites with imperfect interfaces, with focus on the mechanical and thermal properties of composites at elevated temperatures. For nanocomposites subjected to thermomechanical loading, the analysis will concentrate on examining the load transfer, conductivity and heat dissipation efficiency of composites with particular emphasis on interactions between heat transfer and separation at the interface. The study will also examine the effect of nanomaterial alignment and volume ratio on the thermomechanical properties of composites. [1] A. Turon, P.P. Camanho, J. Costa, C.G. Dvila, A damage model for the simulation of delamination in advanced composites under variable-mode loading. Mechanics of Materials. Mechanics of Materials Vol. 38 (11) pp. 1072-1089, 2006.

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Title: Calibration and Validation of a Thermal Model of Laser-Induced Melt Pools in SS 17-4PH

Author(s): *Yi Shu, *Stanford University*; Daniel Galles, *Oak Ridge Institute for Science and Education*; Nancy Yang, *Sandia National Laboratories*; Xiaohan Zhang, *Stanford University*; Wei Cai, *Stanford University*; Adrian Lew, *Stanford University*;

In Additive Manufacturing, microstructures and residual stress depend heavily on the thermal history of the material points and are essential to the mechanical properties of the printed parts. SS 17-4PH is a low carbon martensitic stainless steel which exhibits several phase changes when heated to different temperatures. We induce melt pools on SS 174-PH blocks by lasers with different power distributions and spot sizes along straight lines. The blocks are then sectioned and etched, showing several curved boundaries as results of phase changes. We then use a three-dimensional heat transfer model to reproduce such boundaries in simulations. The model considers both conductive and convective heat transfer, and as such, is based on solving the incompressible Navier-Stokes equations in the melt, and incorporating all material nonlinearities and Marangoni forces driving the flow. The parametric space of laser power and spot size is scanned to match the liquidus curve boundary identified in the section images. After the calibration of the parameters, the model is capable of reproducing the liquidus boundaries observed in the experimental samples. The other phase transformation temperatures are determined and compared to those obtained from quasi-equilibrium-state phase diagrams. We also contrast the model against one with only heat conduction, through sensitivity studies and a comparison of temperature fields and cooling rates. Key words: SS 17-4PH, Thermal Convection, Phase Transformation, Incompressible Navier-Stokes

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Title: Achieving Both Convenience and Performance in Matrix Assembly Using Trilinos

Author(s): Timothy Fuller, *Sandia National Laboratories*; Mark Hoemmen, *Sandia National Laboratories*; William McLendon III, *Sandia National Laboratories*; *Christopher Siefert, *Sandia National Laboratories*;

Many applications do not ghost sufficient information to do finite element assembly on non-owned elements, therefore data derived from the computed element stiffness matrices must be migrated as part of matrix assembly process. Historically, the Trilinos library has provided a convenience layer which allows for arbitrary off-rank insertion. However the performance of this layer was poor and it introduced a number of barriers to thread-parallelism. We present a new interface for matrix-assembly that we believe offers convenience for application programmers, while offering reasonable performance on next generation computing platforms. Computational results using MPI-everywhere and MPI+OpenMP to will be shown.

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Title: The Peridynamic Splice Method

Author(s): *Stewart Silling, *Sandia National Laboratories*;

The “splice” method was proposed several years ago as a way to couple subregions with different horizons in a peridynamic body [1]. In this method, material points near the coupling interface have two force states associated with them corresponding to the two values of the horizon. In computing the acceleration of a point near the interface, only the force states with the same value of horizon as that point are used. By a straightforward extension, the splice method can also be used as a technique for local-nonlocal coupling. Some results on the accuracy of the splice method were derived in [1], including ghost forces. The present talk reports on recent experience in implementing the splice method in the Emu code to achieve multiscale mechanics, grid refinement, and local-nonlocal coupling. Applications to practical problems in multiple dimensions are presented. [1] Silling S, Littlewood D, Seleson P. Variable horizon in a peridynamic medium. Journal of Mechanics of Materials and Structures 10 (2015) 591-612.

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Title: Topology Optimization of Labyrinth Seals

Author(s): Shahin Ranjbarzadeh, *University of Sao Paulo*; *Emilio Carlos Nelli Silva, *University of Sao Paulo*;

Uncontrolled CO2 and CH4 emissions can have a great influence on climate impacts. The emission occurs in a variety of ways; such as leakage from mechanical seals on compressors, turbines, and also from pneumatic devices, which are designed to vent gas as part of the operation. Studies show that the major emission sources are related to pneumatic devices/pumps and equipment leaks, accounting for approximately 60% of emissions. In the quest to reduce the climate effects caused by CO2 and CH4 emissions, the improvement of the Labyrinth Seals in multi-stage pumps, and compressors becomes a necessity. This paper discusses the Topology Optimization of Ionic Polymer-Metal Composite (IPMC) integrated Labyrinth Seal. Main advantages of IPMCs compared to conventional smart materials consist of large deformation, low voltage actuation, and low weight. Due to these characteristics, IPMCs are a promising candidate for manipulation of the fluid. The interaction of the IPMC with flow inside the Labyrinth Seals absorb their energy and release at an appropriate phase. A model is developed by coupling equations of governing IPMC deformation (chemo-electro-mechanical) and Navier-Stokes equation to describe IPMC-fluid interaction. This model implementation is based on commercial software COMSOL Multiphysics to allow us coupling a wide range of physics including the fluid-structure interaction (FSI) and the Topology Optimization. Then, a Topology Optimization Method consists of density method, fluid domain introduced by Borvall, Solid Isotropic Material with Penalization and Method of Moving Asymptotes (MMA) is coupled with chemo-electro-mechanical model and Navier-Stokes equations to simulate the behavior of the IPMC integrated Labyrinth Seals and to optimize the performance of the Labyrinth Seals leakage. Extending the topology optimization method to these physical domains generally involves some rethinking of the design problem to determine suitable design objectives. Post processed results e.g. Topology optimization design, fluid flow and pressure contour, etc. will be produced to employ in IPMC integrated labyrinth seal design. The results show the optimum design of Labyrinth Seals with minimum leakage.

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Title: Enrichment for GFEM in Composite Media

Author(s): Ivo Babuska, *University of Texas, Austin*; Robert Lipton, *Louisiana State University*; *Paul Sinz, *Michigan State University*; Michael Stuebner, *Global Engineering and Materials*;

We present a computationally efficient method for implementing domain decomposition for multiscale problems in composite media. Our approach is to use nearly optimal local bases functions within the Generalized Finite Element Method. Here optimality is measured in terms of the Kolomoragov n-width. In this talk we describe the new approach and provide new mathematically rigorous convergence rates. Several computational examples are provided. We demonstrate the how this method scales favorably with problem size.

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Title: Survey of Optimization Under Uncertainty Methods for a Multi-Objective Mechanical Analysis of a Composite Structure

Author(s): *Alyssa Skulborstad, *Sandia National Laboratories*; Stacy Nelson, *Sandia National Laboratories*;

Fiber reinforced composite structures lend themselves to tailored designs that take advantage of their directional properties. Variables such as fiber volume, ply thickness, ply orientation, and stacking sequence may be prescribed to meet specific performance criteria. In practice, structures must balance multiple, often conflicting, performance objectives. In this work, a composite cylinder design framework is analyzed for the optimization of two performance objectives under uncertainty. For example, uncertainties in composite simulations may occur due to uncertainties related to the fabrication process including ply orientation and thickness, or due to uncertainties in mechanical and thermal properties derived from experiments. The goal of this study is to compare the performance of three optimization under uncertainty (OUU) methods available within Sandia's Dakota toolkit. The uncertainty methods examined within the OUU framework include a Latin Hypercube sampling method, a form reliability method, and a stochastic expansion method. The multiple objective optimization problem is formulated with the Multi-Objective Genetic Algorithm (MOGA), where ply orientation of the three composite layers are optimized for the two objectives while also subject to uncertainty due to fabrication processes. One of the objective terms is to minimize the max principal stress that results from the composite curing cycle due to different thermal properties for the composite constituents. The other objective terms is to maximize the fundamental frequency of the composite structure. The relative computational cost and uncertainty statistics are assessed for each of the methods and conclusions are drawn regarding the best OUU approach to employ for future optimization studies.

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Title: Estimating Pressure Dependent Outflow Facility for the Human Eye

Author(s): *David Smith, *University of Western Australia*; Bruce Gardiner, *Murdoch University*;

Estimating parameters controlling intraocular pressure is important for identifying possible causes of elevated intraocular pressure, the primary risk factor for glaucoma (glaucoma is the leading causes of irreversible blindness in the world today). Consequently there is great interest in estimating the 'outflow facility' of the eye. Based on the fundamental physiology of fluid flow across membranes and using a new, unambiguous notation, we develop a new pressure-dependent outflow model for the human eye. We conservatively estimate the total pressure dependent fluid outflow rate in apparently normal, aged adults to be about 6.0 microlitres/min, and the average outflow facility is around 0.55 microlitres/mm Hg. This estimated pressure dependent outflow is more twice as large as usual estimates of total aqueous outflow through the anterior chamber (i.e. 2.5 microlitres/min). The analysis finds a substantial fraction (around half) of aqueous fluid production in the eye exits through the choroidal vasculature via the retinal pigmented epithelium (RPE) at the back of the eye. We explain that this RPE flow is consistent with the known experimental evidence of the retinal-choroidal interface. We show the new pressure-dependent outflow model can, for the first time, explain eye pressure elevation upon the introduction of a silicone oil tamponade into the vitreous chamber. We also explain how for certain parameter combinations the intraocular pressure may become unstable. This may help explain the origin and significance of this independent risk factor for glaucoma. Finally we explain the relationship between traditional measures of outflow facility, and the outflow facility predicted by the new pressure-dependent outflow model. Smith, D.W., and Gardiner, B.S. (2017). Estimating outflow facility through pressure dependent pathways of the human eye. PLOS ONE https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0188769

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Title: Efficient Multi-Linear Elastic-Plastic Model Calibration for Accurate Reduced-Order Fastener Models

Author(s): Peter Grimmer, *Sandia National Labs--Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.*; John Mersch, *Sandia National Labs--Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.*; *Jeffrey Smith, *Sandia National Labs--Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.*;

Finite element analysts often need to calibrate material models to experiments. One of the key things that needs to be calibrated for many plasticity models is the hardening curve defining how the equivalent stress evolves with increasing equivalent plastic strain. For a uniaxial tension test, the hardening curve can be directly obtained from the test data up until the specimen necks; after this point the stresses and strains become nonuniform and a direct relationship between load vs displacement, and effective stress and strain cannot be assumed. This issue is commonly resolved by solving an inverse problem where a finite element model of the test is repeatedly simulated while iterating its hardening curve until satisfactory agreement is found between the simulated and tested load vs displacement curves. The final result is a hardening curve that enables the analysis model to reproduce the experimental load-displacement response, and this calibrated model is typically extended to more complicated loading than the original tension test. Conventional multivariate optimization routines calibrate analytical hardening curves (e.g., power law hardening) to test data, defining the cost function as the total error between the loading history of the test and the simulation. It is impractical to calibrate an MLEP curve with a large number of separate points with more traditional optimization methods as the number of design variables (e.g., each individual effective stress value) becomes very large. Moreover, the sensitivity of the cost function to each individual design variable is low, in contrast to using a hardening curve that's defined by an analytic function where each parameter has a direct influence on the entire load-displacement response. An alternative approach developed at Sandia National Labs (described on page 18 in Ref. [1]) utilizes the history dependence of how plasticity evolves in a test specimen subjected to monotonic boundary conditions. Instead of running the entire model each iteration, we use an incremental approach in which small portions of the load-displacement are individually simulated so that corresponding portions of the hardening curve can be optimized. This allows the experimental load vs displacement response to be matched very closely. We modified the previously developed tool to be used for more general models beyond uniaxial tension; here we present the results of utilizing the method to generate accurate reduced-order nonlinear fastener models, calibrated to fastener tension tests. [1] G. Wellman, "A simple approach to modeling ductile fracture," Sandia National Laboratory, Albuquerque, NM, SAND2012-1343, 2012.

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Title: Advanced Computational Framework for the Automated Image-Based Modeling of Composite Materials

Author(s): *Soheil Soghrati, *The Ohio State University*; Anand Nagarajan, *The Ohio State University*; Ming Yang, *The Ohio State University*; Bowen Liang, *The Ohio State University*; Hossein Ahmadian, *The Ohio State University*;

We present an integrated computational framework relying on a novel virtual microstructure reconstruction algorithm and a new parallel non-iterative mesh generation technique for creating high fidelity finite element (FE) models and simulating the failure response of composite materials. A NURBS-based reconstruction algorithm is introduced to synthesize the material microstructure by packing arbitrary shaped particles, morphologies of which are extracted from digital data such as scanning electron microscopy (SEM) and micro-computed tomography images. A genetic algorithm (GA) based optimization phase is then employed to replicate target statistical microstructural descriptors. The FE model is then generated using a meshing algorithm named Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) algorithm, which transforms an initial structured mesh into a high-quality conforming mesh. CISAMR can handle problems with highly intricate geometries, including material interfaces with sharp edges/corners and pre-existing cracks. The parallel implementation of CISAMR is also introduced, which is capable of generating meshes with hundreds of millions elements while achieving a super-linear speedup. We show the application of the computational framework built by integrating these reconstruction/meshing algorithms for simulating the micromechanical behavior and damage process in various materials systems, including fiber reinforced/particulate composites, and lithium ion battery electrodes. Some of these problems involves highly nonlinear simulations, involving continuum damage and cohesive-contact models.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Fluid-Structure Interaction for Large Scale Assemblies

Author(s): *Jerome Solberg, *LLNL*;

Heat exchangers are often composed of thousands of tubes composed in arrays with stochastic design variables as a result of tolerance stack-up and assembly variation, and may involve many thousands of contacts, at specific points, along edges, and along surfaces. The analysis of the vibration characteristics of these structures by themselves is challenging, as a result of the contact- and friction-induced nonlinearities, the stochastic nature of the assembly, and the scale and number of components. In a heat exchanger these issues are further complicated by the presence of flowing fluid around and inside the tubes and in the gaps. Similar issues exist in the context of fabrics and composite structures. Starting with the work of Merzari, et. al. [1], and inspired in part by the work of Hassan [2] and Pettigrew [3], we apply a combination of methods, including verification via two-way-coupled FSI on representative subassemblies and one-way-coupled FSI via similarity methods, PSD's, and simulation-tuned empirical models, to analyze representative large-scale engineering heat exchangers and related structures. [1] E. Merzari, H. Yuan, A. Kraus, A. Obabko, P. Fischer, J. Solberg, S. Lee, J. Lai, M. Delgado & Y. Hassan "High-Fidelity Simulation of Flow-Induced Vibrations in Helical Steam Generators for Small Modular Reactors", Nuclear Technology, 205:1-2, 33-47 (2019). [2] Hassan, M. Gerber, A. and Omar, H., "Numerical Estimation of Fluidelastic Instability in Tube Arrays", J. Pressure Vessel Technol 132(4), 041307 (Jul 29, 2010). [3] Pettigrew, M.J., and Taylor, C. E., 'Vibration analysis of shell-and-tube heat exchangers: an overview—Part 1: flow, damping, fluidelastic instability", Journal of Fluids and Structures Volume 18, Issue 5, Pages 469-483 (November 2003).

15th U.S. National Congress on Computational Mechanics
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Title: The Shifted Boundary Method: A New Approach to Embedded Domain Computations of Waves and Shallow Water Flows

Author(s): *Ting Song, *Duke University*; Alex Main, *Duke Univerisity*; Guglielmo Scovazzi, *Duke University*; Mario Ricchiuto, *INRIA Bordeaux--Sud-Ouest*;

We present a new embedded boundary method for wave equation problems in time domain. Embedded boundary methods obviate the need for continual re-meshing in many applications involving rapid prototyping and design. Unfortunately, many finite element embedded boundary methods for incompressible flow are also difficult to implement due to the need to perform complex cell cutting operations at boundaries, and the consequences that these operations may have on the overall conditioning of the ensuing algebraic problems. We present a new, stable, and simple embedded boundary method, which we call “shifted boundary method” (SBM), that eliminates the need to perform cell cutting. Boundary conditions are imposed on a surrogate discrete boundary, lying on the interior of the true boundary interface. We then construct appropriate field extension operators, with the purpose of preserving accuracy when imposing the boundary conditions. We demonstrate the performance of the proposed method in simulations of problems in acoustics and shallow water flows.

15th U.S. National Congress on Computational Mechanics
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Title: 3D Image Based Inspection and Simulation Applied to Additive Manufactured Spinal Truss Medical Implants

Author(s): Kerim Genc, *Synopsys Inc.*; Ali Kiapour, *4Web Medical*; Herminso Villarraga-Gómez, *Nikon Metrology Inc.*; Patrick Tompsett, *Synopsys Inc.*; David Milner, *Thornton Tomasetti*; Yunjie Wang, *Thornton Tomasetti*; Philippe Young, *University of Exeter*; *Thomas Spirka, *Synopsys Inc.*;

Spinal fixation is currently a standard of care for patients suffering from traumatic and chronic injuries that lead to reduced mobility and increased pain in the back, neck, and limbs. New manufacturing technologies such as additive manufacturing (AM) are becoming more popular in the production of orthopedic devices, such as spinal fixation devices, due to inherent benefits that include a potentially larger set of mechanical design options that are enabled by the production of parts derived directly from the part-design without dedicated tooling. 4WEB Medical's proprietary Truss Implant Technology™ is one such example. The U.S. Food and Drug Administration (FDA) approved titanium additive manufactured Truss Implant Technology™, which leverages a mechanobiologic mechanism inherent to its truss design that could stimulate an osteogenic response to facilitate fusion in the spine and provide joint stability during the healing, or fusion, process. Despite the popularity and proven clinical significance of AM truss implants, many questions in terms of accuracy, quality, strength, and reliability of AM parts remain still relatively unanswered and therefore challenge manufacturers of medical devices. These challenges lead manufacturers to ask the following question: "What are the differences between my design and the part that is actually manufactured and how will these differences affect performance in reality?" Today, manufacturing companies typically rely on 3D imaging techniques such as industrial computed tomography (CT) for inspection and reverse engineering of AM parts. From the CT scan data, users can typically quantify porosity, crack/defect size, and dimensional deviations in geometry when compared to reference/nominal design. However, this information, in and of itself, does not necessarily convey how these defects and deviations may affect the AM parts' functional performance in real-world applications. We will describe a proof-of-concept workflow intended to better understand the functional differences between as-designed and as-built AM truss implants. The workflow begins with CT imaging of the manufactured part, followed by 3D image-based measurements, and finite element (FE) simulations.. We will then compare these results with the computer-aided design (CAD) model, i.e., the base design, through geometric analyses, simulations, and physical test results. This workflow allows users to close the design loop, better understand how defects (e.g., porosity, cracks, delamination etc.) as well as dimensional deviations in the manufactured parts may affect the performance of AM devices, particularly in medicine, and potentially adjust the additive manufacturing process or the design itself to minimize functional differences.

15th U.S. National Congress on Computational Mechanics
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Title: Behavior of Frustrated Antiferrmagnets in Random Field

Author(s): *Siddhartha Srivastava, *University of Michigan*; Aaditya Lakshmanan, *University of Michigan*; Veera Sundararaghavan, *University of Michigan*;

Geometrically frustrated magnetic systems open up the possibility to have unconventional magnetic order or even novel spin liquid states without any long-range spin order at low temperatures. These are systems in which all the spin interactions cannot be simultaneously satisfied because of the connectivity of the lattice. From the point of view of real crystalline materials, there are many examples in which the magnetic ions are arranged on non-bipartite lattices based on triangular units like the 2-dimensional Triangular and Kagome, and the 3-dimensional pyrochlore lattices [1]. They have been the object of many theoretical and experimental studies for several decades now with a plethora of models dedicated to understanding the behavior of these magnetic materials. Critical properties associated with classical and quantum phase transitions have been successfully described via simple nearest neighbor interaction models. However, it has been long believed that the experimental realization of these systems may harbor some randomness in the ideal parameters. This randomness often presents itself as an aleatoric uncertainty in the applied magnetic field [2], the behavior of which becomes increasingly relevant at lower temperatures. In this talk, we will present the statistical behavior of the Ising model on these frustrated lattices in the presence of a spatially uncorrelated magnetic field at low temperature. We model the noise in the applied field as a Gaussian distribution. We show that an increase in the standard deviation of this distribution leads to a more paramagnetic nature of sampled spins. The behavior is characterized using the absolute magnetization and the expected neighboring spins. The computations for estimating minimal energy states are performed using a physical quantum annealing processor (c.f [3]). The advantage of this system is that it directly simulates the transverse-field Ising model and allows direct sampling of ground states in the desired lattice. We conclude by presenting how uncertainties in applied field propagate forward in the Ising model. References [1] Sen, Arnab, et al. "Triangular and kagome antiferromagnets with a strong easy-axis anisotropy." Physical review letters 102.22 (2009): 227001. [2] Pastor, A. A., V. Dobrosavljevi?, and M. L. Horbach. "Mean-field glassy phase of the random-field Ising model." Physical Review B 66.1 (2002): 014413. [3] King, Andrew D., et al. "Observation of topological phenomena in a programmable lattice of 1,800 qubits." Nature 560.7719 (2018): 456.

15th U.S. National Congress on Computational Mechanics
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Title: Guaranteed Element Quality Overlay Tetrahedral Mesh Generation with CAD Feature Capture

Author(s): *Matthew Staten, *Sandia National Laboratories*; David Noble, *Sandia National Laboratories*; Corey McBride, *Elemental Technologies*; C. Riley Wilson, *Sandia National Laboratories*;

Many variations of overlay grid approaches to tetrahedral mesh generation have been published [1]. They are particularly popular with level set data to capture iso-surface type geometries. However, difficulties using overlay grid approaches to mesh CAD models are documented in literature due to difficulties capturing the CAD curves and vertices without sacrificing element quality. We present a new approach to overlay grid tetrahedral mesh generation with element quality guarantees and captures most CAD surface, curves and vertices. Overlay grid approaches start from an overlay grid with excellent quality, followed by either snapping overlay nodes, or cutting overlay cells to geometry intersections. Our design principle is capture as much geometry as possible without sacrificing element quality. We accomplish this design principle with snapping only (i.e. no element cutting) by iterating between first, moving overlay grid nodes towards their target locations on CAD features but only to the point of maintaining a user specified element quality threshold, and second, tetrahedral topology changes to improve the quality of tetrahedra in the neighbor of the moving nodes, which will enable nodes to move closer to their targets in subsequent iterations. While there is no guarantee that all nodes will ever reach their target locations, in practice, greater than 99.9% of overlay nodes do reach their targets. This guarantees the resulting element quality at the expense of geometry capture. The higher the requested guaranteed element quality, the lower the geometric fidelity and vice versa. We couple this guaranteed element quality with the target location identification described by Staten et. al. [2] to capture CAD features with tetrahedral meshes in distributed memory parallel. Updates on the latest progress of this approach will be presented. [1] F. Labelle, J. R. Shewchuk. ”Isosurface Stuffing: Fast Tetrahedral Meshes with Good Dihedral Angles.” ACM Transactions on Graphics, 26(3):57.1-57.10, July 2007. Special issue on Proceedings of SIGGRAPH 2007. [2] M. L. Staten, D. R. Noble, C. R. Wilson, C. L. McBride, M. K. Bhardwaj. “Massively Parallel Tet Meshing With Size-Dependent Feature Capture on CAD Models, Proceedings 27th International Meshing Roundtable, 2018. *Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

15th U.S. National Congress on Computational Mechanics
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Title: Experimental Validation of Residual Stress Predictions for LENS 304L Stainless Steel

Author(s): *Michael Stender, *Sandia National Laboratories*; Lauren Beghini, *Sandia National Laboratories*; Michael Veilleux, *Sandia National Laboratories*; Christopher San Marchi, *Sandia National Laboratories*; Michael Hill, *University of California, Davis*; Christopher D'Elia, *University of California, Davis*;

This talk will discuss the validation of a part-scale multi-physics model of metal additive manufacturing with experimental measurements residual stresses. Validation is an essential element in the deployment of modeling methodologies and will enable higher confidence predictions for future modeling efforts. Experimental builds and simulations are based on the Laser Engineered Net Shaping (LENS®) process; a subclass of directed energy deposition (DED) additive manufacturing. LENS involves a continuous spray of metal power aimed into the focal point of a laser that melts the incoming metal powder. To help elucidate the nature of residual stresses, a thermal-mechanical Lagrangian finite element workflow is used to model the LENS deposition process throughout the history of a build. In this study, two different geometries; a wall and a hollow cylinder made from 304 L stainless steel were built and simulated. Inherent to the LENS process with 304L stainless steel, are spatially varying residual stresses with magnitudes often on the order of the material yield strength. Such high stresses can affect mechanical performance and are an essential design consideration motivating the capability to accurately predict residual stresses. Simulation predictions of residual stresses are compared to experimental residual stress measurements, using several residual stress measurement techniques, for critical areas of the LENS build including the part/baseplate interface. Differences between experimental measurements and model predictions will be discussed, and uncertainty quantification of critical model parameters will also be explored. This work will help to develop a validated method for the prediction of residual stresses for LENS build parts intended for critical high consequences engineering environments. *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

15th U.S. National Congress on Computational Mechanics
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Title: Dakota: What's New?

Author(s): *John Stephens, *Sandia National Laboratories*; Brian Adams, *Sandia National Laboratories*; Gianluca Geraci, *Sandia National Laboratories*;

The Dakota software package is a widely-used collection of tools for performing optimization, sensitivity analysis, uncertainty quantification, and model calibration on black box computational simulations. Begun as an internal research project at Sandia National Labs almost 25 years ago, we estimate it now has thousands of users worldwide in academia, government, and industry. This talk is a brief introduction to and review of Dakota's history and capabilities. Special attention is given to recent developments in algorithms and usability, such as Dakota's new graphical interface, multilevel/multifidelity sampling methods, and HDF5 output.

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Title: Advances in Quasistatic and Dynamic Phase-Field Implementation for Ductile Failure in SIERRA

Author(s): *Andrew Stershic, *Sandia National Laboratories*; Jakob Ostien, *Sandia National Laboratories*; Brandon Talamini, *Sandia National Laboratories*; Michael Tupek, *Sandia National Laboratories*;

Computational modeling of the fracture and failure of ductile metals remains a challenging problem in mechanical engineering. This problem is relevant to diverse applications, such as metal cutting processes and ballistic impacts on metals. While continuum damage models have long been applied to model this problem, an area of rapid development within the computational fracture community is phase-field modeling. By introducing a regularization length scale, the phase-field approach motivates damage growth through a continuum approximation of a discrete crack in a way that alleviates the spurious strain localization endemic to damage models in the softening regime. Only recently has the phase-field approach been applied to characterize ductile failure. In this work, we introduce a novel approach to ductile phase-field fracture modeling which is implemented in a scalable multi-physics finite element code, SIERRA. This model has been developed in a way that is inherently consistent with finite deformation mechanics and is modular with regard to the hardening component of the plastic constitutive model. We first provide an over-view of the mathematical and implementational aspects of this ductile phase-field model in SIERRA. We then discuss the implementation of explicit time integration of the model for dynamic simulations and the advantages and drawbacks thereof. Next, we provide a model validation study using experimental fracture data on 6061-T651 aluminum collected at Sandia National Laboratories. Lastly, we will discuss future directions of this work. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

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Title: Adjoint Analysis Tools in the libMesh Finite Element Library

Author(s): *Roy Stogner, *University of Texas at Austin*; Vikram Garg, *University of Texas at Austin*;

We discuss techniques for adjoint-based analyses of Boundary Value Problems using Galerkin and stabilized finite element formulations, along with the libMesh finite element library software patterns which have been developed to improve the ease of use of those techniques. Adjoint consistency is discussed for raw quantities of interest, but also for superconvergent quantity of interest calculations obtained via heterogenous adjoint boundary conditions or via stabilized QoI approximations, including a newly-devised approximation for use with variational multiscale formulations. Error estimation and error reduction via goal-oriented refinement are discussed, as are the corresponding software interfaces which libMesh makes available to users to abstract away some of the complexity of these operations and to make various tradeoffs between accuracy, computational expense, and code development time. Finally, parameter sensitivity operations are also discussed, including software abstractions developed for easier coupling to third-party physics codes.

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Title: Nondimensionalization and Adaptive Integration of a Semi-Analytic Heat Conduction Solution for Additive Manufacturing

Author(s): *Benjamin Stump, *ORNL-MSTD*;

Solidification dynamics affect the final microstructure of additively manufactured parts. Multi-physics models can help provide insight into how phenomena such as fluid flow, keyholing, and porosity affect the solidification dynamics but are unable to simulate actual builds due to computational expense. On the other hand, analytic and semi-analytic solutions for moving heat sources in an infinite domain are capable of efficiently predicting solidification conditions in regimes where keyholing and other phenomena are negligible. Though the rudimentary implementation of these solutions are thousands of times faster than multi-physics models, there is still substantial room for improvement. This presentation goes over utilizing the combination of several methods which build upon each other to make the integration of these solutions more generalized and provides substantial speedup for long length and time scales. Several applications of this solution for additive manufacturing are also reviewed.

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Title: Enriched Isogeometric Analysis on Stitched NURBS Patches

Author(s): Chun-Pei Chen, *Purdue University*; *Ganesh Subbarayan, *Purdue University*;

We propose a new form of approximation to perform isogeometric analysis on geometries “stitched” together using multiple NURBS patches. The concept of the proposed methodology is to use lower-dimensional NURBS entities with appropriate enrichment to “stitch” trimmed NURBS domains of a higher dimension. Specifically, we extend the previously developed enriched isogeometric analysis (EIGA) formulation in which the behavioral field is constructed to form partition of unity by a weighted composition of base approximation and boundary (or interfacial) approximation [1]. The neighborhood of the boundary is appropriately enriched based on the a priori knowledge of the local behavior. For instance, the stitching interface can be as simple as the boundary curve joining NURBS patches of identical material, or to couple NURBS patches of dissimilar materials that has discontinuous gradient of fields across the stitching boundary. The stitching naturally leads to “watertight” boundaries. The technique allows a complex domain to be composed by multiple trimmed NURBS patches with different discretization and/or distinct materials using a bottom-up Boolean compositional strategy. The proposed method leads to tight CAD-CAE integration by using the trimmed NURBS geometries directly imported from commercial CAD systems for analysis. Convergence studies and patch tests are performed, and several numerical examples of elatostatics problems are demonstrated to show the advantages of the proposed methodology. References: [1] A. Tambat and G. Subbarayan, “Isogeometric enriched field approximations,” Comput. Methods Appl. Mech. Eng., vol. 245, pp. 1–21, 2012.

15th U.S. National Congress on Computational Mechanics
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Title: Numerical Integration of Homogeneous Functions on Curved Geometries

Author(s): Eric B. Chin, *UC Davis*; *N. Sukumar, *UC Davis*;

Integration over curved geometries has become a growing need in many emerging computational methods such as the extended finite element method, embedded interface methods such as CutFEM [1], and the virtual element method [2]. In this talk, we present an extension of the homogeneous numerical integration (HNI) technique [3] to two-dimensional domains bounded by parametric curves such as rational and polynomial Bézier curves, NURBS curves, and cubic Hermite curves. The HNI method combines Euler's homogeneous function theorem and Stokes's theorem to reduce integration to the boundary of the geometry. In Chin et al. [3], regions of integration are limited to those bounded by affine edges, such as convex and nonconvex polygons, and by homogeneous algebraic curves, such as circular arcs. We establish that the HNI approach can be readily extended to regions bounded by arbitrary parameterized curves. This provides a means to efficiently and accurately integrate positively homogeneous functions on such geometries. Further, if the curved boundary is defined as a polynomial curve and the integrand is polynomial, the HNI method delivers exact integration with an appropriate Gauss quadrature rule. The benefits of the HNI approach for polygonal domains carry over to curved domains, namely eliminating the need for partitioning the domain and reducing the dimension of integration, which considerably reduces the number of cubature points required for accurate integration. We will present several numerical examples to highlight the capabilities of the HNI method for integrating curved geometries, and also discuss extensions to three- dimensional domains containing weakly singular integrands. REFERENCES [1] Burman E, Claus S, Hansbo P, Larson MG. CutFEM: Discretizing geometry and partial differential equations. Int J Numer Methods Eng 2015; 104(7): 472—501. [2] Beirão da Veiga L, Russo A, Vacca G. The Virtual Element Method with curved edges. ESAIM Math Model Numer Anal 2018; in press. [3] Chin EB, Lasserre JB, Sukumar N. Numerical integration of homogeneous functions on convex and nonconvex polygons and polyhedra. Comput Mech 2015; 56(6): 967—981.

15th U.S. National Congress on Computational Mechanics
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Title: Deep Learning Enabled Data-driven Discovery of Nonlinear Governing Laws

Author(s): Zhao Chen, *Northeastern University*; Yang (Emily) Liu, *Northeastern University*; *Hao Sun, *Northeastern University*;

Harnessing data to discover the governing equations and scientific laws of complex systems remains a critical challenge in many science and engineering areas. Although the explosive growth of data and advances in computation make possible to use AI algorithms (e.g., machine learning) for exploration of mathematical governing laws in a data-driven manner, intractable issues arise associated with the preparation of massive data for complex physical systems and the inevitable noise of acquired data. Thus, there is an urgent need to develop transformative AI techniques, grounded with available physics information, to address this discovery issue in the presence of scarce/sparse, noisy data. To this end, we develop an innovative, rigorous data analytic pipeline, within the framework of deep learning and based on sparse representation theory, for discovering nonlinear governing laws termed as a set of partial differential equations in a data driven manner. The parameterized governing equations will be encoded into the deep learning model through augmenting the loss function. Determination of the unknown parameters will rely on a sparsity representation which bypasses a brute-force large search over all possible candidate solutions. We will demonstrate the generalizability and scalability of the proposed approach on a wide range of physical systems with different complexities, under various scenarios of rich, scarce/sparse, and noisy data, including dynamical structural systems, fluid transport, chaotic dynamical systems, etc.

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Title: Bound-Preserving Algorithms for Fully Implicit Formulation of Multi-Phase Flow in Porous Media

Author(s): *Shuyu Sun, *King Abdullah University of Science and Technology (KAUST)*; Yiteng Li, *King Abdullah University of Science and Technology (KAUST)*;

Simulation of multiphase flow in porous media has been a major effort in many fields. For example, it assists petroleum engineers to manage existing petroleum fields and to develop new oil and gas reservoirs, while it helps environmental scientists to investigate and compare various schemes to inject and store CO2 in subsurface geological formations, such as depleted reservoirs and deep saline aquifers. One basic requirement for accurate and robust modeling and simulation of multiphase flow is to have the predicted physical quantities sit within a physically meaningful range. For example, the predicated saturation should sit between 0 and 1 in immiscible multiphase flow models. Unfortunately, popular simulation methods used in petroleum industries do not preserve physical bounds. Bound violation may crash the simulator, as saturations are often applied to a function involving logarithm in order to get the capillary pressure. A commonly used fix in industry to this problem is to simply apply a cut-off operator. However, this cut-off practice does not only destroy the local mass conservation but it also damages the global mass conservation, which seriously ruins the numerical accuracy and physical interpretability of the simulation results. In the talk, we will present our recent work on bound-preserving discretization and solvers for subsurface flow models based on a fully implicit framework. We reformulated subsurface multiphase flow using variational inequalities that naturally ensure the physical feasibility of the physical quantities including saturations (and concentrations if modeling composition). We applied a mixed finite element method and the implicit backward Euler scheme with adaptive time stepping. The resultant nonlinear system arising at each time step was then solved by a generalized Newton method, i.e., active-set reduced-space method, and then the ill-conditioned linear Jacobian systems were solved with a Krylov subspace method combined with a nonlinear preconditioner based on overlapping additive Schwarz type domain decomposition and nonlinear elimination. Numerical results will be presented to examine the performance of the newly developed algorithm on parallel computers. This presentation is partially based on the joint work [1-3] with Haijian Yang (Hunan University), Chao Yang (Beijing University), and Yiteng Li (KAUST). [1] H. Yang, S. Sun, Y. Li, and C. Yang, Computer Methods in Applied Mechanics and Engineering, 330: 334-350, 2018. [2] Yang, S. Sun, and C. Yang, Journal of Computational Physics, 332: 1-20, 2017. [3] H. Yang, C. Yang, and S. Sun, SIAM Journal on Scientific Computing, 38(4): B593–B618, 2016.

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Title: A Cooperative Two-player Game for Data-driven Discovery of Elasto-plasticity Knowledge Represented in Directed Graph

Author(s): Kun Wang, *Columbia University*; *WaiChing Sun, *Columbia University*; Qiang Du, *Columbia University*;

We introduce a multi-agent meta-modeling game to generate data, knowledge, and models that make predictions on constitutive responses of elasto-plastic materials. We introduce a new concept from graph theory where a modeler agent is tasked with evaluating all the modeling options recast as a directed multigraph and find the optimal path that links the source of the directed graph (e.g. strain history) to the target (e.g. stress) measured by an objective function. Meanwhile, the data agent, which is tasked with generating data from real or virtual experiments (e.g. molecular dynamics, discrete element simulations), interacts with the modeling agent sequentially and uses reinforcement learning to design new experiments to optimize the prediction capacity. Consequently, this treatment enables us to emulate an idealized scientific collaboration as selections of the optimal choices in a decision tree search done automatically via deep reinforcement learning.

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Title: New Approaches in Modeling Belt-flesh-pelvis Interaction Using Obese GHBMC Models

Author(s): *Zhaonan Sun, *University of Virginia Center for Applied Biomechanics*; Bronislaw Gepner, *University of Virginia Center for Applied Biomechanics*; Jason Kerrigan, *University of Virginia Center for Applied Biomechanics*;

Obesity is associated with higher fatality risk and altered distribution of occupant injuries in automotive collisions. This is partially because of the substantial effect that obesity has on occupant-restraint interaction. Restraining obese occupants becomes a challenge due to their higher body mass, unfavorable belt placement, and larger forward excursion within the occupant compartment. An increased depth of abdominal soft tissue, results in delayed and limited engagement of the lap belt with the pelvis and increases the risk of pelvis “submarining” under lap belt, exposing occupant’s abdomen to belt loading. Previous modeling studies have shown that pelvis submarining could not be replicated using existing obese human body models (HBMs) (Gepner, 2018). This study aims to explore a new numerical approach to modeling adipose tissue that has the potential of facilitating large tissue deformation observed during submarining. HBM simulations were performed using one of the available obese GHBMC models (Hu, 2012), following the belt pull tests described by Kim et al. (2015). Several models with varied tissue parameters were used in this study. First, several material models and mesh formulations of adipose tissue were investigated. Second, pelvis to flesh connectivity was redefined, and sliding contact was implemented to facilitate large tissue deformations. Third, a smooth particle galerkin (SPG) meshless method was used to model the adipose tissue. Regardless of force input, adipose tissue material model, and mesh quality, the original model failed to replicate large shear deformation kinematics observed in the experiment. Although similar overall kinematics can be replicated by implementing a sliding contact between the pelvic bone and the abdominal adipose tissue, deformation was facilitated by relative motion between the flesh and pelvis instead of adipose tissue shearing. SPG meshless method gave promising results by enabling large deformation within the abdominal flesh, replicating the observed submarining kinematics. This is the first study proposing model modifications on the obese GHBMC model to replicate submarining kinematics observed in the belt pull experiments. This study used a novel SPG method to model soft tissue in large shear deformation, which paves the way for its application in robust tissue modeling. Reference: Kim, T. et al. (2015). Abdominal Characterization Test Under Lap Belt Loading. ESV Hu, J. et al. (2017). UMTRI Morphed Human Models Based on GHBMC M50?O v4.4. Gepner, B. et al. (2018). Performance of the Obese GHBMC Models in the Sled and Belt Pull Test Conditions. IRCOBI

15th U.S. National Congress on Computational Mechanics
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Title: The End-Point Path Design of the Structural Motion using the Bending Behavior of a Photo-Responsive-Polymer

Author(s): *Heejun Sung, *Seoul National University*; Hongseok Kim, *Seoul National University*; Hyunsu Kim, *Seoul National University*; Maenghyo Cho, *Seoul National University*;

In this paper, we focus on overcoming the limitations of the basic behavior of self-deforming structures through structural design. It is widely known that azobenzene-added liquid crystal polymers react with UV light. Typical photo-reactive self-deforming structures have non-contact bending behavior based on their position when the light of a specific wavelength is irradiated. In repeated bending behavior, it is difficult to return to the initial state after avoiding obstacles or rotating motion because it moves periodically in the same path. In this study, we designed the motion that could not be designed on the existing bending behavior by attaching the joint part to the photo-responsive-polymer structure. In the first experiment, the photo-reactor was designed to continuously rotate the gear structure through the introduced bending behavior. Typical bending movements push the gear back in the opposite direction when returning the reactor back to its original position, which makes it difficult to move the gear in a certain direction. In this study, the bending behaviors of the upper and lower parts of the photo-responsive-polymer structures were independently moved around the joint, so that when the tooth was rotated, the lower bending was used. When returning to the original position, so that it can be returned to its initial position without making a contact to the teeth of the gear and push the next teeth of the gear in the same direction. In the second experiment, the same principle as the first experiment was applied to a soft-robot walking mechanism and implemented the continuous walking using the bending behavior through the joint structures. All the behaviors were constructed and verified through experiments. It is expected that a more diverse behavior can be designed by continuous research on the photo-responsive-polymer structures.

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Title: Thermodynamic Consistency of Beam Mathematical Models in the context of Classical and Non-classical Continuum Mechanics and a Thermodynamically Consistent New Formulation

Author(s): *Karan Surana, *University of Kansas*; Dhaval Mysore, *University of Kansas*; J. N. Reddy, *Texas A&M University*;

In order to enhance currently used beam theories in R2 and R3 to include mechanisms of dissipation and memory, it is necessary to establish if the mathematical models for these theories can be derived using the conservation and the balance laws of continuum mechanics in conjunction with the corresponding kinematic assumptions. This is referred to as thermodynamic consistency of the beam mathematical models. Thermodynamic consistency of the currently used beam models will permit use of entropy inequality to establish constitutive theories in the presence of dissipation and memory mechanism in the currently used beam theories. This is the main motivation for the work presented in this paper. The currently used beam theories are derived based on kinematic assumptions related to the axial and transverse displacement fields. Using stress and strain measures, energy functional is constructed over the volume of the beam consisting of kinetic energy, strain energy and potential energy of loads. The Euler's equation(s) extracted from the first variation of this energy functional set to zero yields the differential equations describing the evolution of the deforming beam. Alternatively, principle of virtual work can also be used to derive mathematical models for beams. For linear elastic behavior with small deformation and small strain the two approaches yield same mathematical models. In this paper we examine whether the currently used beam mathematical models can be derived using the conservation and balance laws of classical continuum mechanics or non-classical continuum mechanics to ensure that the mathematical models so derived ensure thermodynamic equilibrium. Currently used Euler-Bernoulli and Timoshenko beam mathematical models that are representative of most beam mathematical models are investigated. This is followed by details of general and higher order thermodynamically consistent beam theory that is free of kinematic assumptions and other approximations and remains valid for slender as well as deep beams. Model problem studies are presented for slender as well as deep beams. The new formulation presented in this paper ensures thermodynamic equilibrium as it is derived using the conservation and the balance laws of continuum mechanics and remains valid for slender as well as non-slender beams.

15th U.S. National Congress on Computational Mechanics
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Title: Tunable Architected Materials Using Topology Optimization

Author(s): S. M. Tareq Zobaer, *The Ohio State University*; Zhi Zhang, *The Ohio State University*; Jaejong Park, *Prairie View A&M University*; *Alok Sutradhar, *The Ohio State University*;

Designing multi-functional structures with multi-material involves multiscale consideration. The structure in macro level needs to satisfy the space, functional, visual and load-transfer requirements. Additional considerations of stress-patterns and localized stress-concentrations to improve the effectiveness and functionality can be increased using architected materials in macro, meso and micro level structures. Topology optimization is a numerical tool that is suitable for obtaining optimized geometries under several constraints. Earlier efforts used inverse homogenization technique to attain the microstructures of geometries. These equivalent material models would be more feasible when there is a significant dimensional difference between the large and the small scales. With recent advances, 3D printing of multiscale multi-material structures is realizable. We present an approach to design architected materials and structures, which can be tunable and tailor localized geometric and stress patterns. We develop a topology optimization framework to design the architecture materials in different scales, which can vary smoothly within the design domain. The preliminary study shows easy control in connectivity and provides more topological variability. The designs using the methodology in this work are 3D printed, and their performance is studied using mechanical testing.

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Title: A Nonlinear SUPG Method for High-speed Compressible Flows

Author(s): *Yoshifumi Suzuki, *Altair Engineering, Inc.*;

In this paper we present a nonlinear streamline-upwind Petrov-Galerkin (SUPG) method for high-speed compressible flows. It is well known owning to Godunov's barrier theorem that a numerical method higher-than first-order requires nonlinearity in algorithm for capturing shock and contact discontinuity monotonically. However, the original SUPG method is a linear method, and later developed nonlinear discontinuity-capturing operators do not necessary guarantee monotonicity. In the new method, nonlinearity is introduced directly into the Petrov part of test function, making the method nonlinear and monotonicity preserving. At first, Fourier analysis is conducted to study the order of accuracy of the original Galerkin and SUPG methods with consistent or lumped mass matrix. It turns out that, for unsteady equations, adding the SUPG dissipation term is not sufficient to degrade the Galerkin method to first-order accurate which is necessary for monotonicity; mass lumping is also necessary to make the SUPG method to be truly first-order accurate. Once we establish the baseline first-order accurate SUPG method for shock and contact discontinuity capturing, we develop a nonlinear blending function to turn on or off the SUPG dissipation term where it is needed. If a solution is smooth, we do not need the dissipation term, and the original Galerkin discretization itself provides higher-order accurate results. A key is how to detect where the dissipation is needed. Here, we borrow the concept of nonlinear limiters originally developed in finite-volume community. In summary, the method compares a solution gradient in an element to its neighboring elements, and determines if the solution is in oscillations (sign changes) or not. If it is in oscillations, a limiter turns on and the SUPG dissipation term drives the method toward first-order accurate. Conversely, if a solution is in a smooth region, a limiter diminishes the SUPG dissipation term so that the original Galerkin method is recovered. Firstly, the method is tested on the one-dimensional unsteady linear advection equation with a smooth and non-smooth initial conditions. Convergence studies are conducted to confirm Fourier analyses. Secondly, the Burgers' equation is used to examine nonlinear effect, and later the study extends to the isothermal and Euler equations to capture both linear and nonlinear waves such as shock, contact discontinuity, and expansion fan.

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Title: On the Thermal Conductivity Degradation across Cracks in a Model Capturing Brittle and Ductile Fracture Using the Phase-field Method

Author(s): *Lampros Svolos, *Columbia University*; Curt Bronkhorst, *University of Wisconsin–Madison*; Haim Waisman, *Columbia University*;

Dynamic loading of polycrystalline metallic materials can lead to brittle or ductile fracture depending on the loading rates, geometry, and material type. For materials which possess limited plastic deformation mechanisms, brittle fracture is observed, in which cracks rapidly develop with minimal plasticity and heat dissipation. At high strain rates for materials which can accommodate plastic deformation, material instabilities known as shear bands, can occur. Shear bands are narrow localization bands which reduce the stress-bearing capacity of the material and act as a precursor to fracture. A unified model, which accounts for the two aforementioned failure processes simultaneously, is employed. In this model, the phase-field method is used for crack initiation and propagation, which is coupled to a temperature dependent visco-plastic model for shear bands. In this presentation, an improvement to the unified model is presented to capture the heat transfer behavior across cracks, which is extremely important for high strain rate loadings. To this end, we propose a novel thermal conductivity degradation function based on a micromechanics void extension model due to fracture. We investigate the behavior of the aforementioned technique on a set of dynamic fracture benchmark problems and show the advantages of the micromechanics model compared with the conventional quadratic degradation function.

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Title: OpenKIM: Reliable Interatomic Models for Atomistic and Multiscale Simulations

Author(s): *Ellad Tadmor, *University of Minnesota*; Ryan Elliott, *University of Minnesota*; Daniel Karls, *University of Minnesota*;

Atomistic and multiscale simulations of materials using empirical interatomic potentials play a key role in realistic scientific and industrial applications. The Open Knowledgebase of Interatomic Models project (https://OpenKIM.org) [1,2] includes an automated user-extendable framework for testing the predictions of potentials for a host of material properties. Visualization tools have been developed to compare potential predictions to help select the most appropriate one for a given application. Verification checks ensure the integrity of the potentials. The potentials in OpenKIM conform to the KIM application programming interface (KIM API), which means that they can be seamlessly used with several major molecular simulation codes that support the KIM standard. This talk will describe the OpenKIM project and how the testing framework can assist materials researchers. [1] "The Potential of Atomistic Simulations and the Knowledgebase of Interatomic Models", E. B. Tadmor, R. S. Elliott, J. P. Sethna, R. E. Miller and C. A. Becker, JOM, 63, 17 (2011). [2] "NSF Cyberinfrastructures: A New Paradigm for Advancing Materials Simulation", E. B. Tadmor, R. S. Elliott, S. R. Phillpot and S. B. Sinnott, Current Opinion in Solid State and Materials Science, 17, 298–304 (2013).

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Title: Automatic Hexahedral Meshing based on the Quantization of a Delaunay Mesh

Author(s): *Reza Taghavi, *SIW Corporation*;

Given a closed triangulated surface, its interior is meshed using constrained Delaunay tetrahedralization. The resulting elements are sorted based on the number and topological configuration of their internal edges and faces. This results in a partition of the volume into more than a dozen groups. Further reorganization results in a partition into four groups labeled 0D, 1D, 2D and 3D. A similar logic applied to element faces leads to a partition of triangular faces into three groups, 0D, 1D and 2D. We show that 0D tetras have four 0D faces. 1D tetras have one 0D and three 1D faces. 2D tetras have two 1D and two 2D faces, and 3D tetras have four 2D faces. We call this a quantization of the object. A colorization of tetrahedra by label exhibits stacks of 2D tetrahedra, book-ended by 3D tetrahedra, forming a network of generalized prisms aligned with the edges of the object and enclosing swaths of extrudable sub-volumes especially prominent when the object is thin. More precisely, the longitudinal edges of the generalized prisms subdivide the initial surface mesh into numerous extrusion source and target patch pairs. A sub-volume sandwiched between any source and target pair can be meshed into hexahedra by extruding the quadrilateral mesh resulting from the paving of an average mid-patch mesh. The mid-patch is built by slicing half-way through all the 1D tetrahedra connecting the source and target patches. The remaining volume is composed of isolated 3D tetrahedra, interconnected by a network of generalized prisms. Therefore, the remaining volume can be trivially meshed into hexahedra -compatible with existing extruded mesh blocks- by splitting each 3D tetra into 4 and each prismatic block into 3 hexahedral mesh blocks. This method is essentially an automated hex-meshing that uses a volume decomposition resembling mid-surface decomposition. Computationally, the method relies on simple local mesh manipulation operations such as edge spitting and collapse, which should lend itself to parallelization. Discussion of necessary and sufficient conditions, or whether every solid lends itself to such a decomposition, or whether this approach is a reasonable way of building hexahedral meshes for every solid are valid and open discussions which are not addressed in this presentation. Several examples of all-hexahedral meshes of high-aspect ratio (very thin) mechanical parts commonly seen in electronics, composites and light-weight structural applications are presented.

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Title: Artificial Intelligence Data Driven Model for Adolescent Idiopathic Scoliosis: Analysis, Prediction, and Treatment

Author(s): *Mahsa Tajdari, *Northwestern University*; Hengyang Li, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

Scoliosis, 3D deformation of the human spinal column, is characterized by a lateral deviation of the spine, accompanied by axial rotation of the vertebrae. This study primarily focuses on Adolescent Idiopathic Scoliosis (AIS) which is the most common type of scoliosis affecting children, mostly between ages 8 to 18 when bone growth is at its maximum rate. Studies reported that the asymmetric growth of the spine causes the vertebral rotation and development of scoliotic curves. The treatment of scoliosis is highly dependent on the scoliosis curve. Currently, the treatment method is only guided by available medical devices which mostly are based on the surgeon's experience. Therefore, developing a clinically validated patient-specific model of the spine would aid surgeons to understand the AIS during the early stages and propose an efficient method of treatment for individual patients. In this study, a clinically validated patient-specific FE model of the human spine including vertebral, vertebral growth plate and intervertebral discs is generated using human DICOM images. The initiation and induction of scoliosis are studied focusing on the middle column. The spine FE model considers the axial and transverse growth of both the vertebral bodies and intervertebral discs. The axial growth of the vertebra utilizes the existing 1D growth model. The growth model parameters are calibrated through the experimental data. The results obtained by the FE simulation can be implemented to generate a database of spinal curve progression over a particular period and for a variety of variables such as initial spinal geometry, patient weight, and daily activity. The developed database will be combined with a system of neural networks to predict the curve progression over the years as stated by initial spine geometry. Moreover, the model can be combined with an effective therapy program to target the affected area and modify curvatures in an optimized way.

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Title: Peridynamics Study on Irreversible Deformation of Glass under Indentation

Author(s): *Yoichi Takato, *AGC Inc.*; Kohei Fujita, *National Institute of Technology, Gifu College*; Ryoichi Shibata, *National Institute of Technology, Gifu College*; Madoka Ono, *AGC Inc.*; Satoshi Miyasaka, *AGC Inc.*; Shingo Urata, *AGC Inc.*;

Glass is a well-known brittle material that fractures easily if excessively loaded. An indentation test to determine the hardness of a glass exhibits irreversible deformations including densification, plastic flow, and crack, depending on glass composition and the shape of an indenter. To capture the complex mechanical behaviors of glasses under indentation, numerical simulations are suited. However, use of numerical simulations on the basis of standard continuum mechanics including finite element analysis is still challenging due to discontinuous deformation fields formed in the indented glass. To overcome the shortcoming we employed Peridynamic theory, which can cope with crack propagation naturally because of its non-local formulation of continuum mechanics. In this talk we present composition dependent deformations observed in the numerical indentation tests for oxide glasses. In addition, we applied the test to copper nanoparticles embedded soda-lime silica glasses, which were confirmed in our experiments to be tougher than the base glass. The mechanical properties required to implement the Peridynamics simulations for the composite glass were determined using reactive molecular dynamics (RMD) simulations with nanoscale models in which an approximately spherical nanoparticle is embedded. The results of RMD and Peridynamics simulations show that the presence of copper nanoparticles in the composite glass makes its surface softer and in turn improves crack resistance of the oxide glass.

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Title: Fully-Coupled Numerical Framework for Dynamic Simulations on Two Scales

Author(s): *Erik Tamsen, *Technische Universität Dresden*; Daniel Balzani, *Ruhr University Bochum*;

Micro-heterogeneous materials under dynamic loading can give rise to wave propagation and distinct stress distributions at the microscale, thus resulting in a complex macroscopic material behavior. A well known example are certain meta materials, that exhibit a negative bulk modulus at specific loading frequencies. Another example are for instance strain-hardening cement-based composites, where the favorable energy absorption behavior under impact loading results from breaking of the concrete matrix and fiber pullout. We present an FE² framework for large strains where for each macroscopic integration point of a structural finite element problem a microscopic boundary value problem is solved using a finite element discretization of a representative volume element. An energetically consistent scale-bridging is achieved by using homogenization operators, taking into account the extended Hill-Mandel principle of macro-homogeneity [1,2]. A direct kinematic coupling, based on kinematic admissibility [1], is implemented using Lagrange multipliers to enforce the displacement coupling condition. Thereby, the often applied restriction of prescribing zero displacements to specific nodes can be avoided, which allows for a rather arbitrary choice of microstructure. The presentation includes the principals on which the framework is based, the formulation of the displacement constraint and the derivation of the consistent tangent moduli. Selected numerical simulations will be given to show the influence of microscale inertia on the macroscopic material response. [1] E.A. de Souza Neto, P.J. Blanco, P.J. Sánchez, R.A. Feijóo. An RVE-based multiscale theory of solids with micro-scale inertia and body force affects, Mechanics of Materials, 80:136-144, 2015. [2] C. Liu and C. Reina. Variational coars-graining procedure for dynamic homogenization. Journal of the Mechanics and Physics of Solids, 104:187-206, 2017.

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Title: A Fully Coupled Non-Ordinary State-Based Peridynamics Model for Functionally Graded Materials under Thermal Shock

Author(s): *Yang Tan, *Wuhan University of Technology*; Qiwen Liu, *Wuhan University of Technology*; Mingwei Chen, *Wuhan University of Technology*; Lisheng Liu, *Wuhan University of Technology*;

In this study, a fully coupled non-ordinary state-based peridynamics (NOSB-PD) model for functionally graded materials (FGMs) is introduced to simulate dynamic damage process of FGMs under thermal shock loading. The formulation includes coupling of both thermal and mechanical fields. The material properties of FGMs are supposed to vary exponentially along speci?c direction and temperature-dependent material properties are also taken into consideration. Validation of the proposed numerical model is conducted by comparison with finite element results. Good agreements are obtained by comparing the results obtained from the NOSB-PD model with finite element results. Subsequently, the crack propagation of a FGM plate with a pre-existing crack is investigated under thermal shock loading. The crack propagation paths and temperature distributions are given. The effects of the material gradient and the coupling parameter on dynamic crack propagation and branching in FGMs are analyzed.

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Title: Energy-based Matching Boundary Conditions for Stable Simulation of Non-ordinary Peridynamics in One Space Dimension

Author(s): *Shaoqiang Tang, *Peking University*; Siqi Zhu, *Peking University*;

In this talk, we describe a class of matching boundary conditions (MBC) for simulating non-ordinary peridynamics in one space dimension. Over a finite computing domain to simulate the dynamics for the whole infinite domain, one is lack of information at exterior material points, leaving the interial material points dynamics unclosed. Numerical boundary conditions are thus needed. MBC's are expressed as additional linear constraints among the displacement and velocity at selected material points near the numerical boundary. The coefficients in MBC's are adjusted to best avoid spurious wave reflection. Due to the complexity of peridynamics governing equation, and in particulalr its nature of non-nearest neighboring interaction, special treatments are proposed in this work, using an energy-based approach. More precisely, we first formulate a suitable form of MBC's such that the selected energy functions (Lyapunov functions) are non-increasing. Then we determine the coefficients to optimize wave transmission at selected wave numbers. Reflection coefficient analysis and numerical tests are performed to demonstrate the effectiveness of the proposed boundary treatments. In particular, we avoid the indefinite growth that was related to zero-energy mode. Furthermore, by Laplace transform we can describe the asymptotics of a relevant drift.

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Title: Effect of Collagen-Elastin Microstructure Architecture on Heterogeneous Response in Trachea and Bronchial Regions

Author(s): *Mehrzad Tartibi, *Delbeat, LLC*; Mona Eskandari, *University of California Riverside*;

Advancements in lung mechanics rely on accurate material characterization of airways. Recent experimental and constitutive models of porcine bronchi have emphasized anisotropic and heterogeneous tissue mechanical behavior. The uniform alignment of collagen and elastin fibers along the axial direction rationalizes anisotropy, explaining axially loaded samples' greater stiffness modulus (slope of stress-strain response in the small deformation regime) [3]. Remarkably, heterogeneity is observed only amongst circumferentially loaded specimens, with distal small airways exhibiting increased stiffness modulus [2]. While preliminary studies of tissue content did not find region-dependent collagen composition, seminal histology images comparing proximal to distal bronchi demonstrates the evolution of fiber architecture from folded to taut, potentially explaining heterogeneity [2]. Established worm-like chain networks and undulation models could justify the variation in material response if considering behavioral differences caused by loading parallel to fiber alignment [1]; however, bronchial region-dependent mechanics is exclusive to loading transverse to fiber orientation. To investigate this phenomenon, we computationally explore a microstructural finite element model with characteristic meshed stiff fibrous substructures and soft extrafibrillar matrix substrate. The mechanics of structurally reinforced crimped or straightened fibrous tissue, as observed in proximal and distal bronchi histology images respectively, is systematically compared to experimental tensile measures of specimens' force-displacement response. Bronchial tissue mechanics is found to be dictated by fiber density and degree of crimp, even for loads transverse to the fiber direction. Identifying and simulating the role of microstructure in bronchial heterogeneity facilitates understanding tissue remodeling caused by pulmonary disease and injury, where degradation and reorientation of fibers alter lung mechanics. [1] Chen, H. et al. (2011). A micromechanics finite-strain constitutive model of fibrous tissue. J Mech and Phys Solids. [2] Eskandari, M. et al. (2018). Mechanical Properties of the Airway Tree: Heterogeneous and Anisotropic Pseudoelastic and Viscoelastic Tissue Responses. J App. Physiol. [3] Teng, Z. et al. (2012). Anisotropic material behaviours of soft tissues in human trachea: an experimental study. J Biomech.

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Title: Optical Recognition of Alphanumeric Codes on Ceramic Bowls Used in Lost-wax Casting

Author(s): Tiago Roque, *Instituto de Ciência e Inovação em Engenharia Mecânica e Engenharia Industrial, Faculdade de Engenharia, Universidade do Porto, PORTUGAL*; Valter Costa, *Instituto de Ciência e Inovação em Engenharia Mecânica e Engenharia Industrial, Faculdade de Engenharia, Universidade do Porto, PORTUGAL*; *Joao Manuel R.S. Tavares, *Instituto de Ciência e Inovação em Engenharia Mecânica e Engenharia Industrial, Faculdade de Engenharia, Universidade do Porto, PORTUGAL*;

Abstract The industry is currently going through a new industrial revolution know as Industry 4.0, that consists in an exponential increase in automation and information exchange among different production phases with the goal of building "smart factories", where it is possible to have full control and feedback on all production stages. Hence, this work consisted on the development of a new computer system that fits within this philosophy; specifically, a system based on computer vision to recognize alphanumeric codes engraved along the edge of ceramic bowls commonly used in lost-wax casting. Because it is mainly an Optical Character Recognition problem (henceforth OCR), the first step was to enhance the input image using several image pre-processing techniques; then, the text region was detected and the alphanumeric code segmented and finally, recognized using a well-known OCR engine. The developed computational solution was implemented and optimized in a Raspberry Pi based system with a Pi camera. The experimental tests, conducted under different acquisition conditions, were very promising, leading to high accuracy rates and low processing times. References [1] S. Choi, J. P. Yun, K. Koo, S.W. Kim, “Localizing slab identification numbers in factory scene images”, Expert Systems with Applications, 39(9):7621-7636, 2012 [2] P. P. A. Burry, V. Kozitsky, “License Plate Optical Character Recognition Method and System”, US8644561B2 patent, 2014 [3] N. Islam, Z. Islam, N. Noor, “A Survey on Optical Character Recognition System”, Journal of Information & Communication Technology, 10(2), 2016 [4] R. P. Foundation, “Raspberry Pi Documentation.”, Available at: https://www.raspberrypi.org/documentation/ (last access on January 2019)

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Title: Towards Simulating Microstructure Evolution of 3D Printed Stainless Steel Using the Cellular Automata Finite Element Model

Author(s): *Kirubel Teferra, *US Naval Research Laboratory*; David Rowenhorst, *US Naval Research Laboratory*;

Additive manufacturing (AM) is a promising materials technology because of its ability to generate components according to prescribed CAD-based geometries with tight tolerances. The AM build process generates highly localized thermal cycles that induces rapid phase changes in the material. The frequency, localization, and speed of the thermally-driven phase changes is significantly different than the annealing processes associated with traditionally processed materials, often leading to different microstructural and constitutive properties. Since microstructure influences material properties, it is important to statistically characterize the features of these novel microstructures and develop models to simulate their morphology for subsequent analysis. Furthermore, since the optimally designed geometries enabled by AM processing often results in structural members of relatable sizes to microstructural length scales, structural member properties must be analyzed using principles of stochastic volume element analysis, which explicitly involves analysis of polycrystals. There are a range of modeling approaches for simulating microstructure morphology in terms of fidelity of incorporated physics. The least physical approach is purely statistical methods based on simulating the parameters of a tessellation model, with the drawback that these models are too simplistic to capture the complex morphologies of AM microstructures. The most physical approaches are phase field models that incorporate the kinetics of microstructure evolution into an energy functional to be minimized. While this approach enables studying effects of competing mechanisms, it is too computationally demanding to simulate large microstructures. The cellular automata finite element approach is a compromise between the two extremes. The heat equation is solved based on the laser scan history to compute the temperature field and its gradient during microstructure evolution. The cellular automata approach is used to simulate the epitaxial grain growth from the base plate of the AM build by incorporating empirical models for analyzing competitive growth, such as preferential crystallographic growth or thermal gradient driven growth. This model is developed and utilized to simulate the microstructure evolution of 316L stainless steel and qualitatively compared to 3D serial section data.

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Title: Machine Learning Materials Physics: Integrable Deep Neural Networks Enable Scale Bridging by Learning Free Energy Functions

Author(s): *Gregory Teichert, *University of Michigan*; Anirudh Natarajan, *University of California-Santa Barbara*; Anton Van der Ven, *University of California-Santa Barbara*; Krishna Garikipati, *University of Michigan*;

The free energy of a system is central to many material models. Although free energy data is not generally found directly, its derivatives can be observed or calculated. In this talk, we present an Integrable Deep Neural Network (IDNN) that can be trained to derivative data, then analytically integrated to recover an accurate representation of the free energy. The IDNN is demonstrated by training to the chemical potential values of a binary alloy with B2 ordering. The resulting DNN representation of the free energy is used in a phase field simulation and found to predict the appropriate formation of antiphase boundaries in the material. In contrast, a B-spline representation of the same data failed to represent the physics of the system with sufficient fidelity to resolve the antiphase boundaries.

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Title: NURBS-based Finite Element Framework for Kohn-Sham Density Functional Theory

Author(s): *Ilker Temizer, *Bilkent University*; Phani Motamarri, *University of Michigan*; Vikram Gavini, *University of Michigan*;

A computational framework is presented for real-space electronic structure calculations using finite-element discretizations of the Kohn-Sham density functional theory. The focus of the framework is on higher-order discretizations through non-uniform rational B-splines (NURBS) where the order and the resolution of the discretization can easily be controlled through degree-elevation and knot-refinement algorithms. The resulting generalized eigenvalue problem is solved through a Chebyshev-filtered subspace iteration method. In order to address the efficiency of the NURBS-based approach versus Lagrange-based discretizations in comparable settings, series of one-dimensional (radial) and three-dimensional problems are investigated, ranging from all-electron calculations on single-atom configurations to local and non-local pseudopotential studies on small multi-atom systems. For the latter, the size of the system ranges from the hydrogen and methane molecules to a 172-atom Aluminum cluster and the C60 molecule. In addition to an emphasis on optimal convergence rates, the studies demonstrate that in many cases comparable errors in total energy can be obtained through NURBS with coarser and lower-order discretizations. Various shortcomings of the NURBS-based approach, such as the cost of quadrature and the apparent need for a generalized eigenvalue problem setting, will also be discussed.

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Title: Geometry Conforming Parallel Mesh Generation and Adaptation for Large Scale Flow Simulations

Author(s): *Saurabh Tendulkar, *Simmetrix Inc.*; Mark Beall, *Simmetrix Inc.*; Rocco Nastasia, *Simmetrix Inc.*; Kenneth Jansen, *U. Colorado Boulder*;

The CFD Vision 2030 study [1] foresees that 10-100 billion element meshes will be normal in 2030. Such meshes must be adaptively obtained in parallel using in-memory functional interfaces with the solver to avoid I/O and serialization bottlenecks. The initial mesh must itself be sufficiently fine in order to obtain an accurate converged solution efficiently, and so must be generated in parallel as well. The generated as well as adapted meshes must conform to the geometric model inclusive of complexities where the flow physics needs to be accurately resolved. For efficient resolution of complex flow physics, conditions of anisotropy, grading and spacing control should be met by the mesher. Adaptation should be supported in the unstructured mesh region as well as in the boundary layer mesh in the in-plane and thickness directions. We will discuss recent advances in mesh generation and adaptation technologies that successfully address the above needs of large scale, parallelization, in-memory solver interfacing, gradation control, anisotropy and conformance to geometry. A number of complex flow simulations where such meshes were used will be presented. In particular, we will address efforts targeting meshes satisfying these requirements with element counts in the CFD Vision 2030 normal range, i.e. tens of billions of elements. [1] J. Slotnick et al., "CFD vision 2030 study: a path to revolutionary computational aerosciences," NASA Langley Research Center, NASA/CR-2014-218178, Mar. 2014.

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Title: Predictive Model of Skin Growth in Response to Stretch Calibrated Experimentally with a Porcine Animal Model of Tissue Expansion

Author(s): Tianhong Han, *Purdue University*; Elbert Vaca, *Northwestern University*; Sergey Turin, *Northwestern University*; Lindsay Janes, *Northwestern University*; Arun Gosain, *Northwestern University*; *Adrian Tepole, *Purdue University*;

Skin responds to chronic stretch beyond its physiological regime by growing in area. This adaptive capability of skin has led to tissue expansion (TE), a common technique in reconstructive surgery that enables growth of sizable flaps to correct large skin defects or in breast reconstruction after mastectomy. However, despite its popularity, current TE protocols are arbitrary, based on each surgeon's experience and training, rather than quantitative engineering knowledge. As a consequence, TE leads to complications such as lack of enough skin growth to close a defect, or asymmetric and unnatural breast shape. To address the current shortcomings of TE, we have previously proposed a phenomenological skin growth model and a custom finite element implementation of TE scenarios that resulted in predictions aligned with clinical experience [1]. We also introduced an experimental model of TE in the swine [2]. Here we show the use of our animal model to inform, for the first time, the parameters of the phenomenological growth model. We tattoo four rectangular 10x10cm grids on the back of two one-year old Yucatan minipigs. We surgically implant two tissue expanders, one frontal, one caudal, with the corresponding contralateral side as control. We inflate the expanders to 60cc in a single inflation step, then sacrifice the animals and excise the skin at time points: 1 hr, 1 day, 3 days and 7 days. We acquire three-dimensional (3D) photos throughout the procedure. From the 3D photos we extract the coordinates of the grid points and fit a spline surface to them. We then use a custom isogeometric analysis implementation to compute the deformation gradient between any two pairs of surfaces. Comparing surfaces of the in vivo state between the beginning of the protocol and right before skin excision yields the total deformation. Excising the patches of the expanded side reveals the elastic deformation. Excising the control patches reveals prestrain. Growth is determined from total, elastic and prestrain deformations. We fit two growth models to these data, one is a linear growth rate, the other is a Hill function. We implement the growth laws into our finite element model of TE. In conclusion, we use an animal model of TE to calibrate a phenomenological model of skin growth and incorporate this knowledge into a predictive finite element model. [1] Tepole, Vaca, …, Gosain A. JoVE, 2017. [2] Lee, Vaca, Ledwon,…, Tepole. J Mech Behav Biomed Mat, 2018.

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Title: A Variational Framework for Two-scale Thermo-mechanical Coupled Problems

Author(s): *Kenjiro Terada, *Tohoku University*; Seishiro Matsubara, *Tohoku University*;

A variational framework is presented for two-scale thermo-mechanical coupled problems, which enables us to analyze both mechanical and thermal behaviors in composite materials simultaneously. The framework can be regarded as an extended version of the thermo-mechanical coupled incremental variational framework [1] and is formulated with the so-called generalized Hill-Mandel principle [2], by which microscopic inertia effects can be considered. Thanks to the principle, the rate of change of macroscopic thermo-mechanical coupled potential is equivalent to the volume average of the microscopic one. Along the lines of [2], the corresponding two-scale Euler-Lagrange equations are formulated along with the appropriate boundary conditions for the microstructure. The primary contribution of the proposed framework is that all of the features of variational structures are inherited. For instance, the symmetry of Hessian in the global problem, i.e., the two-scale consistent tangents, is guaranteed, and thus achieve numerical efficiency during the Newton-Raphson procedure. Also, if selected materials are “variational” in the sense of [1], the heat-exchange efficiency from the inelastic dissipation is automatically calculated without additional modeling. The capability of our proposed framework is demonstrated by solving several numerical examples for thermo-hyperelastic and standard dissipative composites in comparison with the conventional approach [3], which is close to our proposed framework. REFERENCES [1] Q. Yang, L. Stainier and M. Ortiz, “A variational formulation of the coupled thermo-mechanical boundary-value problem for general dissipative solids”, J. Mech. Phys. Solids, 54, 401-424 (2005) [2] E. A. de Souza Neto, P. J. Blanco, P. J. Sanchez and R. A. Feijoo, “An RVE-based multiscale theory of solids with micro-scale inertia and body force effects”, Mech. Mater., 80, 136-144 (2015). [3] G. R. Ramos, T. dos Santos and R. Rossi, “An extension of the Hill–Mandel principle for transient heat conduction in heterogeneous media with heat generation incorporating finite RVE thermal inertia effects”, Int. J. Numer. Mech. Engng., 111, 553-580 (2017)

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Development of Validated High-accuracy Interatomic Potentials Using DAKOTA for Large-Scale Atomistic Simulation of Materials

Author(s): *Aidan Thompson, *Sandia National Laboratories*;

Molecular dynamics (MD) is a powerful materials simulation method whose accuracy is limited by the interatomic potential (IAP). SNAP is an automated quantum data-driven approach to IAP generation that balances accuracy and computational cost. The energy is formulated in terms of a very general set of geometric invariants that characterize the local neighborhood of each atom. The SNAP approach has been used to develop potentials for studying plasticity in tantalum, site defects in indium phosphide, and plasma surface interactions in tungsten and beryllium.The SNAP coefficients are fit to a large quantum-mechanical data set of energy, force, and stress values using weighted linear least squares. On top of this, the DAKOTA optimization package is used to define a set of objective functions that characterize how well each SNAP IAP will perform in MD simulations of the intended materials science application. Genetic search algorithms are used to explore the space of SNAP hyperparameters, including atomic neighborhood distance cutoffs, weighting of different training data components, number of bispectrum components, etc. The best-performing SNAP IAP that emerges from the genetic search is subjected to further cross-validation against unseen quantum data to check for overfitting. The resultant SNAP potentials enable high-fidelity MD simulations of a wide variety of materials systems with thousands to millions of atoms.

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Title: Simulating Failure of Cortical Bone With an Energy Based Discrete Fracture Model

Author(s): *Tim Thompson, *University of Waterloo*; Mohammadreza Hirmand, *University of Waterloo*; Katerina Papoulia, *University of Waterloo*;

We present simulations of human cortical bone at the osteon level and at the macroscale. The microscale model is an energy based approach to generalized cohesive fracture. A two-field discontinuous Galerkin finite element method is used which treats the displacement field and crack opening displacements as separate variables. In contrast to Newtonian approaches, the explicit minimization of the material energy consisting of bulk and cohesive parts allows for a smooth transition of material points from the undamaged to the cohesive state in the sense that the nodal forces are continuous functions of the displacements. The approach results in a non-differentiable, non-convex constrained optimization problem that is solved with a block coordinate descent algorithm and a Nitsche flux constrains interelement interfaces to either remain closed or follow a cohesive traction-separation model. Comparison is made to available results in the literature. The macroscale model consists of the same fracture approach of the bulk but also introduces a novel cohesive approach for fracturing of fibers, which results to the anisotropic behavior observed in the material. Failure envelopes are derived from the approach. Comparison is made with experimental results and with distributed modeling of fracture using a damage model. References Non-differentiable energy minimization for cohesive fracture, K. D. Papoulia, Int. J Fract, 204:143–158, 2017 Block-coordinate-descent energy minimization for dynamic cohesive fracture, M.R. Hirmand and K.D. Papoulia, Computer Meth Appl Mech Eng, in revision.

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Title: The Porous Microstructure Analysis (PuMA) Software for Image-Based Microscale Modeling

Author(s): *John Thornton, *STC at NASA Ames Research Center*; Federico Semeraro, *UIUC at NASA Ames Research Center*; Joseph Ferguson, *STC at NASA Ames Research Center*; Francesco Panerai, *University of Illinois at Urbana-Champaign*; Nagi Mansour, *NASA Ames Research Center*;

Many spacecraft thermal protection systems are comprised of porous materials. Understanding the material response of these materials during atmospheric entry requires accurate knowledge of their material properties. To this end, the Porous Microstructure Analysis (PuMA) software [1] has been developed. This software can compute effective material properties such as thermal conductivity, surface area, porosity, and tortuosity from micro-computed tomography (micro-CT) images of a porous material microstructure. PuMA operates on a three-dimensional domain obtained by segmenting grayscale micro-CT images using a basic thresholding method in which a grayscale cutoff value is specified to separate regions representing different materials in the images. This method has been sufficient for random fibrous media where a large difference in density exists between constituent materials, however for materials containing many different constituents or constituents of similar density, more advanced segmentation techniques are required. For these materials, a PuMA plugin has been developed for Dragonfly [2], a commercial software for advanced image analysis and visualization. Dragonfly includes many advanced segmentation techniques including a machine learning engine, watershed and superpixel methods. The plugin includes the PuMA methods for computing material properties but allows for use of the advanced segmentation techniques and other features offered by Dragonfly. In this presentation, we will look at woven materials as an example, in which segmenting using the thresholding method is difficult due to the tight bundling of fibers. We will show how various methods affect the quality of the segmentation as well as the material properties computed using PuMA. [1] J. C. Ferguson, F. Panerai, A. Borner, N. N. Mansour, PuMA: the Porous Microstructure Analysis software, SoftwareX 7 (2018): 81-87. [2] Dragonfly 3.6 [Computer software]. Object Research Systems (ORS) Inc, Montreal, Canada, 2018; software available at http://www.theobjects.com/dragonfly.

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Title: Immersed Boundary Methods for Fluid-structure Interactions

Author(s): *Fang-Bao Tian, *University of New South Wales, Canberra, ACT 2600, Australian*;

Abstract: This talk introduces two versions of immersed boundary methods: an adaptive immersed boundary-lattice Boltzmann method (IB-LBM) [1] and an IB-WENO (Weighted Essentially Non-oscillation)/TENO (Targeted Essentially Non-oscillation) method [2]. The adaptive IB-LBM is introduced for the fluid–structure interaction (FSI) problems at moderate and high Reynolds numbers. This method employs an improved IBM based on a feedback scheme where the feedback coefficient is explicitly approximated. The Lagrangian force density is divided into two parts: one is the traction caused by the predicted flow velocity, and the other is caused by the acceleration of the immersed boundary. Such treatment significantly enhances the numerical stability for modelling FSI problems involving small structure-to-fluid mass ratios. A novel dynamic geometry-adaptive refinement is applied to provide fine resolution around the immersed geometries and coarse resolution in the far field. Finally, large eddy simulation models are incorporated into the framework to model turbulent flows at relatively high Reynolds numbers. The IB-WENO/TENO method combines the first-order IBM with a finite difference method where the convective term of the compressible viscous Navier-Stokes equations is discretized by a fifth-order WENO or a fifth-order TENO scheme, the viscous term is discretized by a fourth-order central difference scheme and the temporal term is treated by the third-order Runge-Kutta scheme. With this method, the aeroacoustics field generated by the moving boundaries and the associated flows is inherently solved. Extensive benchmark cases are presented to validate the accuracy and efficiency of these solvers. We also explain why the low order IBM works well for fluid-structure-acoustics interactions, where it can be used and where the highly accurate IBM should be used. The principal contributions to the field include the improved IBM with a simple adaptive mesh and the simple IBM for fluid-structure-acoustics interactions. Key words: IB-LBM; fluid-structure interaction; fluid-structure-acoustics interaction. References: [1] Xu, L., Tian, F. B., Young, J. & Lai, J. C. S. A novel geometry-adaptive Cartesian grid based immersed boundary-lattice Boltzmann method for fluid-structure interactions at moderate and high Reynolds numbers, J. Comput. Phys., 2018, 375: 22-56. [2] Wang, L., Currao, G. M. D., Han, F., Neely, A. J., Young, J. & Tian, F. B. An immersed boundary method for fluid-structure interaction with compressible multiphase flows, J. Comput. Phys., 2017, 346: 131-151.

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Title: Multiphysics and Multimaterial Topology Optimization for Programmable Ferromagnetic Soft Active Structures

Author(s): *Jiawei Tian, *Department of Mechanical Engineering, State University of New York at Stony Brook, Stony Brook, NY 11794, USA*; Shikui Chen, *Department of Mechanical Engineering, State University of New York at Stony Brook, Stony Brook, NY 11794, USA*; Xuanhe Zhao, *Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*;

Soft materials can generate flexible movement and change configurations through large deformations when subjected to an external environmental stimulus. They can be engineered to ‘soft machines’ such as soft robots, flexible actuators, compliant electronics, or biomimetic medical devices. Those soft machines make a distinguished difference from their conventional rigid-body counterparts where motions are generated by the change in the relative positions of rigid components. Among the various manipulation strategies such as the electric field, acoustical field, optical field, or thermal field, the manipulation via magnetic field can provide numerous remarkable advantages including remote and non-contact control, safe and biological-friendly stimulation, relatively high manipulated force and torque as well as small scaled target actuation. Ferromagnetic soft elastomers can undergo large deformation under the actuation of external magnetic field by embedding ferromagnetic particles into the soft elastomer matrix, where there exists a magnetic torque acting on the magnetized soft matter and forcing it to rotate to a new configuration so the direction of the internal magnetization vector within the soft material is parallel to the direction of the exterior magnetic flux density. By taking advantage of this physical property, soft active structures undergoing desired motions in response to external magnetic stimuli can be generated by tailoring the layouts of the ferromagnetic soft elastomers with different magnetized ferromagnetic particles. Structural topology optimization has emerged as an attractive tool to achieve innovative structures by optimizing the material layout within a design domain, and it can be utilized to architect ferromagnetic soft active structures. In this paper, the Neo-Hookean hyperelastic model is employed to predict the nonlinear stress-strain behavior of the ferromagnetic soft elastomers, and the level-set-based multimaterial topology optimization method is employed to achieve optimized soft active structures. The objective function is formulated as a minimization of the difference between nodal displacement and targeted nodal displacement within the design domain. Shape sensitivity analysis is derived from material time derivative and adjoint variable method. Since shape sensitivity result contains gradient and divergence terms, causing challenges in constructing the design velocity, two processes, are investigated to construct descent design velocity fields . To verify the feasibility and effectiveness of the proposed method, three benchmark examples including a bending rectangular beam, an expanding or contracting block structure, and a mask are implemented and studied. The optimized results illustrate that the designed structure can achieve programmable ferromagnetic soft active structures with the desired large deformation.

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Title: Investigating Viscous Effects in a Pumping Heart

Author(s): *Oguz Ziya Tikenogullari, *Stanford University*; Francisco Sahli Costabal, *Pontificia Universidad Católica de Chile*; Vijay Vedula, *Stanford University*; Ellen Kuhl, *Stanford University*; Alison Marsden, *Stanford University*;

In this study we use the recent advancements in the experimental characterization and material modeling of the human heart to investigate the effects of viscosity on the blood pressure and flow throughout the cardiac cycle. Experimental studies have quantified the viscous behavior of human heart tissue (Sommer et al., 2015) and recent constitutive models provide an adequate framework for capturing the experimentally observed viscous orthotropic behavior (Liu, Holzapfel, Skallerud & Prot, 2018). Here we assume the heart tissue to be thick walled, orthotropic, viscoelastic, and electrically active. To reproduce realistic contraction sequence throughout the organ, we mathematically represent the heart tissue by following the fully coupled electromechanics framework (Göktepe & Kuhl, 2010) and solve it on the organ level using the finite element method with explicit time integration. We handle the electrical to mechanical coupling by using the active stresses that depend on the transmembrane potential and deformation fields. Passive behavior of the material is reflected by a Holzapfel-type anisotropic viscoelastic material model complemented by the multiplicative split of kinematics into elastic and viscous parts. Passive material properties are chosen to conform to the experimental results of Sommer et al. (2015). Significance of this study lies in the use of a realistic four-chamber human heart model. Using this model, we compute and compare pressure-volume readings resulting from the use of elastic and viscoelastic materials against experimental measurements. We probe whether viscous effects play an important role towards an accurate modeling of the myocardium at the tissue level. References: 1. Sommer, G., Schriefl, A. J., Andrä, M., Sacherer, M., Viertler, C., Wolinski, H., & Holzapfel, G. A. (2015). Biomechanical properties and microstructure of human ventricular myocardium. Acta biomaterialia, 24, 172-192. 2. Liu, H., Holzapfel, G. A., Skallerud, B. H., & Prot, V. (2019). Anisotropic finite strain viscoelasticity: Constitutive modeling and finite element implementation. Journal of the Mechanics and Physics of Solids, 124, 172-188. 3. Göktepe, S., & Kuhl, E. (2010). Electromechanics of the heart: a unified approach to the strongly coupled excitation–contraction problem. Computational Mechanics, 45(2-3), 227-243.

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Title: Uncertainty Quantification in Heterogeneous Material Microstructures with a Large Number of Random Parameters

Author(s): *Ramakrishna Tipireddy, *Pacific Northwest National Laboratory*; Varun Gupta, *Pacific Northwest National Laboratory*;

Geometric and material uncertainties in heterogenous materials at microscale are in general modeled with a large number of random parameters. For example, the composite materials with polymer matrix reinforced by non-circular fiber particles can have variations in geometry of each particle and their relative location in the matrix. Similarly, metal alloys can have varied grain structure and phases. In this work, we model microstructural randomness by treating some of these features as random variables resulting in a very high dimensional stochastic microstructure. Here, we are interested in propagating and quantifying uncertainty in the constitutive relationship at macroscale. Propagating uncertainty form random microstructural properties to macroscopic constitutive relation is a daunting task due to a large number of random variables (parameters). Although the macrostructural constitutive behavior depends on a large number of microstructural features, it resides in a low-dimensional manifold spanned by a small set of random variables due to the concentration of measure. This will extend our prior work [2,3] on stochastic dimensional reduction methods to develop efficient uncertainty propagation method for deriving constitutive behavior at the macroscale. [1] Clément, A., Soize, C., & Yvonnet, J. (2013). Uncertainty quantification in computational stochastic multiscale analysis of nonlinear elastic materials. Computer Methods in Applied Mechanics and Engineering, 254, 61-82. [2] Tipireddy, R., & Ghanem, R. (2014). Basis adaptation in homogeneous chaos spaces. Journal of Computational Physics, 259, 304-317. [3] Tipireddy, R., Stinis, P., & Tartakovsky, A. M. (2018). Stochastic Basis Adaptation and Spatial Domain Decomposition for Partial Differential Equations with Random Coefficients. SIAM/ASA Journal on Uncertainty Quantification, 6(1), 273-301.

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Title: Part-Scale Process-Microstructure Simulation during Laser Power Bed Additive Manufacturing

Author(s): *Albert To, *University of Pittsburgh*; Santanu Paul, *University of Pittsburgh*; Qian Chen, *University of Pittsburgh*; Jian Liu, *University of Pittsburgh*; Yunhao Zhao, *University of Pittsburgh*; Wei Xiong, *University of Pittsburgh*;

This work presents a novel part-scale process-microstructure simulation method for simulating grain growth during the laser powder bed fusion process. In the process simulation, a new hybrid part-scale thermal process model that combines the analytical solution in the near-field and finite element method (FEM) in the far-field has been developed. The near-field incremental temperature field due to the scan lines of one step is calculated by a newly derived analytical transient solution for a single scan line. This near-field incremental temperature field is superposed on the FEM model at the end of a time step. The FEM model then solves the heat transfer in the remaining part, while energy input is added at every time step as a superposition of incremental temperature field. In the microstructure model, an efficient model is proposed to simulate the competitive growth of epitaxial columnar dendritic grains by geometrically tracking the tip of the constituent stable primary dendrite arms. In this model, the solidification front is discretized into a number of seed dendrites, where each dendrite is modeled as a growing line segment and its current growth direction is determined by the local thermal gradient and its crystallographic orientation. Note that the local thermal gradient along the liquidus isotherm is obtained from the hybrid part-scale thermal process model. Since a dendritic grain is the sum of its constituent dendrites, by tracking the tip locations of each dendrite at each time step, the grain growth during solidification can be simulated. The proposed model also considers situations arisen from competition between converging dendrites and secondary dendrite growth from diverging dendrites. By linking the thermal process model and grain growth model, the grain structure for the entire part produced by laser powder bed fusion can be predicted.

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Title: A Characteristic-based low-dissipative shock capturing method for Compressible Large-eddy Simulation

Author(s): *Niccolo' Tonicello, *INSA et Université de Rouen*; Guido Lodato, *INSA et Université de Rouen*; Luc Vervisch, *INSA et Université de Rouen*;

Within the context of shock waves turbulence interaction (SWTI) problems numerical dissipation is a key factor to describe properly the coexistence of many complex phenomena which are indeed fundamental in modern design engineering processes. The presence of strong density variations in the fluid domain implies many difficulties regarding both theoretical and numerical treatment of the problem. How is kinetic energy transferred along scales? How is physically described the interaction between dilatation and viscous dissipation along this process? How to model it? The coupling between compressibility effects and classical vorticity-driven contributions to turbulence are of big interest in many industry applications. That’s why in the last few decades more and more attention has been focused on artificial viscosity (AV) methods to smooth shocks as well as on eddy-viscosity models for turbulence energy transfer description (in both LES and RANS settings). The two aspects need to be treated harmoniously without any loss of information. In this sense, in the present paper a low dissipative shock-capturing procedure involving physical viscosities (with particular attention to bulk viscosity) coupled to a classical eddy-viscosity model for LES is presented and studied. The addition of the spurious terms associated to the two separate techniques is controlled in both cases via modal detectors for turbulence under-resolution and shock discontinuities, respectively. How much the sensors are decoupled one another is fundamental to preserve a good description of the two phenomena simultaneously. Keeping this is mind, the shock wave sensor is based on acoustic characteristic variables and the turbulence detector on the mean kinetic energy. Due to its many positive features a high-order numerical discretisation (namely the Spectral Difference scheme) has been employed in the present work. The use of a high-order procedure is of fundamental importance for the intrinsic definition of the sensors themselves. Many different canonical test cases have been studied in both one, two and three dimensions. Particular attention has been focused on the preservation of entropy shock behaviour (mostly for one- and two-dimensional problems) and on the injection of physically consistent dissipation through artificial viscosity. The main aim of the ongoing research is the development of a unified compressible model able to deal automatically with both turbulence and shock waves simultaneously.

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Title: On Domain Symmetry and Its Use in Structural Optimization

Author(s): *Daniel Tortorelli, *Lawrence Livermore National Laboratory and University of Illinois at Urbana Champaign*; Mathias Wallin, *Lund University*;

Group representation theory has frequently been applied to reduce the cost of finite element simulations of linear elastic structures that exhibit domain symmetry. However, the theory is seldom used in design optimization. This is despite the fact that the designs of many structures exhibit such symmetries. Indeed, those familiar with the structural optimization have seen the topologically optimized Messerschmidt-Bolkow-Blohm (MBB) beam in which domain symmetry is often used to halve the structural domain and thus reduce the computational burden of the problem. What is never seen, however, is the use of domain symmetry in the even more popular cantilever beam topology optimization problem. Here too, domain symmetry can be utilized to halve the structural domain. In this talk we revisit the group representation theory as it applies to linear and nonlinear elastic bodies that exhibit domain symmetry. We consider the usual structural analysis as well as those for homogenization purposes which require the application of periodic boundary conditions. Interestingly, in the latter case, the imposition of the periodic boundary conditions is no longer required, so the domain symmetry reduces the computational burden and simplifies the analysis. Topology optimized structures and unit cells that exhibit both linear and nonlinear elastic response are presented to exemplify the methods. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore Laboratory under Contract DE-AC52-07NA27344. The financial support from the Swedish research council (grant ngb. 2015-05134) is also gratefully acknowledged.

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Title: 2D to 3D Shallow Water and Transport Coupling Within The Adaptive Hydraulics Suite

Author(s): *Corey Trahan, *United States Army Corps of Engineers (USACE), Engineering Research and Development Center (ERDC), Information and Technology Laboratory (ITL)*; Gajanan Choudhary, *The University of Texas in Austin, The Institute for Computational Engineering and Sciences (ICES)*; Clint Dawson, *The University of Texas in Austin, The Institute for Computational Engineering and Sciences (ICES)*; Gaurav Savant, *United States Army Corps of Engineers (USACE), Engineering Research and Development Center (ERDC), Coastal Hydraulics Laboratory (CHL)*; Lucas Pettey, *Science Applications International Corporation, PETTT HCPMP*;

The Adaptive Hydraulics (AdH) software suite is a flagship, DoD-wide, high fidelity, finite element resource for 2D and 3D shallow water (SW) modeling and transport applications. It supports a host of features vital to most hydraulic and transport-engineering applications, including for example, spatial and temporal adaption, surface wave and wind-wave stress coupling, flow through hydraulic structures (weirs, flap gate, etc.) and vessel flow interactions. The AdH suite is also internally linked to a number of process-oriented libraries for cohesive/non-cohesive sediment transport, meteorological forcing and friction and turbulence applications. Recently, the AdH framework was redesigned to allow for both monolithic and flux coupling of the software's internal models. The coupling mechanisms are both conservative and easy to implement. In this talk we specifically present the coupling formulation between AdH's 2D and 3D SW and transport models along with verification and validation results. The primary motive behind 2D/3D SW coupling is (1) to improve the efficiency of 3D baroclinic applications by approximating some part of the global domain as 2D and (2) to incorporate wetting and drying regions into 3D SW domains.

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Title: A Comparison of Image-Based Meshing Methods on Geometry and Transport Properties of Lithium-Ion Battery Electrode Reconstructions

Author(s): *Bradley Trembacki, *Sandia National Laboratories*; David Noble, *Sandia National Laboratories*; Scott Roberts, *Sandia National Laboratories*;

Advances in the imaging and subsequent computational representation of lithium-ion battery electrodes have made it possible to perform mesoscale simulations on reconstructed electrode particle beds. Particle-scale simulations inform large-scale battery simulations, most notably through effective transport properties. For these simulations to be representative and robust, quality computational meshes that represent the true microstructure must be achieved. Both the particles and the surrounding void space must be meshed to simulate surface-dominated electrochemistry as well as relevant transport in all materials. Converting high resolution imaging results (i.e. X-Ray CT, SEM) to computational meshes is an ongoing area of research across various fields. There are two main metrics by which to judge resulting computational meshes: geometric representation and mesh cell/element quality. Additionally, the workflow from images to mesh can be time-intensive, making an automated process desirable. We compare several methods for converting high resolution image data to a computational tetrahedral mesh, including the conformal decomposition finite element method (CDFEM), Sandia's CUBIT/Sculpt module, and TetWild, along with mesh improvement algorithms. Both element quality and workflow/automation metrics will be discussed, and we evaluate the resulting meshes by measuring both the geometric accuracy of the particle beds (surface area, volume) as well as comparing results from relevant physical transport simulations such as electrical and thermal conduction. The comparison will demonstrate the strengths and weaknesses of each technique, providing valuable guidance for future efforts in the image-based simulation field. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Title: A Multi-Omic Approach to Predict Protein Functions and Cancer Cell States for Patient-Specific Therapy

Author(s): *Cyanea Van Trieu Do, *University of Texas at San Antonio*; Yidong Chen, *UT Health San Antonio*; Xiaowei Zeng, *UT San Antonio*; Kathryn Mayer, *UT San Antonio*; Yusheng Feng, *UT San Antonio*;

The complexity of cancer poses many challenges for diagnosis, prognosis, and treatment. One of the fundamental issues is how cancer cells behave and their responses to various therapies. Investigation of these issues requires multi-disciplinary efforts such as biology, biophysics, biochemistry, and biomechanics. In this study, we focus on developing methods to predict cancer cell states and cell behaviors. This study follows the Central Dogma of Biology: from DNA to RNA to Protein. Using DNA mutation status, gene expression dysregulation, and DNA copy number alteration, we determined a gene's activity score, gain or loss of function status based on the protein concentration that deviates from its normal state. By selecting specific proteins and their associated signaling pathways, and utilizing the signaling pathway's network representation, these proteins' concentration levels and their rate of change can be determined. The level and rate of change of protein concentrations, coupling with its genomic alternation, will lead to the alteration in cells' behavior. Generally speaking, many cancer studies show that alternation in gene level is the major cause of aggressive cancer growth. Leveraging big genomic data generated in last few decades with advanced technologies for DNA and RNA profiling and their manifestation by gene mutation, copy numbers, and indices of recurrence, we have developed a predictive model that can be used to design targeted drug based on the prediction of relationship between protein function and cellular states. Mathematically, a signaling transduction pathway in cells is represented as a connected network of proteins, which is further modeled by a system of ordinary differential equations (ODEs). Using a fuzzy logic model, we will demonstrate how to determine the protein loss and gain functions in a cell. The network provides the necessary information to construct protein function on a speci?c signaling transduction pathway, thus to predict the rate of change of components within the pathway. The cell states can be further determined by the protein concentrations and their rates of change. In addition, to verify the predictability of the proposed model, the genomic data obtained from a real patient will be used to compare with the computational results. Our results have shown that the computationally predicted cell states match the histological results very well.

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Title: Hierarchical Multiscale Modeling of Microtextured Regions in Ti-6242 during Alpha/beta Processing

Author(s): *Timothy Truster, *University of Tennesse*; Ran Ma, *Columbia University*;

Ti-6242 is a near alpha titanium alloy, which has excellent high-temperature creep resistance and is widely used in jet engine compressors. This alloy is susceptible to creep fatigue failure under dwell loading below 473 K. The existence of microtextured regions (MTRs) contributes significantly to this fast crack propagation. Mechanical processing in alpha + beta region has been employed to eliminate MTRs, but the efficiency depends significantly on the applied strain path. Previous investigations based on crystal plasticity finite element (CPFE) simulations have demonstrated the relationship between breakdown efficiency and loading direction. Therein, MTRs with regular geometry and pure initial orientation were utilized to isolate the effect of loading direction from initial microstructure. In this talk, the behavior of MTRs with realistic initial microstructure is presented using a hierarchical multiscale modeling framework, and the microscale results are analyzed in detail to understand the behavior of MTRs under different loading conditions. It is shown that a hierarchical multiscale model with realistic initial microstructure at the microscale can reflect the influences from different strain paths, initial orientation distributions, and positions of the region simultaneously. The combined effect of initial orientation distribution and loading direction on the MTR breakdown efficiency is discussed in detail.

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Title: Embedded/Immersed Methods for ALE and Particle Discretizations

Author(s): Mike Puso, *Lawrence Livermore National Laboratory*; *Paul Tsuji, *Lawrence Livermore National Laboratory*; Carly Arthur, *Lawrence Livermore National Laboratory*; Chad Noble, *Lawrence Livermore National Laboratory*; Dana Goto, *Lawrence Livermore National Laboratory*; Ted Orzechowski, *Lawrence Livermore National Laboratory*;

An approach to couple overlapping finite element meshes and SPH or other particle discretizations in an immersed or embedded context is presented. This format is particularly useful in simulations of explosives where explosives are treated as fluids and fragments can be treated as Lagrange solids. The ability to handle contacting fragments immersed in a background fluid is unique to this approach. A solid-solid and fluid-solid coupling scheme that is provably stable for transient analysis will be highlighted. Finally, focus will be made on a number of analytical and experimental validations in the area of blast.

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Title: Calibration of Reaction-Diffusion Glioma Model with Mass-Effect by Longitudinal Magnetic Resonance Imaging

Author(s): *B. Tunc, *Oden Institute*; D.A. Hormuth, *Oden Institute*; G. Biros, *Oden Institute*; G. J. Rodin, *Oden Insitute*; T. E. Yankeelov, *Oden Institute*;

We discuss the calibration of a biophysical tumor growth model using animal- based longitudinal multi-parametric images. The goal of the project being to develop a model which can be calibrated using the least set of data to accurately predict tumor growth at future time points. In this experiment we apply our approach to a murine model of glioma, a form of primary brain tumor. The reaction diffusion model is a single species nonlinear PDE and is one of the most commonly used in practice. One twist in our model is that we include mechanical deformations of the brain due to tumor. In this study, we present a comparison of three models: reaction-diffusion, mechanically coupled reaction-diffusion model without the effects of advection, and mechanically coupled reaction-diffusion model including the effects of advection, for the case of a murine model of glioma. The first two models have previously used to predict glioma growth in a cohort of animals. Dimensional analysis was performed to determine the effect of advection prior to the prediction of tumor growth. For the mechanically coupled models, the level set method was utilized to track the deformations of the brain resulting from tumor growth. The data for model calibration was provided by MRI which gives several measures of tumor status in 3D. MRI data was collected for five animals at 5 to 7 time points over a 10-day period. More specifically, diffusion weighted MRI and dynamic contrast enhanced MRI was used to estimate the concentration of tumor cell number and segment the tumor regions, respectively. T2-weighted MRI was used to provide anatomical information to identify tissue deformations within the brain as a result of the growing tumor. All models were implemented using FEM method and FEniCS library. For each animal, we use the image at the first time point to provide our initial conditions. We used the images at subsequent time points to calibrate each model by solving a parameter estimation problem (for 3-10 parameters) using derivative free optimization. We used the remaining time points (i.e., the total number of time points minus the first three time points) for validation. The objective function of the optimization considers both the tumor concentration mismatch and the deformation mismatch. We use level sets to track the latter. We compare the predictive capability of the models as well as the variability of the estimated parameters across models. Results are discussed in this presentation.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Seismic Resistance for High-rise Buildings Using Multi Tuned Liquid Dampers Considering the Liquid - Tank Wall Interaction

Author(s): *Bui Tuong, *HCMUTE*; Phan Huynh, *HCMUTE*; Nguyen Son, *HCMUTE*;

In recent years, considerable attentions have been paid to research for the development of structural control devices, particularly focusing on the mitigation of wind and seismic's effects. The use of water tanks at roof as resistant solutions, which are known as Tuned Liquid Dampers (TLD), for high-rise buildings is considered in this paper. In the literature, TLD has shown significant advantages and can be one of excellent methods to control high-rise building's vibration. Liquid storage tank is designed to achieve its natural frequency same as that of the building. As a result, the resonant phenomenon will occur and contribute to the building's balance. Besides using TLD to analyze the seismic resistance for high-rise buildings, this paper is also considered the interaction between the liquid and tank wall for with/without using water tank at roof as seismic resistance devices. Results showed that the maximum displacements at the top of buildings can be decreased from 50% to 80% and internal stresses are also reduced meaningfully. Moreover, the result is also checked on the shaking table to show the good agreement between theory and experiment.

15th U.S. National Congress on Computational Mechanics
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Title: Coupled Simulation of Metal Additive Manufacturing Processes at the Fidelity of the Microstructure

Author(s): *John Turner, *Oak Ridge National Laboratory*; James Belak, *Lawrence Livermore National Laboratory*;

Additive manufacturing (AM), or 3D printing, of metals is transforming the fabrication of parts, in part by dramatically expanding the design space, allowing optimization of shape and topology. However, although the physical processes involved in AM are similar to those of welding, a field with decades of experimental, modeling, simulation, and characterization experience, qualification of AM parts remains a challenge. While modeling approaches and simulation tools for welding and similar processes are quite mature, they are inadequate for AM processes. The Exascale Computing Project (ECP, https://exascaleproject.org/) is a U.S. Dept. of Energy effort developing hardware, software infrastructure, and applications for systems capable of performing 1018 floating point operations per second (one “exaop”). The Exascale Additive Manufacturing Project (ExaAM) is one of the applications selected for development of models that would not be possible on even the largest of today’s computational systems. In addition to ORNL, partners include Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), the National Institute for Standards and Technology (NIST), and key universities such as Purdue Univ., UCLA, and Penn. State Univ. We will describe physics components that comprise our simulation environment (extensions of existing simulation software and newly developed capabilities) and report on progress to date using highly-resolved melt pool simulations to inform part-scale finite element thermomechanics simulations, drive microstructure evolution, and determine constitutive mechanical property relationships based on those microstructures using polycrystal plasticity. The coupling of melt pool dynamics and thermal behavior, microstructure evolution, and microscale mechanical properties provides a unique, high-fidelity model of the process-structure-property relationship for additively manufactured parts. We will report on the numerics, implementation, and performance of the nonlinearly consistent coupling strategy, including convergence behavior, sensitivity to fluid flow fidelity, timestepping challenges. We also discuss plans for verification and validation through collaboration with efforts such as AM-Bench (https://www.nist.gov/ambench), a set of benchmark test problems under development by a team led by NIST. (*) James Belak, co-PI (LLNL), Nathan Barton (LLNL), Matt Bement (LANL), Curt Bronkhorst (Univ. of Wisc.), Neil Carlson (LANL), Robert Carson (LLNL), Jean-Luc Fattebert (ORNL), Neil Hodge (LLNL), Zach Jibben (LANL), Brandon Lane (NIST), Lyle Levine (NIST), Chris Newman (LANL), Balasubramaniam Radhakrishnan (ORNL), Matt Rolchigo (LLNL), Stuart Slattery (ORNL), and Steve Wopschall (LLNL). This work was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

15th U.S. National Congress on Computational Mechanics
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Title: Prediction of the Viscoelastic Properties of Thermosetting Polymers from Molecular Dynamics Simulations

Author(s): *Robin Unger, *Institute of Structural Analysis, Leibniz Universität Hannover, Germany*; Wibke Exner, *Institute of Composite Structures and Adaptive Systems, DLR (German Aerospace Center), Braunschweig, Germany*; Behrouz Arash, *Institute of Structural Analysis, Leibniz Universität Hannover, Germany*; Raimund Rolfes, *Institute of Structural Analysis, Leibniz Universität Hannover, Germany*;

The precise knowledge of the time and temperature dependent material behavior under loading of polymers is of great importance for engineering applications. It is worthwhile to reduce the extensive experimental testing required for the characterization of viscoelastic materials by using molecular dynamics (MD) simulations that are already utilized to predict elastic material properties [1]. However, a direct determination of time dependent material properties from MD simulations is not possible, since feasible simulation times in MD calculations are in the order of nanoseconds. The challenge of bridging the different time scales can be overcome by identifying parameters for viscoelastic theories to predict the material response over a broad time and temperature range. Several physically motivated theories follow the fundamental theory of Eyring, which assumes the viscoelasticity to be a thermally activated rate process [2,3]. The Eyring theory states that the viscose flow and the macroscopic deformation are the result of molecule movements at atomistic length scale, caused by externally applied stresses or strains. The present study focuses on the prediction of the viscoelastic material response at experimental time scales over a broad range of temperatures in the glassy regime. MD simulations of a commercially available epoxy system are utilized for the parameter identification of existing theories. A qualitative assessment and experimental validation are presented based on tensile test results, obtained over a range of strain rates and temperatures. The presentation discusses the challenges and opportunities of MD simulations with respect to the viscoelastic material properties of thermosetting polymers. References [1] C. Li & A. Strachan; Molecular scale simulations on thermoset polymers: A review; Journal of Polymer Science Part B: Polymer Physics 53, 103–122 (2015) [2] H. Eyring; Viscosity, Plasticity, and Diffusion as Examples of Absolute Reaction Rates; The Journal of Chemical Physics 4, 283–291 (1936) [3] A. Argon; A theory for the low-temperature plastic deformation of glassy polymers; Philosophical Magazine 28, 839–865 (1973)

15th U.S. National Congress on Computational Mechanics
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Title: Thermal Characterization of Multi-terminal Nanotube Junctions Using Phonon Transport Phenomenon

Author(s): *Vinu Unnikrishnan, *West Texas A&M University*; Sushan Nakarmi, *The University of Alabama*;

Nanotube junctions have unique thermal properties with promising engineering applications in thermal management of devices, nano-fins, and composite fillers. However, development of topologically accurate computational models of these junctions are necessary to study their thermal properties. The complexity in creating topologically accurate computational models of nanotube junctions had been a road-block. An efficient CAD based approach that uses optimization techniques and remeshing strategies [1, 2] have been used to construct topologically accurate atomistic models of 3T-junctions that are energetically stable. The thermal transport properties of these 3T-junctions have been investigated using molecular dynamic simulations and variation in the transport of phonons through the junction are studied using phonon wave packet method [2]. The phonon transport phenomenon in junctions having three angles (30o, 60o and 90o) are investigated. It can be seen that the presence of non-hexagonal defects in the junction impedes the thermal transport in nanostructures. The 60o junction with lowest number of defects (six heptagons) was shown to have a lower thermal resistance compared to 30o and 90o junctions. Since phonons are the major heat carriers in carbon nanotubes, the study of vibrational modes and frequency of phonons provides important insight to the thermal property of nanotube junctions. Thus, the phonon density of states of atoms near junctions shows a shift in higher frequency phonon modes while compared with pristine nanotubes. This decreased thermal conductivity in a junction in comparison with pristine nanotubes is due to phonon scattering that occurs in the junction because of non-hexagonal defects and an extra path available for phonon transport. References 1. Nakarmi, S., et al., Computer-aided design of three terminal (3T-) zig-zag SWCNT junctions and nanotube architectures. Composites Science and Technology, 2018. 2. Varshney, V., et al.,"Developing nanotube junctions with arbitrary specifications," Nanoscale, 2018,10, 403-415 3. Lee, J., et al., Single mode phonon energy transmission in functionalized carbon nanotubes. The Journal of chemical physics, 2011. 135(10): p. 104109.

15th U.S. National Congress on Computational Mechanics
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Title: A Hierarchical Multiscale Modeling with Electrostatic Interaction at Finite Temperature; Validation for an Amorphous Oxide Glass

Author(s): *Shingo Urata, *AGC Inc.*; Takahiro Murashima, *Tohoku University*; Shaofan Li, *University of Califorinia, Berkeley*;

Recently, we have extended a multiscale modeling, which employs atomistically-informed constitutive relation in continuum method, to apply to amorphous materials using a representative sampling cell (RS-cell) composed of multiple atoms. Because the atomistic clusters in the RS-cell can capture irreversible microstructure rearrangements, the multiscale method contains potential shear-transformation-zones to describe a variety of amorphous plasticity behaviors, such as plastic flow stress, inelastic hysteresis loops under cyclic loading, and strain localizations at macroscale. We therefore name the method as a multiscale shear-transformation-zone (MSTZ). In order to apply the MSTZ to realistic materials, we further extend the method to include both long-range electrostatic interaction and temperature effect on the mechanical response. To do so, we first modified our in-house code to couple with a general purpose molecular dynamics (MD) code, LAMMPS, enables us to utilize various interatomic interaction models and electrostatic interaction. In general, MD codes employ a symmetrically constrained unit cell, i.e. the cell shape tensor should be upper triangular matrix. Contrarily, the RS-cells embedded into every quadrature points of macroscale finite elements do not have the restriction. We therefore developed an algorithm to couple with the conventional MD code and MSTZ by decomposing the RS-cell shape tensor into an upper triangular matrix and a rotation matrix. In this study, we compared the novel coupling method and our previous code by applying several asymmetrical deformation to the RS-cell including a FCC copper crystal, ensured the accuracy and validity of the algorithm. Then, the MSTZ was applied to simulate uniaxial and shear deformations of a continuum model for (SiO2)80(Na2O)20 oxide glass in a continuum model, wherein RS-cells including 2,000 atoms are embedded. Because the interatomic interaction is composed of short-range interaction, repulsive interaction and long-range Coulomb potential as a function of partial charges, Ewald method was used to evaluate the electrostatic interaction. In comparison with a MD simulation with a larger unit cell including 20,000 atoms at room temperature, the MSTZ simulation overestimates the stress-strain curve of the simple deformations. This is because the current version of the MSTZ employs conjugate-gradient method to minimize the potential energy in each RS-cell, does not consider temperature effect. We therefore tried to take finite temperature into account in the multiscale modeling with using both molecular dynamics and force-biased Monte Carlo methods. In this talk, we would demonstrate how the MSTZ method works for oxide glasses at finite temperature.

15th U.S. National Congress on Computational Mechanics
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Title: Microstructure Particle Identification and Morphology Correlation with Effective Transport Properties Applied to Battery Modeling, and High-Performance Computing of Anode Microstructure Lithiation.

Author(s): *Francois Usseglio-Viretta, *National Renewable Energy Laboratory*; Kandler Smith, *National Renewable Energy Laboratory*; Andrew Colclasure, *National Renewable Energy Laboratory*; Peter Graf, *National Renewable Energy Laboratory*; Jeffery Allen, *National Renewable Energy Laboratory*; Justin Chang, *National Renewable Energy Laboratory*; Thomas Heenan, *University College London*; Daniel Abraham, *Argonne National Laboratory*;

Battery performance is strongly correlated with electrode microstructural properties. Of the relevant properties, the tortuosity factor of the electrolyte transport paths through microstructure pores is important as it limits battery maximum charge/discharge rate, particularly for energy-dense thick electrodes for automotive application. Tortuosity factor is often correlated with porosity, using microstructure-dependent coefficients (e.g. generalized form of the empirical Archie's law). Such relationships, however are only valid for the specific microstructure morphology for which their empirical parameters are fit, limiting their extensibility [1, 2]. Indeed, it is well known porosity alone cannot reflect the impact of the complex microstructure on the diffusion path: particle orientation, presence of additives, sinuosity and constriction are other contributions often quoted in the literature. In this work, a set of nickel-manganese-cobalt (NMC) and graphite electrodes with various porosity and particle morphology has been imaged with X-ray computed tomography. Both solid and pore domains exhibit a very high connectivity (percolation) preventing a straightforward particle identification. A novel particle identification physics-based algorithm has been developed to label each particle individually [3]. It has been found the new algorithm shows less over segmentation compared with a standard watershed approach, thus providing a better, less noisy, particle labelling. Particle morphology has been then quantified, and a strong correlation has been found between the particle orientation and the tortuosity factor. Especially, particles oriented along the electrode thickness significantly improve the effective diffusion compared with microstructures of similar porosities but with particles oriented along the electrode plane. Such result has practical application as electrode manufacturing techniques exist to align particles (e.g. magnetic alignment). In addition, the pore domain has been skeletonized, based on the pores labeled using the same original algorithm but applied to the pore phase, and the geometric tortuosity as well as the factor of constriction has been deduced and positively correlated with the tortuosity factor. Furthermore, half-cell geometries have been meshed based on these tomography images using a free mesh generation third-party toolbox (Iso2mesh) embedded in an in-house Graphic-User Interface to accelerate the workflow. Fast charging has been then calculating, using High Performance Computing, to investigate the impact of particle heterogeneities on the anode lithiation. It has been found particle size and morphology variations impact local charging state and favor degradation. [1] F. Usseglio-Viretta et. al., Journal of The Electrochemical Society,165(14) A3403-A3426 (2018) [2] F. Usseglio-Viretta and K. Smith, ECS Transactions, 77 (11) 1095-1118 (2017) [3] Article in preparation.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Robust Algebraic Level Sets on Immersed Boundaries for Enriched Isogeometric Analysis

Author(s): *Pavan Kumar Vaitheeswaran, *Purdue University*; Ganesh Subbarayan, *Purdue University*;

We propose an explicit interface tracking algorithm for immersed boundaries using signed algebraic level sets. The algebraic level sets are constructed from implicitized low-degree NURBS surfaces. The theory of resultants in algebraic geometry provides implicit level sets that extend to infinity. In our past work, we developed [1] signed algebraic level sets using the Dixon resultant to carryout Boolean compositions of complex geometries purely algebraically. The sign of the level sets helps classify points as lying inside or outside the region enclosed by the surface. We also carried out isogeometric analysis on the composed geometries using the algebraic level sets. However, the Dixon resultant based method does not produce signed algebraic level sets on all surfaces. For instance, it fails in implicitizing cylindrical and spherical surfaces. Also, for surfaces such as spheres, the generated level sets are unsigned, thus failing to classify points as inside/outside. The present work extends the resultant based method to generate algebraic level sets for most parametric surfaces. A submatrix approach [2] is used to recover implicitizations for failed surfaces, while a polynomial root procedure is developed for recovery of sign. These robustness enhancements are one-time operations for a given geometry and do not add cost in distance computation. As an application, 3D void growth due to electromigration is simulated. Since the analysis of behavior is based on algebraic level sets, topological changes such as void coalescence can be captured purely algebraically on these level sets [1]. The algebraic procedure circumvents the need for intersection computations and collision detection, common challenges in explicit interface methods. As an example, multiple voids interacting under electromigration is demonstrated. In summary, the developed method, provides the advantages of explicit, exact representation of boundary surfaces, enabling sharp interface, simpler governing equations, together with the ability to model topological changes as easily as implicit boundary methods such as the phase-field method. REFERENCES 1. K. Upreti and G. Subbarayan, Signed algebraic level sets on NURBS surfaces and implicit Boolean compositions for isogeometric CAD–CAE integration, Computer-Aided Design, 82, 2017. 2. D. Kapur, T. Saxena and L. Yang, Algebraic and geometric reasoning using Dixon resultants, Proceedings of the international symposium on Symbolic and algebraic computation, 1994

15th U.S. National Congress on Computational Mechanics
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Title: Automatic Variationally Stable Analysis for FE Computations of Convection-Dominated Diffusion Problems

Author(s): *Eirik Valseth, *South Dakota School of Mines and Technology*; Albert Romkes, *South Dakota School of Mines and Technology*; Victor Calo, *Curtin University*;

We introduce the automatic variationally stable finite element (AVS-FE) method [1] for linear scalar-valued convection-diffusion problems. The AVS-FE method uses a first order system integral formulation of the underlying partial differential equations (PDEs) and, in the spirit of the discontinuous Petrov-Galerkin (DPG) method by Demkowicz and Gopalakrishnan [2, 3], employs optimal test functions to ensure discrete stability. The 1AVS-FE method distinguishes itself by using global H and H(div) conforming FE trial spaces and broken Hilbert spaces for the test spaces. The broken topology of the test spaces allows us to compute numerical approximations of the local restrictions of the optimal test functions in a completely decoupled fashion, i.e. element-by-element. The test functions can be computed with sufficient numerical accuracy by using the same local p-level as applied for the trial space. We present 2D numerical results of convection-dominated dif- fusion problems which show optimal asymptotic convergence rates and present preliminary results for goal-oriented a posteriori error estimates. References [1] V.M. Calo, A. Romkes, and E. Valseth. Automatic variationally stable analysis for FE com- putations: An introduction. Preprint submitted to Lecture Notes in Computational Science and Engineering, arXiv preprint arXiv:1808.01888., 2018. [2] L. Demkowicz and J. Gopalakrishnan. Analysis of the DPG method for the Poisson equation. SIAM Journal on Numerical Analysis, 49(5):1788–1809, 2011. [3] L. Demkowicz and J. Gopalakrishnan. A class of discontinuous Petrov-Galerkin methods. II. Opti- mal test functions. Numerical Methods for Partial Differential Equations, 27(1):70–105, 2011.

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Title: Uncertainty Analysis of Fiber Misalignment on Fiber-Matrix De-bonding in Composite Materials Using Cohesive Zone and Embedded Element Modeling

Author(s): *Dirk Vandepitte, *KU Leuven, Mechanical Engineering Dept.*; Pavel Druzhinin, *KU Leuven, Mechanical Engineering Dept.*; Qiang Liu, *KU Leuven, Materials Engineering Dept.*; Stepan Vladimirovich Lomov, *KU Leuven, Materials Engineering Dept.*; Larissa Gorbatikh, *KU Leuven, Materials Engineering Dept.*;

One of the failure mechanisms in composite materials is de-bonding between filaments and matrix.. De-bonding initiates when the traction between both constituents exceeds a threshold value. At de-bonding the energy which was stored in the interface is released and separation takes place. Also stress redistribution takes place and the area of de-bonding may or may not extend. This phenomenon is sensitive to incorrect alignment of the filament with respect to the direction of loading and it is a source of uncertainty in damage modeling in composite materials, which is usually conducted in a multi-scale approach. Finite element modeling at the micro-scale requires detailed meshes and conventional models with matching interfaces have huge numbers of degrees of freedom. The concept of embedded elements (EE) in combination with a cohesive zone model (CZ) releases some of the geometrical constraints, with the filament being meshed independently from the matrix mesh. The present paper discusses the application of the EE-CZ model to modeling of damage in misaligned uni-directional fiber bundles and in textile composites. A first section concerns the implementation in the finite element model. The outer surface of cohesive elements is embedded into the matrix, which means that only the interface nodes on the outer surface of a cohesive element are coupled with the matrix, while the fiber mesh is not embedded. Several load cases are considered to validate the modeling concept first: (1) fiber-matrix de-bonding in transverse tension and (2) fiber pull-out for straight and wavy fibers. The main section of the paper discusses a uni-directional composite with misaligned filaments which is loaded along the fiber direction. An EE-CZ model calculates the onset and extent of de-bonding. Different model realizations are generated with average fiber misalignments in the order of 3.5° to 4° yet with non-interpenetrating filaments and the relation between applied strain and de-bonded area is monitored. The mechanical behaviour of fibrous plies with damage may then further be used at the meso-level in a multi-scale modeling approach. [1] Vorobiov, O., S. A. Tabatabaei and S. V. Lomov. "Mesh superposition applied to meso-FE modelling of fibre reinforced composites: cross-comparison of implementations." Int J Num Meth Eng 111: 1003-1024, 2017. [2] Tabatabaei, S. A., E. Bedogni, A. R. Melro, D. S. Ivanov and S. V. Lomov. "Meso- FE simulation of progressive damage in textile composites using mesh superposition method". ECCM-17, Munich, s.p., 2016

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Title: Design and Manipulation of 3D-Printed Soft Silicone Architectures with Programmed Magneto-Capillary Reconfiguration

Author(s): *Orlin Velev, *North Carolina State University*; Sangchul Roh, *North Carolina State University*; Lilian Okello, *North Carolina State University*; Jameson Hankwitz, *North Carolina State University*; Joseph Tracy, *North Carolina State University*;

We will discuss the principles of design and manipulation of soft matter structures that are programmed to reshape and reconfigure under magnetic fields. Examples of such structures include magnetically percolated gel networks, reconfigurable microbot clusters [1], microswimmers, and 3D printed architectures. The focus of this talk will be on a new class of smart elastomeric architectures that undergo complex reconfiguration and shape change in applied magnetic fields while floating on the surface of water [2]. These magnetoactive soft actuators are fabricated by 3D printing with Homocomposite Thixotropic Pastes (HTPs) - a capillary ink consisting of silicone microbeads, liquid silicone and water [3]. The magneto-capillary actuators are reversibly laterally contracted and expanded by controlling the normal magnetic field applied from below the vessel. The tensile and compressive moduli of the actuators are easily determined by their topological design. Their shape change can be programmed by engineering the pattern of the elastin-type mesh while taking into account the lateral capillary forces [2]. The HTP 3D printing method makes possible the fabrication of soft architectures with different actuation modes, such as isotropic/anisotropic contraction and multiple shape changes. Similar architectures that reconfigure in magnetic fields in response to external stimuli could find a broad range of applications, such as making 2D auxetic materials, soft actuators and soft robots with non-contact actuation. [1] K. Han, C. Wyatt Shields, N. M. Diwakar, B. Bharti, G. P. López, O. D. Velev, Science Adv. 3, e1701108 (2017). [2] S. Roh, D. P. Parekh, B. Bharti, S. D. Stoyanov, O. D. Velev, Adv. Mater. 29, 1701554, 1 (2017). [3] S. Roh, L. B. Okello, N. Golbasi, J. P. Hankwitz, J. A.-C. Liu, J. B. Tracy, O. D. Velev, Adv. Mater. Technol, in press (2019).

15th U.S. National Congress on Computational Mechanics
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Title: A High-Order Unstructured Solver for Fluid Structure Interaction Using the Flux Reconstruction Approach

Author(s): *Brian Vermeire, *Concordia University*;

The development of novel discretizations has been critical in the advancement of fluid structure interaction (FSI) modelling on moving and deforming domains. In practice, such applications often involve complex geometries, necessitating the use of mixed-element unstructured meshes. Furthermore, high-order accurate numerical methods are often required to represent the flow solution and the propagation of coherent structures, such as turbulent wakes, over long distances. To address these issues, in the current work we present a novel High-ORder Unstructured Solver (HORUS) for FSI using the flux reconstruction (FR) approach [1]. FR utilizes a piecewise polynomial representation of the solution on each fluid element, allowing for arbitrarily high-orders of accuracy on mixed-element unstructured meshes. Previously, the accuracy and efficiency of FR has demonstrated for Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) of static bodies [2]. In the current work we extend the utility of the FR approach to FSI, adapting it to moving and deforming domains via the Arbitrary Lagrangian Eulerian (ALE) framework. We first present a summary of the FR approach and necessary conditions for an accurate and efficient ALE framework using both explicit and implicit temporal schemes. We then verify that our implementation in HORUS can obtain arbitrarily high-orders of accuracy in both space and time on moving and deforming domains. The approach is then validated against a set of benchmark FSI problems including a cylinder under forced vibration, a plunging and pitching airfoil, and a vertical axis wind turbine, including comparisons against existing numerical and experimental data. Then we explore a range of acceleration techniques including unsteady polynomial adaptation and mixed implicit-explicit temporal schemes. Finally, we will present an LES demonstration case, using HORUS for unsteady scale-resolving simulations of turbulent flows on moving and deforming domains. It is expected that this approach may allow for more efficient and accurate simulations of general FSI problems on complex geometries. [1] H.T. Huynh, A FR approach to high-order schemes including DG methods, 18th AIAA CFD Conference, Miami, 2007. [2] B.C. Vermeire, F.D. Witherden, and P.E. Vincent. On the utility of GPU accelerated high-order methods for unsteady flow simulations: A comparison with industry-standard tools. Journal of Computational Physics 334:497-521, 2017.

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Title: Influence of Grain Interfaces on the Mechanical Behaviour of Polycrystalline Materials

Author(s): *Miguel Vieira de Carvalho, *Faculty of Engineering of the University of Porto, Portugal*; Daniel de Bortoli, *Institute of Science and Innovation in Mechanical and Industrial Engineering, Portugal*; Francisco Andrade Pires, *Faculty of Engineering of the University of Porto, Portugal*;

The increasing demand for new alloys with enhanced mechanical properties has motivated the development of advanced high-strength steels (AHSS) that simultaneously exhibit high strength and good ductility. The 3rd generation of AHSS often incorporates the so called TRIP effect (transformation-induced plasticity), which increases the strain hardening capacity of multiphase steels. These materials show a highly non-linear response to mechanical loadings resulting from intricate phenomena at the microstructural level, due to the complex interplay of deformation mechanisms influencing their elasto-plastic response (such as plastic slip and phase transformations) [1]. In addition, it is known that brittle failure in polycrystalline materials is related to inter-granular fracture, whereas a ductile response is associated to trans-granular fracture, where cracks propagate from grain interfaces to their interior. Thus, grain interfaces directly influence the overall mechanical material behaviour [2]. In this work, the impact of such interfaces on the overall mechanical response of multi-phase polycrystalline materials is studied, under a variety of loading conditions, considering both the slip-plasticity and martensitic transformation regimes. To do so, a large-strain fully implicit, RVE-based multi-scale finite element code is used [3]. The grain interfaces are modelled using cohesive elements, which are based on a traction-separation relationship. RVE homogenisation is then performed to study the influence of microstructural parameters (crystalline grains and interfaces) on the resulting behaviour. References: [1] Tjahjanto et al. “Crystallographically based model for transformation-induced plasticity in multiphase carbon steels”. In: Continuum Mechanics and Thermodynamics 19 (2008) [2] Akbari et al. “On the effect of grains interface parameters on the macroscopic properties of polycrystalline materials”. In: Computers & Structures 196 (2018) [3] Reis and Andrade Pires. “An adaptive sub-incremental strategy for the solution of homogenization-based multi-scale problems”. In: Computer Methods in Applied Mechanics and Engineering 257 (2013)

15th U.S. National Congress on Computational Mechanics
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Title: Fbar Based Hyper-reduction for Hyper Elastoplastic Material Models

Author(s): *Soumianarayanan Vijayaraghavan, *University of Luxembourg*; Lars Beex, *University of Luxembourg*; Ludovic Noels, *University of Liège*; Stéphane Bordas, *University of Luxembourg*;

The work is concerned with the formulation of a Reduced Order Model (ROM) that can accurately represent the physical behavior of elastoplastic deformations of metals. Many nonlinear solid mechanics problems are computationally expensive as they have (i) many Degrees Of Freedom (DOFs) and (ii) many integration points that need to be visited for each iteration in each increment. We employ a ROM based on the snapshot variant of Proper Orthogonal Decomposition (POD) method that reduces the DOFs of the system. The extension of hyper reduction to the POD method allows enforcing the numerical effort only at the most dominant deformed locations. The hyper reduction strategy focuses on generating a grid of integration points that can alleviate the burden of the full integration of the fine discretization used to generate the snapshots [1]. The grid from the proposed approach has fewer elements than the original model. The idea of imposing the incompressibility constraint as an approximate average within the element in a normal FEM [2] is incorporated in the ROM. The construction of a modified deformation gradient tensor (Fbar [2]) in the hyper reduced model, enables to overcome the volumetric locking problem that is generally encountered during the pointwise enforcement of incompressibility constraint. The computational efficiency of the developed ROM is demonstrated with numerical examples considering the hyper elastoplastic material model. [1] Hyper-Reduction Method Using Adaptivity to Cut the Assembly Costs of Reduced Order Models. Hale, J.S.; Schenone, E.; Baroli, D.; Beex, L.; Bordas, S. A Unpublished Manuscript.\\ Available online: http://orbilu.uni.lu/handle/10993/36557 [2] Design of simple low-order finite elements for large-strain analysis of nearly incompressible solids, EA de Souza Neto, D Perialc, M Dutko and DRJ Owen, International Journal of Solids and Structures, Vol 33, Issue 20-22 1996 Elsevier Science Ltd.

15th U.S. National Congress on Computational Mechanics
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Title: High Order Methods for Multiple Scattering Combining Isogeometric Analysis with Farfield Expansions ABC

Author(s): *Vianey Villamizar, *Brigham Young University*; Tahsin Khajah, *University of Texas, Tyler*; Jacob Badger, *Brigham Young University*; Sebastian Acosta, *Baylor College of Medicine*;

Local high order absorbing boundary conditions based on farfield expansions of the scattered wave (FEABC) have been successfully derived and implemented for acoustic scattering from a single obstacle. In this work, we extend its derivation and implementation to scattering from multiple obstacles. To accomplish this, we impose the FEABC on artificial sub-boundaries enclosing individual obstacles. At first, we couple the FEABC with second order finite difference in generalized curvilinear coordinates at each sub-boundary. This coupling takes into account the interaction of the scattered waves from each obstacle. Thus, we obtain accurate results for the scattering from multiple obstacles of arbitrary shape exhibiting only second order convergence. We further exploit the high order nature of the FEABC by combining it with a high order isogeometric finite element method. As a result, we obtain an overall high order method for scattering from complexly shaped scatterers in the full domain. A computational advantageous aspect of the FEABC is its local character. It means only few boundary points or elements are needed to compute the approximate solution at the different stages of the computation. This constitutes a significant improvement over well-known high order absorbing boundary conditions such as the Dirichlet to Neumann whose global nature requires computation over all the nodes or elements at the artificial boundary.

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Title: Equivalence of Local- and Global-Best Approximations and a Simple Stable Local Commuting Projector in H(div)

Author(s): Alexandre Ern, *Université Paris-Est, CERMICS (ENPC)*; Thirupathi Gudi, *Indian Institute of Science Bangalore*; Iain Smears, *University College London*; *Martin Vohralik, *Inria Paris*;

We prove, under minimal regularity, results permitting to localize the global-best approximations by H(div)-conforming finite element spaces. More precisely, we show that the global-best approximation of a given H(div) function in a H(div)-conforming finite element space imposing the normal trace continuity and divergence constraints can be bounded above and below by the sum of the respective local approximations from the elementwise local spaces without any inter-element continuity imposed along the interfaces and without any divergence constraint. Applications of these results leading to optimal a priori error estimates for mixed finite element and least-squares methods are presented. These in particular avoid any notion of an interpolation operator, apply under minimal regularity, and give elementwise best possible estimates. Incidentally, we construct a projector from H(div) to its conforming finite element subspace that is simultaneously locally defined (over patches of elements), simple as obtained via local-best approximation followed by a flux reconstruction, commuting with the L^2-projection, and stable in the L^2 norm. These results are described in [1], in extension of our previous contribution [2] and building upon [3]. [1] A. Ern, T. Gudi, I. Smears, and M. Vohralík. Equivalence of local- and global-best approximations and a simple stable local commuting projector in H(div). In preparation, 2018. [2] A. Ern, I. Smears, and M. Vohralík. Discrete p-robust H(div) -liftings and a posteriori estimates for elliptic problems with H^-1 source terms. Calcolo 54 (2017), 1009–1025. [3] A. Ern and M. Vohralík. Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations. SIAM J. Numer. Anal. 53 (2015), 1058—1081.

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Title: A Thermomechanical Anisotropic Continuum Model for Geologic Materials with Multiple Joint Sets

Author(s): *Oleg Vorobiev, *LLNL*; Miles Rubin, *Technion*;

Jointed rock mass is often mechanically anisotropic due to preferential orientation of joints. The joints often have three main orientations which are nearly orthogonal resulting in elastically orthotropic medium. We have developed a thermomechanical anisotropic elastic-plastic model to model shock wave generation and propagation in jointed rock formations by various sources such as (underground explosions, asteroid impacts, powerful earthquakes). The stress in the rock depends both on elastic deformations (defined in terms of evolution of a triad of microstructural vectors) and specific internal energy. The anisotropic yield surface used in the model is designed to handle slippage along multiple joint sets. We propose a way to calibrate the model parameters using meso-scale simulations of quasi-static loadings of the representative volume of jointed rock in different directions. The joints in these mesoscale simulations are represented as compliant thin elements embedded into an isotropic rock material. The stress equilibrium is assumed between the joint element and the surrounding rock material. It is assumed that a Coulomb friction law is applied at the joints where the maximum shear stress depends on the effective normal stress in the joint. The effective normal joint stress is equal to the joint stress which depends on the joint closure minus the fluid pressure. The fluid pressure is calculated using a Mie-Gruneisen Equation of state of water. Velocity boundary conditions are prescribed at the boundary of the RVE which correspond to a Modified Triaxial Loading (MTRX). Synthetic yield surface obtained during mesoscale simulations is then used to calibrate the parameters of the anisotropic continuum model. Developed anisotropic continuum model provides a substantial computational savings for numerical modeling of large-scale problems involving rock masses with billions of joints.

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Title: A Balanced-Force Level Set Method on Unstructured Meshes for Modeling Powder-Scale Additive Manufacturing Processes

Author(s): *Gregory Wagner, *Northwestern University*; Stephen Lin, *Northwestern University*; Jinhui Yan, *University of Illinois at Urbana-Champaign*;

Multiphase flows involving solid, liquid, and gas are important in many industrial processes. One application is metal additive manufacturing, in which metal powder is melted under laser or electron beam heating and re-solidified, layer-by-layer, to form complex 3D geometries. Forces and fluxes that occur at the molten metal-gas interface drive free surface motion and induce complex flow patterns in both the liquid and surrounding gas, both of which can have a profound impact on the final product quality. Elucidating these phenomena through computational modeling is key to understanding the physics driving the formation of part geometry and material microstructure. In this work, we present a balanced-force level set formulation on unstructured meshes using a control volume finite element method (CVFEM) for large-scale parallel simulations of thermal multiphase flows, including liquid, gas and solid phases. Our goal is to formulate a robust computational framework that is able to resolve the detailed vapor flow in addition to the free surface motion. This formulation is implemented in Nalu, an open source, massively parallel CVFEM flow simulation code. Using this framework, we aim to study the effects of vapor flow and free surface forces on complex phenomena, such as powder denudation, that are observed in additive manufacturing. We demonstrate that the balanced-force algorithm is able to exactly offset surface tension forces through the pressure gradient; validation examples show that this balanced force is necessary to achieve accuracy for flows driven by surface tension. These interfacial forces are significant in additive manufacturing, where highly localized phenomena including melting, evaporation, and flow of molten metal drive the quality of the final as-built product.

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Title: Recent Advances in the Phase Field Method for Fracture of Viscoelastic and Heterogeneous Solids

Author(s): *Haim Waisman, *Columbia University*; Rilin Shen, *Columbia University*;

In this presentation I will discuss our recent contributions to the phase field method for fracture, and in particular concentrate on of viscoelastic solids (e.g. asphalt and ice) and heterogeneous solids (e.g. bones). Fracture of these solids plays an important role in many applications but it is not yet well understood or properly modeled with the phase field method. In both of these cases I will present modifications to the phase field method which makes it more suitable for these classes of materials. For viscoelastic solids, we propose an additional source term in the phase field formulation to account for fracture effects driven by viscous components of the energy. The formulation requires a single additional parameter and is shown to be thermodynamically consistent. Several benchmark problems will be presented such as (i) a bar under creep, relaxation, strain rate and cyclic loading, and (ii) 3-point asphalt-beam bending problems. For heterogeneous elastic solids, we propose a power law relationship between the stiffness and critical fracture energy of the solid. The method is applied to study fracture of a human bone and is shown to predict well the response of the bone observed in the experiment.

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Title: Comparison of Methods for Computing Momentum Enhancement due to Hypervelocity Impact

Author(s): *James Walker, *Southwest Research Institute*; Sidney Chocron, *Southwest Research Institute*; Stephen Beissel, *Southwest Research Institute*; Donald Grosch, *Southwest Research Institute*; Daniel Durda, *Southwest Research Institute*;

Hypervelocity impacts (> 2 km/s) lead to large craters and the liberation of material from the target, referred to as ejecta. Though the ejecta material leaves the impact site at a variety of velocities, it adds up to additional momentum imparted to the impacted body. Computationally modeling momentum enhancement has proved to be quite difficult. Not only is it necessary to model crater formation due to deformation of the target material, but it is also necessary to model the material failure and then model the post-failure behavior, to include the correct speed that the ejecta leaves the crater. Experiments show that momentum enhancement can be large (as much again as the impactor momentum and larger) for impacts into metals and consolidated rock and concrete. The three standard transient large-deformation techniques have all been applied to this problem, namely Eulerian, Lagrangian, and particle methods. A common approach in Lagrangian finite element computations of penetration events is to have an erosion criterion so that elements are discarded when they are highly distorted and invert or otherwise these elements adversely affect the time step. However, to compute momentum enhancement, it is not possible to dis-card material. Thus, we have been using the particle conversion routines in the EPIC hydro-code to study momentum enhancement in the Lagrangian setting. This feature converts a fi-nite element that reaches a failure threshold to a particle, thus conserving mass and momen-tum. We have performed computations where the entire target is initially defined as particles. We also have performed computations with CTH, an Eulerian code. We compare the three methods with an effort to highlight the differences. This talk will present numerical studies with comparisons to experiments performed at Southwest Research Institute. The experi-ments are impacts of aluminum spheres of 2.54 and 4.45 cm in diameter at speeds slightly above 2 km/s into various geological materials, including granite, sandstone, concrete, and pumice. We have also performed some very high velocity impacts (up to 5.77 km/s) with our two-stage light gas gun with 3.00-cm-diameter aluminum spheres into metallic targets. The test data shows a nonlinear size-scaling effect, where more than expected momentum en-hancement occurs as the size increases. Comparing our data with small-scale historical data, though the crater extent scales roughly linearly with projectile size, the liberated material scales with units of fracture toughness, implying the material failure model must have some size or time dependency.

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Title: A Multiscale Method for Embedding One-dimensional Fluid or Solid Models in Three-dimensional Continua with Application to Vascular Tumor Growth

Author(s): *Wolfgang A. Wall, *Technical University of Munich*; Johannes Kremheller, *Technical University of Munich*; Anh-Tu Vuong, *Technical University of Munich*; Bernhard Schrefler, *Technical University of Munich*;

One-dimensional inclusions which are embedded into three-dimensional continua are ubiquitous in engineering applications. In structural mechanics, composite materials consist of slender 1D structures embedded into a three-dimensional matrix. In biomechanics, models for mass transport from the vasculature into the surrounding tissue typically account for the three-dimensional tissue domain through homogenized, porous medium approaches, while the one-dimensional embedded blood vessel domain is considered through corresponding 1D blood flow and species transport equations. Analogous applications occur in geomechanics. In this talk we will present an embedded multiscale method for coupling these problems with heterogeneous dimensionality in a finite element framework [1]. The major advantage of such an approach is that the discretization of the embedded one-dimensional domain and the surrounding three-dimensional tissue domain are completely independent. This is especially beneficial when considering the complex network structure of the microcirculation in-vivo. The main application for which we have adopted the embedded multiscale method is vascular tumor growth. We have coupled it with our multiphase tumor growth model (see [2]) and present some illustrative preliminary results. The method is especially suited to model angiogenesis which is of fundamental importance during tumor growth. Hereby, the tumor triggers the formation of new capillaries from the pre-existing vasculature, which enables efficient nutrient transport towards the tumor and, hence, rapid tumor progression. Our approach consists of a mortar-type coupling between the pre-existing vasculature which we model as discrete, one-dimensional inclusions and the neo-vasculature for which we adopt a homogenized treatment. An equivalent coupling method can be applied in solid or tissue mechanics applications when the embedded structures or fibers are modeled with one-dimensional beam finite elements. [1] J. Kremheller, A.-T. Vuong, W. A. Wall, B. A. Schrefler, A hybrid vascular multiphase tumor growth model based on an embedded multiscale method, in preparation [2] J. Kremheller, A.-T. Vuong, L. Yoshihara, W. A. Wall, B. A. Schrefler, A monolithic multiphase porous medium framework for (a-)vascular tumor growth, Computer Methods in Applied Mechanics and Engineering 340 (2018) 657-683.

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Title: A Gradient-Based Optimization Approach for the Detection of Partially Connected Surfaces Using Vibration Tests

Author(s): *Timothy Walsh, *Sandia National Laboratories*; Wilkins Aquino, *Duke University*; Greg Bunting, *Sandia National Laboratories*; Scott Miller, *Sandia National Laboratories*;

The integrity of engineering structures is often compromised by embedded surfaces that result from incomplete bonding during the manufacturing process, or initiation of damage from fatigue or impact processes. Examples include delaminations in composite materials, incomplete weld bonds when joining two components, and internal crack planes that may form when a structure is damaged. In many cases the areas of the structure in question may not be easily accessible, thus precluding the direct assessment of structural integrity. In this paper, we present a gradient-based, partial differential equation (PDE)-constrained optimization approach for solving the inverse problem of interface detection in the context of steady-state dynamics. An objective function is defined that represents the difference between the model predictions of structural response at a set of spatial locations, and the experimentally measured responses. One of the contributions of our work is a novel representation of the design variables using a density field that takes values in the range [0; 1] and raised to an integer exponent that promotes solutions to be near the extrema of the range. The density field is combined with the penalty method for enforcing a zero gap condition and realizing partially bonded surfaces. The use of the penalty method with a density field representation leads to objective functions that are continuously differentiable with respect to the unknown parameters, enabling the use of efficient gradient-based optimization algorithms. Numerical examples of delaminated plates are presented to demonstrate the feasibility of the approach. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

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Title: Superconvergent Meshfree Collocation Method

Author(s): *Dongdong Wang, *Xiamen University, China*;

Smooth meshfree approximants such as moving least squares or reproducing kernel shape functions are well suitable for strong form collocation methods. Nevertheless, due to the rational nature of these meshfree shape functions, the computation of high order gradients required by collocation formulation is quite complicated and costly. In addition, the basis degree discrepancy and low accuracy are noticeable issues arising from collocation methods, including meshfree collocation approaches. In order to overcome these issues, a gradient smoothing method is proposed to construct the high order gradients of meshfree shape functions. In this method, the first step involves a general gradient smoothing procedure, where the first order smoothed gradients of meshfree shape function are constructed through a meshfree interpolation of the standard derivatives of meshfree shape function. The second order smoothed gradients are then obtained by directly performing differentiations on the first order smoothed gradients. Subsequently, introducing the smoothed gradients into the strong form leads to a superconvergent gradient smoothing meshfree collocation method. A local truncation analysis is performed to prove the superconvergence of the proposed method. The key ingredient attributed to this superconvergence property is that the proposed high order smoothed gradients meet the consistency conditions which go beyond the original basis degree. Moreover, the present formulation enables a convergent collocation scheme when the linear basis function is used in meshfree approximation, which is non-feasible in the conventional collocation formulation. The efficacy of the proposed methodology is validated by numerical results. Acknowledgement: The support of this work by the National Natural Science Foundation of China (11772280) is gratefully acknowledged.

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Title: A Spatially Varying Robin Transmission Condition for Fluid-Structure Coupled Problems with Strong Added-Mass Effect

Author(s): *Guangyao Wang, *Virginia Tech*; Shunxiang Cao, *Virginia Tech*; Kevin Wang, *Virginia Tech*;

In this talk, we present the use of a generalized, spatially varying Robin transmission condition to mitigate the numerical added-mass effect, which has been a key issue limiting the use of partitioned fluid-structure coupling procedures for problems involving incompressible, heavy fluids (e.g., liquids) and slender/thin structures. The basic idea is to substitute the conventional Dirichlet transmission condition by its linear combination with the Neumann transmission condition. This approach introduces a new combination parameter which can be tuned freely without varying the analytical solution of the physical model. A few recent studies have shown that this approach can significantly improve numerical stability, when the parameter value — assumed to be a constant — is carefully chosen. In this work, we generalize the combination parameter to a spatially varying function, and determine its local value basing on the local properties of the structural material and the fluid medium. Specifically, we first study a simple model problem featuring a non-uniform Euler-Bernoulli beam interacting with an inviscid incompressible flow. We show that while the Robin transmission condition introduces a trade-off between accuracy and stability, a spatially varying combination function can lead to a significant improvement (up to 50% in certain cases) in accuracy, compared to constant parameters, with essentially the same computational cost. Next, we present the implementation of Robin transmission conditions in a general CFD (computational fluid dynamics) – CSD (computational structural dynamics) coupled computational framework, focusing on the development of a physics-based model of the spatially varying combination function, and the use of an embedded boundary method to enforce the Robin transmission condition in the context of projection-based incompressible CFD solvers. The salient feature of these methods and algorithms will be demonstrated using both academic benchmark problems (including a modified Turek-Hron problem featuring a non-uniform beam) and application-specific problems related to the design of biomimetic aquatic and aerial propulsors.

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Title: Stochastic Modeling of Uncertainties in Molecular Dynamics Simulations Using a Stochastic Reduced Order Basis

Author(s): *Haoran Wang, *Duke University*; Johann Guilleminot, *Duke University*; Christian Soize, *Université Paris-Est Marne-la-Vall´ee*;

Molecular Dynamics (MD) simulations are widely used in materials and mechanics studies. However, the material behaviors predicted by MD simulations are usually unable to well replicate experimental measurements or first principle calculations. To solve this problem, many studies have been focusing on parametric uncertainties for interatomic potentials. In contrast, this work is aimed to provide a probabilistic framework to assess, model and propagate model-form uncertainties in MD simulations. These uncertainties are typically generated by the a priori selection of functional forms for interatomic potentials. The approach consists in properly randomizing a reduced-order basis, obtained by the method of snapshots in the con?guration space. Various examples involving graphene sheet systems are provided to demonstrate the relevance of the stochastic modeling framework.

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Title: Surrogate Modeling for Vascular Flow Simulations Based on Physics-Constrained, Label-Free Deep Learning

Author(s): *Jian-Xun Wang, *University of Notre Dame*; Han Gao, *University of Notre Dame*; Luning Sun, *University of Notre Dame*;

Computational fluid dynamics (CFD) modeling has become an indispensable tool in hemodynamics for predicting blood flow patterns and hemodynamic forces, which are critical for understanding the physiological mechanisms of cardiovascular diseases. On the other hand, however, CFD simulations are usually computationally expensive, particularly for flows with complex arterial geometry and/or considering fluid-structure coupling. This drawback largely limits its real-time applications for supporting clinicians in their decisions and poses great challenges to many-query analysis, including uncertainty quantification, parameter estimation, and optimization problems arising in cardiovascular modeling. Therefore, there is a strong need to develop efficient surrogates for vascular flow simulations. Deep learning (DL) has shown new promises for surrogate modeling due to its capability of handling strong nonlinearity and high dimensionality. However, the off-the-shelf DL algorithms, success of which heavily relies on large-scale training data, fail to operate in the small data regime. In surrogate modeling, labeled data are often sparse since each data point in the parameter space requires an expensive CFD simulation. In this work, we provide a physics-constrained DL approach for surrogate modeling of fluid flows not relying on any simulation data. Specifically, a structured deep neural network (DNN) architecture is devised to enforce the boundary conditions, and the governing PDEs (i.e., Navier-Stokes equations) are incorporated in the loss function for the DNN training. Numerical experiments are conducted on a number of internal flow cases relevant to hemodynamic applications, and uncertainties in fluid properties and domain geometry are considered. The numerical results show that the DL-propagated uncertainties have a favorable agreement with those propagated through the principled CFD simulations, which demonstrate the merits of the proposed method.

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Title: An Optimization Method for Additive Manufacturing of Two-dimensional Objects with Fine Features

Author(s): *Jingyi Wang, *UC Berkeley*; Panos Papadopoulos, *UC Berkeley*;

We introduce an optimization procedure for the macro-scale simulation of fused filament fabrication using finite element method to achieve desirable geometric properties. The additive manufacturing process is simulated with new elements added at each time step based on previous depositions. The coupled thermo-mechanical problem is solved using a material model capable of representing large temperature gradient. Partial elements are used to more accurately model the topology of the object being built. We choose some crucial and controllable parameters such as speed and size of the deposition as our optimization variables. Appropriate objective functions are then formulated and used for the optimization. Finally, we investigate different optimization methods and apply them to a set of test examples.

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Title: Multiphase Fluid-Material Coupled Computational Analysis of Cavitation-Induced Material Modification

Author(s): Shunxiang Cao, *Virginia Tech*; Guangyao Wang, *Virginia Tech*; Olivier Coutier-Delgosha, *Virginia Tech*; *Kevin Wang, *Virginia Tech*;

The delicate control of cavitation for high-precision material modification has received growing interests in many engineering and biomedical applications, which requires a better understanding about the interaction between bubble collapse and the response of various ductile, brittle, and soft materials in the vicinity. In this regard, this talk presents a computational study on the transient two-way coupling between the shock-dominated gas-liquid flow and the nearby deformable materials with different elastic properties. A three-dimensional CFD (Computational Fluid Dynamics) – CSD (Computational Solid Dynamics) coupled computational model, capable of simulating multi-bubble-material interaction and dynamic fracture, is developed. Specifically, a second-order accurate partitioned procedure is used to couple a two-phase Navier-Stokes CFD solver with a nonlinear finite element CSD solver. The evolution of the bubble surface is captured by solving the level set equation and the solid surface is represented as a dynamic embedded boundary in the CFD solver. The interface conditions are enforced through the construction and solution of local two-fluid and fluid-solid Riemann problems. The CSD solver features the use of a continuum damage mechanics model and an element erosion method to simulate material damage and fracture. After model verification, we investigate a single bubble collapsing near different types of materials, including the primary mechanism of cavitation-induced material damage and the reciprocal effects of the solid material's acoustic impedance, Young's modulus, and Poisson's ratio. Our studies on the collapse of bubble clusters and a few relevant applications, including biofouling control and shock-wave lithotripsy, will also be presented.

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Title: A meshfree stabilized collocation method (SCM) based on reproducing kernel approximation

Author(s): *Lihua Wang, *Tongji University*;

Abstract: Meshfree direct collocation method (DCM) based on strong form suffers low accuracy and instability compared with Galerkin-based meshfree methods. Meshfree weighted least squares collocation method (WLSCM) can improve the accuracy and stability by minimizing the least squares functional corresponding to the governing equation and boundary conditions. However, usage of more discrete points in the least squares solution increases the computational cost which notably reduces the efficiency. In this paper, we propose a new meshfree stabilized collocation method (SCM) and introduce the reproducing kernel function as the approximation. Auxiliary collocation points located in the local subdomains are employed for the stabilization. Their proper positions and corresponding weighting factors for integration using constant and cubic B-spline weighting functions are derived to keep the consistency conditions. Therefore, in this method, the approximation can satisfy the consistency conditions not only on the points, but also in the subdomains. The suggested method has the comparable accuracy and stability compared with WLSCM, and the computation efficiency can match up to DCM. Numerical simulations demonstrate that SCM can surpass DCM in accuracy and stability, and outperform WLSCM in efficiency and conditioning of the matrix according to the discrete equations, where the condition number of matrix is related to the stability. Keywords: stabilized collocation method, reproducing kernel approximation, auxiliary collocation points, accuracy, stability, efficiency

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Title: A Computational Technique for Reliability Analysis of Traffic Barriers

Author(s): *Qian Wang, *Manhattan College*; Hongbing Fang, *The University of North Carolina at Charlotte*;

This work focused on a study of a high-dimensional model representation (HDMR) approach for reliability analysis of crash or impact applications. The HDMR approach is a technique to approximate nonlinear responses using combined component functions of various orders. In the HDMR approach developed in this work, the component functions were created using compacted supported radial basis functions (RBFs) augmented with polynomials. The crash responses of a vehicle impacting a traffic barrier was evaluated based on hi-fidelity numerical simulations. The crash failures of the traffic barrier was defined as the crash response exceeding the prescribed upper limits. Based on the HDMR approach, the performance functions were expressed explicitly in terms of the random variables, and the failure probability was calculated using Monte Carlo simulations (MCS). This proposed approach was applied to solve various mathematical and engineering examples. Accurate reliability analysis results were obtained for the numerical examples. A concrete barrier under the impact of a pickup truck was investigated and the reliability analysis was performed. The vehicular-barrier impact was according to the Manual for Assessing Safety Hardware Test Level 3 conditions. The reliability analysis approach based on combined HDMR and RBFs was efficient and it required a small number of performance function evaluations. The proposed approach is useful for the probabilistic analysis of practical crash and impact problems involving expensive numerical simulations.

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Title: Lightweight Topology Optimization of Multi-material Structures Based on Independent Continuous and Mapping Method

Author(s): *Weiwei Wang, *Beijing University of Technology, Beijing, China*; Hongling Ye, *Beijing University of Technology, Beijing, China*; Yunkang Sui, *Beijing University of Technology, Beijing, China*;

The complex structure systems assembled by multi-components with different materials become more and more widely used in used in engineering. A lightweight topology optimization model with mechanical performance constraints is established for the multi-material structures based on independent, continuous and mapping (ICM) method. The mathematical model with single economic indicator can avoid the difficulty in determining the volume ratio of each phase materials and selecting the weight coefficient of the multi-performances topology optimization. In the process of multi-material structure topology optimization, the MSC.Patran&Nastran is applied to establish the element model and analyze mechanical performances of structures. A class of independent and continuous variables are introduced to recognize the existence or non-existence of elements with different material parameters and a series of filter functions are used to identify the properties of elements. Then the approximate explicit functions between the structural performances (objective and constraints) and the topology variables are established with the help of Taylor expansion and sensitivity analysis. Then the formulation is transformed into a standard quadratic programming model and solved by the dual sequence quadratic programming algorithm. Finally, the optimal topology structures are obtained by inverse mapping the optimal continuous solution into discrete topology variables. A number of numerical examples with displacement, buckling or frequency constraints are presented to illustrate the effective and feasible of this study in topology optimization of structures with multi-materials. The multi-materials structure topology optimization research can realize the integral design of complex structures in engineering.

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Title: Characterizing Complex Morphology of Brain by Imaging and Mechanical Modeling

Author(s): *Xianqiao Wang, *University of Georgia*; Mir Jalil Razavi, *Binghamton University*;

Soft tissues are complex materials with typical nonlinear, anisotropic, inhomogeneous behaviors subjected to large strains and stresses. Growth or atrophy of soft materials in media may lead to instability and formation of surface wrinkling, folding or creasing. The cortical folding of brain, characterized by convex gyri and concave sulci, has an intrinsic relationship to the brain's functional organization. Understanding the mechanism of convolution patterns can provide useful insight into normal and pathological brain functioning. However, despite decades of speculation and endeavors the underlying mechanism of the folding process remains poorly understood. In this work, formation of complex patterns on the surface of brain, during cortical folding phenomenon, is interpreted by both mechanical modeling and imaging. In the modeling part, non-linear finite element (FE) models based on finite growth are employed to present growth, folding and formation of "3-hinges" of the growing brain and in the imaging part all Human Connectome Project (Q3 release) data was used to reconstruct white matter surfaces from structural MR scans of 868 healthy subjects. Then, we developed a robust algorithm to detect gyri lines and also number and location of 3-hinges in the brain in both FE models and images. Results show that after growth, tertiary convolutions and the exact locations of 3-hinges are unpredictable. Results indicate that in all computational models, qualitative features of folds and 3-hinges are similar to each other, but location and type can be quite different. We can observe same variation of 3-hinges locations in different individual brains. We also extracted the dominant patterns of 3-hinges to create a comparison with those taken from brain imaging data. For the imaging part, the dominant patterns of 3-hinge patterns and their percentages in 68 brain subjects were extracted, and for computational part, 30 FE models were used. The comparison indicates that the "Y" shape 3-hinge is the most favorable pattern in real brains as well as in FE models, although the real brain prefers more convoluted 3-hinges. Our study provides a mechanism to explain why locations and patterns of some specific 3-hinges are consistent. The growth, instability and convolution of the growing brain is a dynamic process, and a small difference between two initial states can lead to different 3-hinges patterns at different locations. Therefore, the type and number of 3-hinge patterns in a developing brain could be a new metric to characterize folding of a primate brain.

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Title: Reduced Order Models and Empirical Data in Computational Mechanics

Author(s): *Xiaodong (Sheldon) Wang, *Midwestern State University*;

One of the major challenges in today's science and engineering fields is how to handle complex systems. Reductionist principles have helped the scientists and engineers to develop uncanny understanding of universe range from mechanical to electro-magnetic properties and phenomena. Ever since that famous quote from Albert Einstein, "God does not play dice," people often wonder what happened to seemly obvious uncertainties in nature. The research in chaotic nonlinear systems seems to suggest that even well-defined deterministic nonlinear systems can produce unpredictable results. Is it possible that when a large number of factors or entities interact with each other, a completely different system quantifiable with an entirely different set of phenomenological rules may eventually emerge? In general, chaotic systems are characterized with so-called positive Lyapunov exponents. In this work, through an example on leakage issues of sucker rod pumping systems and other multi-scale and multi-physics models, we demonstrate that simple analytical, or computational, or empirical studies alone are not sufficient for complex systems [1][2][3]. Reduced order models and empirical data are often needed to bridge the gap in direct computational modelling. In fact, using the singular value decomposition, it is possible to identify the hidden spatial and temporal correlations and patterns between variables and material properties. It is hopeful that based on data analysis tools a computational protocol can be established for complex dynamical systems.

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Title: Finite Elements on Prisms and Cones with Polygonal Bases

Author(s): Wenbin Chen, *Fudan University*; *Yanqiu Wang, *Nanjing Normal University*;

We construct lowest-order H1/(H(curl)/H(div) conforming finite elements on prisms and cones with polygonal bases. Note that a 3D convex polytope can be divided into cones by connecting its vertices with a center point. Combined with our method, this provide a practical conforming finite element discretization on convex polytopal meshes. The finite elements are constructed using Bossavit's extrusion and conation techniques, and satisfy the discrete de Rham sequence. Implementation of the elements is simple and efficient.

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Title: Variational System Identification of the Partial Differential Equations Governing Pattern-forming Physics: Inference under Varying Fidelity and Noise

Author(s): *Zhenlin Wang, *University of Michigan*; Xun Huan, *University of Michigan*; Krishna Garikipati, *University of Michigan*;

We present a contribution to the field of system identification of partial differential equations (PDEs), with emphasis on discerning between competing mathematical models of pattern-forming physics. The motivation comes from biophysics, where pattern formation is central to the development of any multicellular organism, and from materials physics, where phase transitions similarly lead to microstructure. In both these fields there is a collection of nonlinear, parabolic PDEs that, over suitable parameter intervals and regimes of physics, can resolve the patterns or microstructures with comparable fidelity. This observation frames the question of which PDE best describes the data at hand. Particularly compelling is the fact that knowledge of the governing PDE immediately delivers deep insights to the underlying physics of the systems. While building on recent work that uses stepwise regression, we present advances that leverage the variational framework, and address the influence of variable fidelity and noise in the data.

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Title: Controlled Shape-Morphing in Elastomers and in Living Composites

Author(s): Cedric Ambulo, *The University of Texas at Dallas*; Laura Rivera, *The University of Texas at Dallas*; *Taylor Ware, *The University of Texas at Dallas*;

Stimuli-responsive polymers often seek to mimic the intelligence of living organisms, where multiple inputs lead to a predictable series of outputs. Here, two orthogonal strategies, one non-living and one living, to create materials that respond in a complex manner to specific environmental conditions will be discussed. First, we will discuss direct ink write printing to control molecular orientation, and therefore the stimulus-response, in liquid crystal elastomers. This processing approach enables 3D structures where stimulus-response, geometry, and activation temperature can be programmed. Using a dual thiol-ene reaction scheme, we control the phase transition temperatures of 3D-printable LCEs from 12 °C to 54 °C. We also 3D print multiple LC inks into single structures to allow for the production of untethered, thermo-responsive structures that sequentially and reversibly undergo multiple shape changes. Towards this end, we demonstrate a sensing gripper that grasps an object at one elevated temperature but bends away from that object at higher temperatures. Notably, the stimulus-response of these structures is derived wholly from physical properties, while the stimulus-response of living organisms is derived in-part from genetic information. To bridge this gap, we will discuss a new strategy to fabricate living cell – synthetic hydrogel composites capable of undergoing programmed shape change. These living composites are acrylic hydrogels embedded with Saccharomyces cerevisiae, Brewer's yeast. As the cells are higher modulus (~100×) than the gel, cell proliferation results in a macroscopic shape change of the composite. Importantly, genetic engineering provides a platform to tune both the perception and responses of the living composite. We have shown that living composites can be synthesized using engineered yeast strains with light-responsive optogenetic Arabidopsis thaliana-derived sensors. As a result, the shape change (up to 300% volume change) of these composites can be patterned spatially and temporally by using low-power blue light. It is expected that these strategies to synthesize 'intelligent' shape-morphing polymers may enable new approaches to engineering challenges from soft robots to smart medical devices.

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Title: Efficient Topology Optimization Under Uncertainty Via Stochastic Reduced Order Models

Author(s): *James Warner, *NASA Langley Research Center*; Miguel Aguilo, *Sandia National Laboratories*;

This work presents a stochastic reduced order modeling approach for the solution of structural topology optimization problems under uncertainty. Relative to their deterministic counterparts, these stochastic topology optimization problems are computationally prohibitive due to the number of model evaluations that are needed to quantify and propagate design uncertainties. This computational complexity is magnified if high-fidelity simulations are used during optimization. A stochastic reduced order model (SROM) approach is applied to (1) alleviate the prohibitive computational cost associated with large-scale, uncertainty aware, structural topology optimization problems; and (2) quantify and propagate inherent uncertainties due to design imperfections. The SROM framework transforms the stochastic topology optimization problem into a deterministic optimization problem that relies only on independent calls to a deterministic analysis engine. This approach enables the use of existing optimization and analysis tools for the solution of large-scale structural topology optimization problems under uncertainty.

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Title: Pelvic Response of a Total Human Body Finite Element (FE) Model During Simulated Under Body Blast Impacts

Author(s): *Caitlin Weaver, *US Army Research Laboratory, Aberdeen Proving Ground, MD*; Berkan Guleyupoglu, *Wake Forest University School of Medicine, Winston Salem, NC*; Joel Stitzel, *Wake Forest University School of Medicine, Winston Salem, NC*;

UBB events in theater are the cause of many serious injuries sustained by the warfighter to the pelvis, spine, and lower extremities. These injuries are often debilitating, resulting in increased healthcare expenses and reduced quality of life. Injury prediction for UBB events continues to be a challenge due to the limited availability of UBB-specific test studies. The objective of this study is to evaluate the pelvic response of a finite element (FE) human body model (HBM) in UBB loading scenarios. The Global Human Body Models Consortium (GHBMC) 50th percentile detailed male model (v4.3) was used for this study. In total, seven simulations were conducted at non-injurious velocities using seat and floor pulses of 4 m/s obtained from experimental UBB testing. Acceleration and rotation data from nodes in the posterior sacral region of the GHBMC pelvis were extracted from the simulations. The extracted FE sacral data were compared to experimentally derived pelvis biofidelity response corridors (BRCs) for x- and z-acceleration and y-rotation. Additionally, maximum principal strain (MPS) data was extracted from the cortical bone elements of the FE pelvis. CORrelation and Analysis (CORA) was used to evaluate the FE pelvic response in comparison to the BRC generated curves. The CORA analysis showed good correlation (0.65 or higher) of the FE pelvic acceleration and rotation for six of the seven tests. Additionally, the strain outputs showed high MPS outputs along the sacrum, specifically at the coccyx. Moderate MPS outputs were also observed at the S3-S5 sacral bodies as well as the ala of the sacrum. The results of this FE study shown good correlation for comparison between PHMS experimental testing and FE human body model acceleration and rotation outputs of the pelvis. There are differences in CORA values between the tests analyzed in this study. The differences are most likely caused by variations in experimental sled and rigs between performers. Future work for this validation effort will examine the biofidelity of the femur and T12 region of the spine. The work performed in this study is part of an on-going development effort to evaluate localized pelvic injury risk in an FE HBM for blunt and blast trauma.

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Title: Hybrid Experimental-Computational (HEC) Methods: Implementation and Validation of Microstructurally Inspired Deformation and Failure Models for Compressive Mechanical Response of Human Skull

Author(s): Stephan Alexander, *SURVICE Engineering Company (ARL)*; C. Allan Gunnarsson, *Army Research Laboratory*; *Tusit Weerasooriya, *Army Research Laboratory*;

Hybrid Experimental-Computational (HEC) Methods: Implementation and Validation of Microstructurally Inspired Deformation and Failure Models for Compressive Mechanical Response of Human Skull Stephan Alexander1, C. Allan Gunnarsson2, Tusit Weerasooriya2 1SURVICE Engineering Company, 2 US Army Research Laboratory Finite element (FE) simulation of blast or impact to the head requires validated mathematical representations (models) of material deformation and failure of the human skull to mechanical loading. Controlled, fully instrumented experiments at larger organ scales are difficult to execute with the needed microstructural measurements. Therefore, before deformation and failure models can be confidently applied to FE simulation of head, they must first be validated with controlled laboratory experiments at smaller scale, including coupon and then skullcap scales, with measured stress and/or strain fields. The complex structural arrangement of bone within the skull challenges the use of biofidelic finer meshes representing the complex microstructure. At the other extreme of simplification, representation by courser homogenous meshes of the skull may be inaccurate due to the lack of conclusively validated models of material deformation and failure that incorporate the microstructural details of the bone. Additionally, the failure initiation and propagation cannot be precisely captured with a coarser (homogeneous) representation of the skull. Power laws relating the modulus and failure of adult human skull to the morphology, specifically the bone volume fraction (BVF), have recently been envisioned at the US Army Research Laboratory (ARL) and the University of Virginia, for compressive and tensile responses of the skull, respectively. Here, the ability of the power laws from ARL to simulate a quasi-static fully instrumented experiment of a skull bone coupon compressed to failure was evaluated by assuming that the deviation from linearity in load-displacement is due to progressive failure of elements, starting with highly porous trabeculae. Ignoring the existence of the complex network of pores, thus enormously simplifying the complex meshing process, a FE mesh based only on the outer geometry of the specimen was used. Elements represented a mixture of both bone and pores, with the corresponding bone material deformation and failure models scaled accordingly. The meshing method, combined with the morphology-based mechanical properties, was able to replicate the initial linear portion as well as the subsequent non-linearity of the experimental response before failure (or complete loss of capacity to resist force), as confirmed by the measured stiffness and by comparison of the measured two-dimensional strain fields and failure over the specimen faces.

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Title: A Meshfree Computational Framework for Modeling Liquefaction-induced Failures of Geomaterials

Author(s): *Haoyan Wei, *University of California San Diego*; J. S. Chen, *University of California San Diego*; Zhijian Qiu, *University of California San Diego*; Ahmed Elgamal, *University of California San Diego*; Jinchi Lu, *University of California San Diego*;

During earthquakes, liquefaction and associated deformations cause extensive damage and destruction. Modeling of such failure processes remains challenging, as conventional numerical methods suffer from mesh distortions. In this work, a stabilized and nodally integrated meshfree approach is developed, aiming to simulate complex damage mechanisms and extreme flow-like material deformations in multiphase geomaterials. To this end, an equal-order reproducing kernel approximation pair in conjunction with fluid pressure projection is adopted in the mixed meshfree formulation [1], which eliminates spurious pressure oscillations caused by the inf-sup condition violation. By adopting the implicit gradient approximation [2], the gradients of strain and fluid flux fields are conveniently added into the mixed formulation to eliminate spurious low-energy modes of nodal integrations at low computational cost. In addition, a set of modified test functions is introduced to ensure variationally consistency [3], leading to a convergent and stable meshfree formulation for multiphase porous media. Under this computational framework, a calibrated UCSD soil constitutive model [4, 5] is integrated and implemented to capture the soil liquefaction and cyclic mobility mechanisms. Finally, the effectiveness of the developed meshfree approach for simulating liquefaction-induced large deformations and material failures is validated by comparing to experimental and field observations. [1] Wei, H., Chen, J. S., & Beckwith, F. (2018). A naturally stabilized semi-Lagrangian meshfree formulation for multiphase porous media with application to landslide modeling. Journal of Engineering Mechanics, under review. [2] Hillman, M., & Chen, J. S. (2016). An accelerated, convergent, and stable nodal integration in Galerkin meshfree methods for linear and nonlinear mechanics. International Journal for Numerical Methods in Engineering, 107(7), 603-630. [3] Chen, J. S., Hillman, M., & Rüter, M. (2013). An arbitrary order variationally consistent integration for Galerkin meshfree methods. International Journal for Numerical Methods in Engineering, 95(5), 387-418. [4] Elgamal, A., Yang, Z., Parra, E., & Ragheb, A. (2003). Modeling of cyclic mobility in saturated cohesionless soils. International Journal of Plasticity, 19(6), 883-905. [5] Yang, Z., Elgamal, A., & Parra, E. (2003). Computational model for cyclic mobility and associated shear deformation. Journal of Geotechnical and Geoenvironmental Engineering, 129(12), 1119-1127.

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Title: Isogeometric Analysis with Boolean Operations

Author(s): *Xiaodong Wei, *École Polytechnique Fédérale de Lausanne, Switzerland*; Pablo Antolin, *École Polytechnique Fédérale de Lausanne, Switzerland*; Riccardo Puppi, *École Polytechnique Fédérale de Lausanne, Switzerland*; Annalisa Buffa, *École Polytechnique Fédérale de Lausanne, Switzerland*;

We present a computational framework for isogeometric analysis (IGA) to directly work on volumetric geometries constructed by Boolean operations, aiming to address the key idea of IGA that utilizes the same geometric representation in both design and analysis. Boolean operations, mainly including difference (i.e., trimming) and union, are universal in Computer-Aided Design systems to create complex geometries from simple primitives such as cubes and cylinders. However, limited effort has been devoted to supporting Boolean operations in IGA, especially when it comes to volumetric NURBS (Non-Uniform Rational B-Spline) representations. Following the precedent work on volumetric trimming [1], we focus on the union operation in this work, where the computational domain is composed of multiple independent domains and each of them has its own parameterization. To make different domains communicate with one another, we need a careful treatment for interfaces of these domains such that numerical integration is accurate on each interface, which requires us to take into account the parameterizations from both domains of an interface. Moreover, after union, generally we have elements of relatively small effective area that lead to the conditioning issue, so we need an effective stabilization scheme to resolve it but in the meanwhile, the stabilization needs to be simple enough such that it does not hinder the algorithm implementation especially in the volumetric case. In the end, we apply the proposed method to solve several benchmark problems and we demonstrate that obtained convergence rates agree with theoretical results. We also present examples with complex geometries built by Boolean operations to show the capability of the method. Reference [1] P. Antolin, A. Bu a, M. Martinelli, Isogeometric Analysis on Vrep: First Results, in preparation (2019).

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Title: A Data-driven Investigation into the Physics of Fetal Brain Morphogenesis

Author(s): *Johannes Weickenmeier, *Stevens Institute of Technology*; Koki Sagiyama, *Imperial College London*; Aishwarya Pawar, *Carnegie Mellon University*; Yongjie Zhang, *Carnegie Mellon University*; Krishna Garikipati, *University of Michigan*;

During fetal development, the human brain undergoes large topological changes and volumetric growth. The corresponding folding of the outer cortex- also known as gyrification- is driven by the migration of neurons from the ventricular zone towards the cortex. The accumulation of neurons in the cortex leads to primary folds that form consistently across all healthy brains around week 10. The development of novel magnetic resonance imaging (MRI) sequences has provided quantitative tools to assess shape, size, and structure of the developing brain; yet, the concise mechanisms behind these folding patterns remain poorly understood. We developed an image registration-based approach to investigate this spatio-temporal evolution of microstructure and topology during gestation. Specifically, we determine the distribution of migrating neurons during the onset of primary folds. Image registration is a powerful approach to quantify such large topological changes [1]. It allows us to compute a transformation map and the neuron density that maximizes the correspondence between images from consecutive gestational weeks. We use MRI data from a fetal brain atlas that is based on 81 fetuses scanned multiple times throughout gestation [2]. Our registration method minimizes a physics-based energy functional that penalizes the correspondence of voxel intensities between two images and the spatial transformation mapping such that it obeys the hyperelastic material response of brain. In order to capture cortical growth, we use a multiplicative split of the deformation gradient into an elastic and a growth part. We assume isotropic volume-growth proportional to the local neuron density and constitute that the elastic response of the brain follows a classical neo-Hookean strain energy. Ultimately, our optimization problem provides the deformation mapping and cell density changes between two consecutive gestational weeks ranging from 21 through 27. By combining these maps, we identify the cell migration patterns underlying the formation of primary folds. Our method will allow us to rationalize the origin of gyrification and provide a novel tool to study the physics behind brain malformations during early development. References [1] Gholipous et al. A normative spatiotemporal MRI atlas of the fetal brain for automatic segmentation and analysis of early brain growth, Scientific Reports (2017) 7:476 [2] Pawar et al. DTHB3D Reg: Dynamic truncated hierarchical B-spline based 3D nonrigid image registration, Communications in Computational Physics (2018) 23:877-898

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Title: 3 Unique Approaches to Additive Manufacturing Constraints in Topology Optimization

Author(s): *David Weinberg, *Autodesk, Inc.*; Nam-Ho Kim, *University of Florida*;

For over a decade Topology Optimization has been remarkably popular in the engineering design community due to its capability on designing lightweight structures by optimally distributing materials to carry loads. Autodesk Nastran has implemented Topology Optimization (TO) since 2014 and rapidly enhancing its capabilities, including multidisciplinary optimization, hierarchical distributed computing, and various manufacturing method-oriented design. This presentation shows how Autodesk Nastran TO handles additive manufacturing constraints so that the designed part can be printable. The pros and cons of three currently available algorithms are introduced. It is also discussed how the users can control parameters to produce a design that is prone to have overhang structures or a design that does not produce overhang structures. In addition we integrate a new method for precise global stress, global displacement, and global temperature constraints. For global stress constraints we only require one adjoint constraint for each stress constraint. For global displacement and temperature constraints we propose a method which allows for either a select set of grid points or all grid points in the model to be included without a substantial loss in accuracy. Examples will include solutions which are compliant in both linear statics and heat transfer and include thermal stress constraints.

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Title: Optimized Fluid Solvers for Biological Fluid-Structure Interaction Problems

Author(s): *David Wells, *University of North Carolina, Chapel Hill*; Boyce Griffith, *University of North Carolina, Chapel Hill*;

Cardiovascular fluid and solid mechanics play a key role in several cardiac diseases. Mathematical modeling, through fluid-structure interaction algorithms, provides a noninvasive way to examine these systems through computational experimentation. At its core, the interaction of the heart tissues (such as muscles and valves) and blood is a fluid-structure interaction (FSI) problem. Such FSI problems in biological applications involve several challenges, such as a range of fluid velocity scales, complex geometries, the added-mass instability, and difficulty in load balancing between the fluid and structure solvers over multiple processors. The Immersed Boundary (IB) method is a common technique for coupling the fluid and structure solvers and allows the use of a Cartesian grid finite difference fluid solver and a standard finite element structure solver, where the two solvers are coupled by computing the force on the fluid and the velocity of the structure by integrating regularized delta functions. In this talk we discuss some recent work to improve the venerable MAC (marker and cell) Navier-Stokes solver in the IBAMR (Immersed Boundary Adaptive Mesh Refinement) library and a sophisticated model of the human heart built on top of IBAMR. We discuss some new analysis tools for understanding the MAC and similar solvers as well as improvements focused on improving the MAC scheme for AMR grids in the Stokes limit.

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Title: Practical Finite-Element Schemes for Subsurface Flow Simulation

Author(s): *Laurent White, *ExxonMobil Research and Engineering*; Dimitar Trenev, *ExxonMobil Research and Engineering*; Jeremy Brandman, *ExxonMobil Research and Engineering*;

Computational simulation of coupled flow and transport in porous media plays an important role for reservoir development and management in the oil-and-gas industry, for predicting the fate of contaminants in groundwater formations as part of soil remediation efforts, and for studying geologic sequestration of carbon dioxide. Here, we mostly focus on multi-phase reservoir flow simulation and recognize that the algorithmic approaches carry over, to a large extent, to other subsurface flow problems. Improving simulation accuracy, which is the driver of this research, is important for making reliable business decisions. Computational models for reservoir flow involve the coupling between discrete approximations to phase velocities and discretized transport equations. In addition to carefully selecting computational approaches for each sub-problem – i.e., the appropriate schemes for velocity and transport discretizations – based on accuracy, speed and robustness, coupling these two computational approaches adds another layer of complexity and restrictions. In particular, the issue of mass conservation (both global and local) is often at the forefront, as spurious mass imbalances not only lead to inaccuracies but can also trigger numerical instabilities, especially for nonlinear multiphase-flow problems. Being heterogeneous and geometrically complex, geologic models are best discretized by unstructured meshes. Because of their ease of implementation and robustness, low-order finite-volume methods have been and continue to be used extensively in commercial reservoir simulators. These schemes, however, can be inaccurate for meshes that are inconsistent with the underlying permeability and for flow exhibiting sharp fronts. By contrast, in this research, we adopt a mixed finite-element approach for velocity and pressure, and a discontinuous-Galerkin method for transported quantities. While velocity and pressure are accurate in the presence of complex heterogeneities, the discontinuous-Galerkin method allows for more accurate resolution of sharp flow features. In addition, these two numerical approaches are consistent with one another: there is no mass imbalance (provided care is taken in discretizing the time derivatives as well). A complete formulation for two-phase flow is presented, where practical – yet rigorous – approximations are made and several numerical examples demonstrate the improved accuracy of the approach. We discuss the extension of the present work to three-phase flow as well as the implications of selecting this numerical scheme from a high-performance-computing standpoint.

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Title: Robust and Efficient Numerical Methods for Phase-field Fracture in Porous Media

Author(s): Sanghyun Lee, *Florida State University*; Andro Mikelic, *Université de Lyon*; Mary F. Wheeler, *UT Austin*; *Thomas Wick, *Leibniz Universität Hannover*;

Currently, fracture propagation is a major topic in applied mathematics and engineering. It seems to turn out that one of the most promising methods is based on a variational setting and more specifically on a thermodynamically consistent phase-field model. Here a smoothed indicator function determines the crack location and is characterized through a model regularization parameter. In addition, modeling assumes that the fracture can never heal, which is imposed through a temporal constraint, leading to a variational inequality system. The basic fracture model problem is augmented with several hints and discussions of serious challenges in developing numerical methods for fracture propagation. Key aspects are robust and efficient algorithms for imposing the previously mentioned crack irreversibility constraint, treatment of the indefinite Jacobian matrix, computational analysis of the interplay of model and discretization parameters, goal-functional evaluations, coupling to other multiphyics problems such as pressurized fractures, (two-phase) fluid-filled fractures, proppant-filled fractures in porous media, fluid-structure interaction, and aspects of high performance computing for tackling practical field problems. References: 1) S. Lee, A. Mikelic, M. F. Wheeler, T. Wick; Phase-field modeling of two phase fluid filled fractures in a poroelastic medium, SIAM Multiscale Modeling and Simulation, 16(4), pp. 1542–1580, 2018 2) A. Mikelic, M.F. Wheeler, T. Wick; Phase-field modeling through iterative splitting of hydraulic fractures in a poroelastic medium, accepted in International Journal on Geomathematics, doi 10.1007/s13137-019-0113-y, 2019 3) S. Lee, M.F. Wheeler, T. Wick; Iterative coupling of flow, geomechanics and adaptive phase-field fracture including level-set crack width approaches, Journal of Computational and Applied Mathematics, Vol. 314 (2017), pp. 40-60

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Title: A Space-time DPG Method for Acoustic Waves in Heterogeneous Media

Author(s): *Christian Wieners, *Karlsruhe, Germany*;

We apply the discontinuous Petrov-Galerkin method (DPG) to linear acoustic waves in space and time using the framework of first-order Friedrichs systems. Based on results for operators and semigroups of linear first-order symmetric hyperbolic systems, we show that the ideal DPG method is well-posed on a suitable subset of the space-time cylinder. Therefore, we use the graph norm of the space-time differential operator, and traces are implicitly defined as distributions. Then, the practical DPG method is analyzed by constructing a Fortin operator numerically, and nonconforming traces are considered by comparison with an equivalent conforming scheme. Moreover, we show the discrete inf-sup constant can be estimated by local eigenvalue problems. For our numerical experiments we introduce a simplified DPG method with discontinuous ansatz functions on the faces of the space-time skeleton, where the error is bounded by an equivalent conforming DPG method. In addition, we provide a Strang-type estimate to bound the quadrature error in case of heterogeneous materials. Examples for a plane wave configuration confirms the numerical analysis, and the computation of a diffraction pattern illustrates a first step to applications. Finally, we present results for a benchmark configuration in seismic imaging with a point source and a small region with measurement points, where we show that the computation on a truncated space-time cylinder allows for a substantial reduction of degrees of freedom. References L. F. Demkowicz, J. Gopalakrishnan, S. Nagaraj, P. Sepulveda. A spacetime DPG method for the Schrödinger equation. SIAM J. Numer. Anal. 55, 1740--1759, 2017. J. Ernesti and C. Wieners. A space-time DPG method for acoustic waves. http://www.waves.kit.edu/downloads/CRC1173_Preprint_2018-15.pdf J. Ernesti and C. Wieners. Space-time discontinuous Petrov-Galerkin methods for linear wave equations in heterogeneous media. http://www.waves.kit.edu/downloads/CRC1173_Preprint_2018-13.pdf

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Title: Discrete-to-Continuum Modeling of Weakly Interacting Incommensurate Lattices

Author(s): Malena Espanol, *The University of Akron*; *J. Patrick Wilber, *The University of Akron*; Dmitry Golovaty, *The University of Akron*;

A graphene sheet is a single-atom thick macromolecule of carbon atoms arranged in a honeycomb hexagonal lattice. When observing a graphene sheet suspended over a substrate, moiré patterns appear driven by lattice and orientation mismatches. In this talk, we start by presenting a formal discrete-to-continuum procedure to derive a continuum variational model for two chains of atoms with slightly incommensurate lattices. The chains represent a cross-section of a three-dimensional system consisting of a graphene sheet suspended over a substrate. We show that the continuum model recovers both qualitatively and quantitatively the behavior observed in the corresponding discrete model. We then extend the discrete-to-continuum procedure to square lattices and give some ideas of how to extend it to honeycomb hexagonal lattices. In all cases, we observe the presence of large commensurate regions separated by localized incommensurate domain walls, in agreement with experiments.

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Title: Multiscale Hybridized Methods for Multiphysics Systems with Applications to Subsurface Flow and Transport

Author(s): *Tim Wildey, *Sandia National Labs*;

Multiphysics systems, such as those occurring in many subsurface applications, are typically strongly coupled, highly nonlinear and characterized by multiple physical phenomena that span a large range of length- and time-scales. Performing direct numerical simulation of such systems that resolves all of the relevant length- and time-scales is often prohibitive, even on the modern leadership-class computing platforms. Consequently, we are interested in developing multiscale methods to allow the incorporation of fine scale information into a coarse scale approximation. The process of injecting information from unresolved, or subgrid, scales into a coarse scale discretization has been pursued in several different ways by different communities. Many of the existing approaches are based on computational homogenization where the objective is to define model parameters on the coarse grid in a consistent manner so that the coarse scale solution is a reasonably accurate numerical approximation of the fine scale solution. While tremendous progress has been made both theoretically and computationally, the process usually requires rather strict assumptions and is difficult to generalize to multiphysics applications. In this presentation, we describe our recent efforts to develop a framework to enable concurrent multiscale approaches for multiphysics systems that do not rely on homogenization and are amenable to moving beyond forward simulation. We describe some of the similarities between our approach and existing methods, e.g., the variational multiscale method, the hybridizable discontinuous Galerkin method, and the multiscale discontinuous Galerkin method. Numerical examples will be presented to illustrate the benefits in using this multiscale approach for a subsurface multiphase flow and transport in a massively parallel computing environment.

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Title: Control of Sound Absorption in a 1-D Magnetorheological Elastomer Based Acoustic Metamaterial

Author(s): *Carson Willey, *UES/AFRL*; Vincent Chen, *UES/AFRL*; Kenneth Scalzi, *UES/AFRL*; Philip Buskohl, *AFRL*; Abigail Juhl, *AFRL*;

Lightweight metamaterials based on weighted elastomeric panels can be used for sound absorption of low frequency noise; however, their attenuation is typically limited to a set of narrowband frequencies. In this presentation, acoustic panels will be fabricated out of magnetorheological elastomers (MRE) composed of magnetic iron particles within a silicone matrix, so that the surface of an MRE panel can be decorated with magnetic masses. The placement and configuration of the magnets affect the mode shapes and corresponding resonance frequencies of the panel vibration, which in turn impacts the band gaps in acoustic transmission or reflection from the panel. Since the magnets are held in place by magnetic force, they can easily be reconfigured to affect a new set of frequencies. A one-dimensional (1-D) reconfigurable metamaterial can be formed by placing these panels in series, separated by acoustic domains. The system is novel in its reconfigurablilty, and uncommon use of placing permanent magnets directly on the MRE layer for tuning. In this work, a finite element model is studied which focuses on the placement and configuration of magnetic masses on a MRE panel and the resulting acoustic transmission.

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Title: Chemo-Thermo-Mechanical Modeling of HMX Based Plastic Bonded Explosives

Author(s): *Cedric Williams, *University of Notre Dame*; Mohammad Shabouei, *University of Notre Dame*; Karel Matouš, *University of Notre Dame*;

Reactive and energetic materials are used in many military, commercial, and industrial settings. As such, a comprehensive understanding of the chemical, thermal, and mechanical behavior of these highly heterogeneous materials is exceedingly desirable. Predictions of this nature involve resolving many inherent spatial and temporal complexities. To do so, a fully coupled chemo-thermo-mechanical (CTM) model is developed and implemented computationally using the Finite Element Method. The developed solver operates in a modular fashion. A finite strain, quasi-steady mechanical solver resolves displacements, stress and strain fields, and etc., by considering nonlinear material behavior modeled by hyperelasticity and J2 plasticity. A fully transient monolithic thermo-chemical solver resolves temperature and chemical reaction evolutions by considering advection, diffusion, and reaction phenomena. These modules operate in a staggered fashion; elastic and inelastic dissipations and displacements produced through the simulated mechanical responses are incorporated into and influence the thermo-chemical module as heating terms and velocity contributions, while thermal expansion due to temperature changes that are resolved by the thermo-chemical module influence the mechanical response. In this work, the solver is used to model HMX based plastic bonded explosives.

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Title: Nonlinear Thermoelectromechanical Modeling and Simulation of Ferroelectric Materials Based on a Variational Formulation

Author(s): *Marius Wingen, *University of Kassel*; Andreas Ricoeur, *University of Kassel*;

Due to their special electromechanical properties, nowadays ferroelectric materials are widely used in many technical applications, mostly as actuators or sensors. Advantages compared to other smart devices are their extremely fast reaction times in a range of $\mu s-ms$ and large actuation forces. In the past, temperature changes inside the material were rather disturbing during the investigation and usage of these materials and were mostly neglected in numerical models, although they may have a non-negligible impact on issues like phase transitions, domain wall motion or reliability and lifetime. One example is the dynamic operation of piezoelectric actuators, resulting in self-heating. In case of insufficient heat dissipation, phase transformations may arise in addition to structural problems due to thermal stresses. In materials with low Curie temperature, such as barium titanate, even depolarization may occur. Experiments have shown, that transient electromechanical fields in ferroelectric materials lead to two types of temperature changes [1,2]. There is a reversible temperature change, which can heat or cool the material and a much stronger irreversible heating caused by domain switching. In this work, the theoretical background and a Finite Element (FE) approach based on a micromechanically and physically motivated nonlinear constitutive model are presented [3]. The model considers the mutual nonlinear coupling of thermal and electromechanical fields. Weak formulations are introduced based on a generalized Hamilton-Jourdain type variational approach. The numerical calculations show the effects of temperature on the electromechanical field quantities and vice versa. They also reveal switching processes in ferroelectrics and associated heating, taking into account their dependence on temperature. Results of temperature changes at a crack tip due to domain switching at subcritical electric loading and of the heating of a bulk specimen are compared to experimental findings, just as polarization hystereses at different temperatures. [1] Chen, H.-S., Pei, Y.-M., Liu, B. and Fang, D.-N.: Rate dependent heat generation in single cycle of domain switching of lead zirconate titanate via in-situ spontaneous temperature measurement. Applied Physics Letters 102, 242912 (2013); doi: 10.1063/1.4811702. [2] Molin, C., Sanlialp, M., Shvartsman, V. V., Lupascu, D. C., Neumeister, P., Schönecker, A. and Gebhardt, S.: Effect of dopants on the electrocaloric effect of 0.92 Pb(Mg1/3Nb(2/3)O3-0.08 PbTiO3 ceramics. Journal of the European Ceramic Society, Volume 35, Issue 7, p. 2065-2071 (2015). [3] Wingen, M. and Ricoeur, A.: Caloric aspects of nonlinear ferroelectric constitutive behavior: modeling and simulation. Continuum Mechanics and Thermodynamics; doi:10.1007/s00161-018-0711-1 (2018).

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Numerical Solution of Shallow Water Equations with Subgrid Corrections Accounting for Unresolved Topography

Author(s): *Damrongsak Wirasaet, *University of Notre Dame*; Andrew Kennedy, *University of Notre Dame*; Diogo Bolster, *University of Notre Dame*; Casey Dietrich, *North Carolina State University*; Amirhosein Begmohammadi, *University of Notre Dame*; Thosmas Sherman, *Univetrsity of Notre Dame*;

In numerical modelling of flow based on 2D shallow water equations, bottom topographical features smaller than the model grid resolution, such as small channels, could in fact represent important flow passages conveying water from one area to another. A performance of the model may suffer significantly from the absence of such subgrid details, especially in inundation and recession zones of flow in previous-dry and wet areas. In this work, we present a set of 2D shallow flow equations with subgrid corrections deriving from applying the volume averaging technique to the conventional 2D shallow water equations. Numerical methods for these equations based on finite-difference and finite-element methods will be presented. Numerical results demonstrate that the subgrid corrections can substantially improve the predictive capability of the coarse-grid solutions with relatively small additional computational expense.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Enriched Finite Volume Methods - Taylored Test Spaces for Flows with Particles

Author(s): *Gabriel Wittum, *AMCS, KAUST*; Susanne Hoellbacher, *AMCS,KAUST*;

We present a fully-implicit and stable finite element and finite volume scheme for the simulation of freely moving particles in a fluid. Our method is based on the Petrov-Galerkin formulation of a vertex-centered finite volume scheme on unstructured grids. Appropriate extension of the ansatz and test spaces lead to a direct formulation. No additional Lagrange multipliers or artificial external forces need to be introduced for the fluid-solid coupling. The interface forces are imposed through the original bilinear form for the fluid. The surface integrals of the finite volume scheme enable a natural incorporation of the interface forces. As a result, only one single solve for the derived linear system for the fluid together with the particles is necessary and the proposed method does not require special time stepping schemes to balance the interaction forces between fluid and particles. For the linear Stokes problem we prove the stability of both schemes. Moreover, for the stationary case the conservation of mass and momentum is not violated by the extended scheme, i.e. conservativity is accomplished within the range of the underlying, unconstrained discretisation scheme. The scheme is applicable for problems in two and three dimensions. We show results of numerical tests.

15th U.S. National Congress on Computational Mechanics
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Title: Interfacing Hydrodynamic and Geotechnical Modeling for the Assessment and Communication of Flooding Risks due to Flood Defense System Failures

Author(s): *Dylan Wood, *The Ohio State University*; Ethan Kubatko, *The Ohio State University*; Mehrzad Rahimi, *The Ohio State University*; Abdollah Shafieezadeh, *The Ohio State University*;

A key aspect of disaster management in preparation for a severe weather event is the assessment of risk due to flooding. Central to these efforts is information on the reliability of flood defense systems, since failures of these systems can lead to catastrophic economic, social and/or environmental losses. Reliability analysis for flood defense structures (\emph{e.g.}, levees, dikes, sheet piles) is often geotechnical in nature, and it should account for different failure mechanisms (e.g., seepage, slope failure, tilting) as well as correlations between these mechanisms in both space and time. In forecasts of flooding risks due to severe weather, many agencies produce predictions of impacts such as hurricane storm surge based on the results of hydrodynamic modeling, but detailed assessments on the reliability of structures are rarely performed concurrently in such analyses, despite that the response of flood defense structures to the loading of flood waters may likely impact patterns of inland flood propagation, especially if these structures were to fail. We present on efforts towards developing and interfacing hydrodynamic and geotechnical modeling methods with the goal of producing an adaptive-resolution storm surge model that responds to the changing state of flood control systems. We may show that hydrodynamic modeling can acceptably assess some hydraulic failures, such as overtopping; however, to effectively assess the risks of structural failure a feedback loop must be integrated between hydrodynamic modeling results and geotechnical reliability models, whereby the reliability modeling can be informed of changes in flow conditions by the hydrodynamic modeling, which can then subsequently inform the hydrodynamic modeling of changes in structures. This dynamic feedback between different engineering modeling techniques will crucially enhance probabilistic assessment of risk due to storm impacts for both short and long-term disaster preparedness efforts.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: The Momentum-Consistent Smoothed Particle Galerkin (MC-SPG) Method for the Extreme Thread Forming Simulation in Flow Drill Screwing Process

Author(s): *C.T. Wu, *LSTC*; Xiaofei Pan, *LSTC*; Wei Hu, *LSTC*; Youcai Wu, *LSTC*; Zeliang Liu, *LSTC*;

Flow drill screwing (FDS) is a modern mechanical fastening technique for joining metal materials in lightweight car structures. Finite element simulation of FDS process probably is one of the biggest challenges for CAE engineers in automotive applications. This is mainly because finite element methods inevitably encounter utmost numerical difficulties associated with meshing issues in modeling the extensive plastic deformation and material failure taking place in the FDS thread forming process. This paper presents a simulation of FDS process using a new particle method. Different from other particle stabilization methods which are obtained by modification of the variational equation using either residual or non-residual stabilization terms, the present method introduces a novel velocity smoothing algorithm to achieve the stabilization effect. It is shown that the semi-discrete equation based on the smoothed velocity field is consistently fulfilling the conservation of linear and angular momentum. Since the new method does not require stabilization terms, it avoids the fundamental difficulty inherent in the stabilization stress computation, thus more computationally efficient. Finally, the stabilized formulation is supplemented with the adaptive anisotropic Lagrangian kernel and bond-based failure criterion to extend the application in severe deformation and material failure analysis. Three numerical benchmarks including one thread forming simulation are utilized to demonstrate the effectiveness of the new approach.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Recent Advances in FSI Using Immersogeometric Techniques

Author(s): *Michael C. H. Wu, *Brown University*; David Kamensky, *Brown University*; Ming-Chen Hsu, *Iowa State University*; Yuri Bazilevs, *Brown University*;

Due to the high demand for greater levels of physical realism in engineering applications, techniques for computational fluid–structure interaction (FSI) continue to be actively developed. Besides boundary-fitted methods, non-boundary-fitted methods, such as immersogeometric analysis (IMGA), have been successfully applied to FSI analysis of bio-systems, especially heart valve simulations. IMGA analyzes a high-order surface representation of the shell structure by immersing it into a non-boundary-fitted discretization of the background fluid domain. For other applications such as helicopter simulation, a hybrid method using both moving-mesh techniques and IMGA is proposed, to obtain high-accuracy results around fluid–structure interfaces with affordable computational power. In this presentation, the fundamentals and some recent advances of the method will be discussed.

15th U.S. National Congress on Computational Mechanics
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Title: Tightly Coupled, Partitioned Fluid-Structure Interaction Analysis of a Horizontal Plate Impact onto a Water Free Surface: Computational Framework and Validation

Author(s): *Wensi Wu, *Cornell University*; Christopher Earls, *Cornell University*;

“Slamming”-induced hydroelastic effects accompanying a horizontal plate impacting a water free surface is investigated numerically using an in-house developed Fluid-Structure Interaction (FSI) solver. The computational framework of the FSI solver involves an implicit, partitioned coupling of an open source computational fluid dynamics (CFD) tool (https://openfoam.org) to an open source computational structural dynamics (CSD) tool (https://github.com/nonlinearfun/CU-BENs/releases). The numerical challenges owing to the added-mass effects accompanying high relative fluid-structure density ratios are mitigated through the use of implicit coupling schemes. The air-water interface is captured by the volume of fluid method in the CFD modeling, while the high strain rates and nonlinear responses due to slamming loads are considered within the CSD modeling context. The hydroelastic responses (i.e., longitudinal strain and out-of-plane deformation) of three types of plates: rigid, moderately deformable, and flexible are considered. The numerical results will be validated against experimental data[1] both qualitatively (i.e., visual comparison) and quantitatively based on a set of validation metrics[2]. This rigorous validation approach allows for the assessment of accuracy within the computational models in terms of the precision within the experimental measurements; thus a series of enhancements in both the computational models and experimental methods can be developed, so that improvements can be made in both the numerical and experimental regimes. Reference: [1] Wang, A., Kim, H., Wong, K., Yu, M., Kiger, K., & Duncan, J. (2018, November). The oblique impact of a flexible flat plate on a water surface. Atlanta, Georgia. [2] Oberkampf, W. L., & Barone, M. F. (2006). Measures of agreement between computation and experiment: Validation metrics. Journal of Computational Physics, 217(1), 5 - 36. (Uncertainty Quantification in Simulation Science) doi: 10.1016/j.jcp.2006.03.037

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Approaches to H and H-P Adaptation and Computational Geometry Access

Author(s): *Nick Wyman, *Pointwise, Inc.*; Steve Karman, *Pointwise, Inc.*;

Recent work in the Pointwise mesh generation software for H and H-P adaptation will be discussed. A cloud of points scheme is used to communicate adaptation requirements in a compact efficient manner. The adaptation scheme allows for refinement and derefinement of a mesh at the curve, surface, and volume levels. Adherence to the supporting computational geometry is maintained at all times. Status of on-going work including mixed order adaptation and H-P adaptation based on solution features will be presented. Finally, an open mesh-geometry associativity schema will be discussed along with examples of how the schema can be used with a geometry kernel to provide efficient access to computational geometry to third-party software.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Non-intrusive Inference Based Reduced Order Model for Fluids Using Deep Neural Network

Author(s): *Xuping Xie, *Oak Ridge National Lab*; Guannan Zhang, *Oak Ridge National Lab*; Clayton Webster, *Oak Ridge National Lab*;

In this effort we propose a data-driven learning framework for reduced order modeling of fluid dynamics. Designing accurate and efficient reduced order models for nonlinear fluid dynamic problems is challenging for many practical engineering applications. Classical projection-based model reduction methods generate reduced systems by projecting full-order differential operators into low-dimensional subspaces. However, these techniques usually lead to severe instabilities in the presence of highly nonlinear dynamics, which dramatically deteriorates the accuracy of the reduced-order models. In contrast, our new framework exploits linear multistep networks, based on implicit Adams-Moulton schemes, to construct the reduced system. The advantage is that the method optimally approximates the full order model in the low-dimensional space with a given supervised learning task. Moreover, our approach is non-intrusive, such that it can be applied to other complex nonlinear dynamical systems with sophisticated legacy codes. We demonstrate the performance of our method through the numerical simulation of a two-dimensional flow past a circular cylinder with Reynolds number Re = 100. The results reveal that the new data-driven model is significantly more accurate than standard projection-based approaches.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Immersogeometric Analysis of Compressible Flows with Application to Aerodynamic Simulation of Rotorcraft

Author(s): *Fei Xu, *ANSYS, Inc.*; Yuri Bazilves, *Brown University*; Ming-Chen Hsu, *Iowa State University*;

We present an Immersogeometric Analysis (IMGA) approach for the simulation of compressible flows around complex geometries. In this method, compressible flow simulations are performed directly on various boundary representations (B-reps) of mechanical designs, circumventing the labor-intensive and time-consuming cleanup of complex geometric models. A new formulation for the weak imposition of essential boundary conditions in the context of non-body-fitted meshes is proposed. The formulation employs the non-symmetric Nitsche method, which yields good performance especially when the penalty parameters are difficult to estimate. We test the proposed immersogeometric formulation on benchmark problems for a wide range of Reynolds and Mach numbers, showing its robustness and accuracy. Finally, the methodology is applied to the simulation of a UH-60 Black Hawk helicopter in forward flight, illustrating the ability of the proposed approach to support the design of real-world engineering systems through high-fidelity aerodynamic analysis.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Inextensional Vibrations of Thin Spherical Shells Using Strain Gradient Elasticity Theory

Author(s): *Rajesh Yadav, *PhD Research Scholar, Indian Institute of Technology Kanpur, Kanpur*; Shakti Gupta, *Associate Professor, Indian Institute of Technology Kanpur, Kanpur*;

Here, we derive frequency expressions for inextensional mode vibrations of a thin spherical shell using Rayleigh's quotient. The material of the shell is considered to be linearly elastic, homogeneous, isotropic and grade-2 [1]. In the Rayleigh's quotient, the strain energy of small deformations is computed using positive and negative strain gradient based constitutive law [2] which includes a strain gradient microstructural parameter and the kinetic energy for the grade-2 material is computed which includes an additional microstructural parameter known as inertia gradient parameter. Both microstructural parameters have dimensions of length. If we neglect the small scale microstructural effects, then the derived frequency expression reduces to that obtained when Hooke's law is used for computation of strain energy. We find that the frequency expressions for inextensional vibrations, predicted by positive and negative strain gradient based constitutive law, differ from the classical continuum theory expressions by a multiplicative factor which further depends on the microstructural parameters. We also observe that the strain gradient theory with positive sign exhibits a saturation-like behaviour of the inextensional mode frequency with the circumferential wave number. In addition, the strain gradient theory with negative sign increases the effective stiffness of the spherical shells and hence it increases the natural frequency of shells. The inclusion of inertia gradient increases the kinetic energy and hence affects the inability of inextensional vibrations of the spherical shells and shifts to the lower circumferential wave numbers for larger inertia gradient parameters. In the recent past in order to accurately model the dynamic behaviour of nanostructures strain gradient theory has been employed by Das et al. [3] without inertia gradient parameter and the current work well agrees qualitatively with the results obtained by Das et al. [3]. REFERENCES 1. Polizzotto C (2012) A gradient elasticity theory for second-grade materials and higher order inertia. International Journal of Solids and Structures 49 2121-2137 2. Altan B S and Aifantis E C (1997) On some aspects in the special theory of gradient elasticity Journal of the Mechanical Behaviour of Materials 8 231-282 3. Das S L, Mandal T and Gupta S S (2013) Inextensional vibration of zigzag single-walled carbon nanotubes using nonlocal elasticity theories International Journal of Solids and Structures 50 2792-2797

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Tuning Strategy of Solving the Hubbard Model by LOBPCG Method on CUDA GPU

Author(s): *Susumu Yamada, *Japan Atomic Energy Agency*; Toshiyuki Imamura, *RIKEN*; Masahiko Machida, *Japan Atomic Energy Agency*;

The Hubbard model has attracted much attentions of physicists, because the model is considered to describe various interesting phenomena such as High-Tc superconductivity in spite of its simplicity. So far, a tremendous number of physicists have tried to solve the model with their theoretical and computational ideas. One of the most precise computational approach is the so-called exact diagonalization method, which directly solves the Hamiltonian matrix as its eigenvalue problem. Since the Hamiltonian matrix is a huge sparse symmetric one, only the ground state (the smallest eigenvalue and the corresponding eigenvector) is demanded. Therefore, the LOBPCG (Locally Optimal Block Preconditioned Conjugate Gradient) method [1] can be utilized as a suitable solver [2]. Since the LOBPCG method is an iteration scheme, the most consuming operation is inside the matrix-vector multiplication part. When we decompose the Hamiltonian based on the physical property, the nonzero elements of the decomposed submatrices can be arranged orderly. Then, the multiplication operation can be easily accelerated with standard tuning strategy. Moreover, most operations except the matrix-vector multiplication operation of the LOBPCG method are basically linear calculations. Therefore, when executing them on CUDA GPU, we can achieve high performance by using cuBLAS library [3]. However, there are still possibilities that some operations can be tuned further by taking account of the character of the algorithm of the LOBPCG method. In this presentation, we propose some tuning strategies of the LOBPCG method for the Hubbard model on CUDA GPU based on the above concepts. Finally, we present results of the numerical tests on NVIDIA Tesla P100 (Reedbush Supercomputer system in The University of Tokyo) and discuss the effectiveness of our strategies. [1] A. V. Knyazev, “Preconditioned eigensolvers - an oxymoron?”, Electronic Transactions on Numerical Analysis, 7: 104–123, 1998. [2] S. Yamada, et. al., “16.447 TFlops and 159-Billion-dimensional Exact-diagonalization for Trapped Fermion-Hubbard Model on the Earth Simulator”, Proc. of SC05, 2005. [3] cuBLAS, URL: https://docs.nvidia.com/cuda/cublas/

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Numerical Verification Procedure for Finite Element Analysis of Contact Problem

Author(s): *Takahiro Yamada, *Yokohama National University*;

Contact problems frequently arise in industrial applications and they are recognized as one of the most important problems in solid mechanics. Despite such importance of contact problems, there are few verification methods for their numerical procedure. The most popular procedure is the comparison with exact solution of the Hertz contact problem and its numerical solution. In this problem, we consider only ideal geometrical shapes and small deformations and hence numerical procedures cannot be verified in practical situations and large deformation ranges. In this work, we propose a verification procedure for contact problems based on the method of nearby problems. The method of nearby problems developed by Roy et al. is a sophisticated verification procedure, in which the problems with exact solutions near the target problem of interest can be generated by a curve fitting of a numerical solution to a continuous function. The authors developed several formulations and techniques that allow us to apply the method of nearby problems to nonlinear finite element analysis of solid. In our approach, equivalent nodal vectors associated with body forces and tractions in a nearby problem can be obtained without calculation of the spatial derivative of stresses. In our application of the method of nearby problems to contact problems, we construct the nearby problem without contact boundary condition from the numerical solution with contact condition imposed. In such a nearby problem, the traction derived from the contact condition in the original problem can be obtained. To verify the solution, the numerical solution of the nearby problem is compared with that of the original problem and we confirm that the traction force of the nearby problem causes the similar deformation to that given by the original contact problem. Furthermore, the traction obtained by the nearby problem can be evaluated in the view of the friction model on the contact surface. Several representative numerical results are presented to show the validity of the present approach.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Thermal Fluid Flows on Moving Domains with Applications to Metallic Additive Manufacturing

Author(s): *Jinhui Yan, *University of Illinois, Urbana-Champaign*;

A thermal fluid flow formulation, considering phase transition, surface tension, Marangoni stress, and interfacial topological changes, is proposed on moving domains through ALE-VMS approach. The formulation is thoroughly validated by a series of benchmark problems. The formulation is applied to model the 2018 NIST additive manufacturing benchmark problem. It is proved that the formulation is able to accurately predict temperature evolution, melt pool dimensions, cooling rate and the 3D surface features of the solidified laser tracks, including the height distribution perpendicular to the laser track and the geometry and spacings of the chevron features. The framework shows great potential in a wide arrange of applications in metallic additive manufacturing.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: A Comparison of Two Commercial Software in Simulating a Selective Laser Melting Manufacturing

Author(s): Ming Liu, *Monash University*; Louis Chiu, *Monash University*; *Wenyi Yan, *Monash University*;

With the rapid development of additive manufacturing (AM) techniques, effective and efficient simulation is required by AM industries. The first generation of commercial software have been developed, enabling the thermal and thermomechanical analysis of different AM processes. Since commercial software are still experiencing rapid development, the strength and limitations of these software are not clearly understood. In this work, two commercial software, Netfabb from Autodesk and Simufact Additive from MSC, were used to simulate a selective laser melting (SLM) process and obtain the temperature evolution during the manufacturing of two simple plates. The simulated results were compared with experimental data obtained by inserting thermocouples at 8 target locations on two plates in Monash Centre for Additive Manufacturing [1]. Netfabb and Simufact Additive employ different modelling strategies to simplify a printing process and reduce computational time. In Netfabb, a process parameter file contains data from simulating the SLM of a 1 mm cube at a micro-scale, which is then mapped to the modelled component in the part-scale simulation. This multi-scale modelling allows for fast and accurate simulation of entire parts. In Simufact Additive, secondary parameters are calculated automatically based on the input parameters and they are used as inputs in multi-layer addition strategy to accelerate computation. The simulated temperatures from both software in this case study were lower than experimental measurements at every thermocouple position. The simulated and measured highest temperatures were 186.59 ? and approximately 258?, respectively. Furthermore, neither software was able to capture a valid peak temperature. Overall, Netfabb predicted more accurate results with less computational time than Simufact Additive. Some simplifications and assumptions, which contribute to the observed discrepancy between the simulated and observed response were identified and discussed. 1. Chiumenti, M., et al., Numerical modelling and experimental validation in Selective Laser Melting. Additive Manufacturing, 2017. 18: p. 171-185.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: New Algorithms for Image-based Virtual Microstructure Reconstruction: Application to Modeling Nonwoven Entangled Fibrous Materials

Author(s): *Ming Yang, *The Ohio State University*; Mingshi Ji, *The Ohio State University*; Soheil Soghrati, *The Ohio State University*;

A new microstructure reconstruction framework is introduced for the virtual reconstruction of heterogeneous microstructures using Non-Uniform Rational B-Splines (NURBS) to explicitly represent morphologies of embedded particles/fibers. As a pre-processing phase, a library of the embedded heterogeneities shapes, parameterized in terms of NURBS functions, is extracted from the image data. Three different algorithms are then employed to reconstruct an initial model of the microstructure. In the first approach for materials with fibrous microstructures, the NURBS curves corresponding to centerlines of fibers are directly used to virtually pack them in the raw microstructure. For particulate composites, the second algorithm implements a set of hierarchical bounding boxes approximating the geometry of each particle to check for overlap. The compacted materials are handled by the third algorithm, which transfers the raw microstructure into a compression model to generate the microstructure with high volume fraction. An optimization phase is then applied to build the final microstructural model, relying either on the Genetic Algorithm to selectively eliminate some of the inclusions or their sequential relocation within the raw microstructure. The target statistical microstructural descriptors such as the volume fraction, size distribution, and spatial arrangement of inclusions are the objectives applied in this optimization phase. In this presentation, we also show the application of the first set of algorithms for analyzing the micromechanical behavior of a fiberglass pack insulation pack with cross-linking between fibers. This nonwoven entangled material has a complex microstructure and highly nonlinear deformation response subject to compressive loads, which are necessary for efficient shipping and handling. After the virtual reconstruction of microstructural models of the insulation pack, we automatically convert them into geometrically reduced-order finite element (FE) models to simulate this behavior. In this approach, fibers are modeled using beam elements, while polymer binder particles providing cross-linking between them are modeled using a truss-shaped set of bushing-like connector elements. Comparison with high-fidelity 3D FE simulations is provided to verify the accuracy of this model. Finally, a comprehensive study is carried out to determine the impact of boundary conditions, size of representative volume element (RVE), cross-linking, and presence of fiber bundles on the micromechanical behavior of the fiberglass packs. Yang, Ming, et al. "Cross-linked fiberglass packs: microstructure reconstruction and reduced-order finite element analysis of the micromechanical behavior". COMPUTERS & STRUCTURES, 209, 182-196 (2018). Yang, Ming, et al. "New algorithms for virtual reconstruction of heterogeneous microstructures". COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING, 338, 275-298 (2018).

15th U.S. National Congress on Computational Mechanics
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Title: A Reproducing Kernel Particle Finite Volume Method for Linear and Nonlinear Mechanics

Author(s): *Saili Yang, *The Pennsylvania State University*; Michael Hillman, *The Pennsylvania State University*;

In the past 20 years, significant effort has been devoted to developing the weak form based Galerkin meshfree methods and the strong-form based collocation meshfree methods. For instance, many treatments have been developed to overcome issues of imposing essential boundary conditions, instability in nodal integration, and quadrature in general. Strong form based meshfree methods do not have these issues, but require other techniques to avoid computing higher order derivatives which incurs a non-trivial cost. A finite volume method based on the reproducing kernel approximation is proposed and developed for linear and nonlinear mechanics. This method follows the global Petrov-Galerkin formulation with a conforming Heaviside test function. The divergence theorem is applied to transfer the integration to be on the cell boundaries, which avoids higher order derivatives. The variational consistency conditions are inherently satisfied, and the method attains optimal convergence rates with low-order quadrature. Furthermore, the essential boundary conditions can be easily imposed by direct collocation, and no instability is observed despite it being a purely node-based method. The proposed approach is developed for linear statics, elastodynamics, as well as nonlinear mechanics under the Total and Updated Lagrangian frameworks. Several benchmark examples are presented to demonstrate the efficiency, accuracy, and stability of the method for linear and nonlinear mechanics.

15th U.S. National Congress on Computational Mechanics
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Title: Goal-oriented Model Reduction of Parametrized Reynolds-averaged Navier-Stokes Flows in Aerodynamics

Author(s): *Masayuki Yano, *University of Toronto*;

We consider goal-oriented model reduction of parametrized Reynolds-averaged Navier-Stokes (RANS) equations to provide rapid and reliable predictions of aerodynamic lift and drag. The key ingredients of our formulation are as follows: the discontinuous Galerkin finite element (FE) method, which provides stability for convection-dominated problems; the dual-weighted residual (DWR) method, which provides effective error estimates for quantities of interest; reduced basis (RB) spaces, which provide rapidly convergent approximations of the parametric manifolds associated with the primal and adjoint solutions; the empirical quadrature procedure (EQP), which provides hyperreduction of the primal problem, adjoint problem, and DWR error estimate while providing a quantitative control of the hyperreduction error; and a weak greedy algorithm, which simultaneously identifies the FE spaces, RB spaces, and EQPs to control the output error. The resulting reduced model provides rapid output predictions and the associated error estimates in the online stage. We demonstrate the approach in the context of flight-parameter sweep and uncertainty quantification for three-dimensional aerodynamic flows.

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Title: An Equal-distance Smoothing Method for a Set of Particles Distributed on an Arbitrary 3D Surface and Remapping of a Surface Particle System

Author(s): *Jin Yao, *Lawrence Livermore National Laboratory*;

We propose a simple method to distribute a set of particles evenly by distance on an arbitrarily specified 3D surface. We also propose a scheme for remapping between particle systems that describe a given surface in space with the proposed smoothing method. We show applications of the proposed equal-distance smoothing method and remapping scheme in 3D front evoluation problems using a mesh-free tracking method.

15th U.S. National Congress on Computational Mechanics
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Title: Nonlinear Finite Element Analysis of Functionally Graded Micro Porous Plates under Thermal-Mechanical Loading

Author(s): *Francisco Yapor Genao, *Western Michigan University*; Jinseok Kim, *Western Michigan University*;

A finite element model of functionally graded micro porous plates based on a general third order shear deformation plate theory (GTPT) is presented. The functionally graded porous material is often applied to thermal-mechanical coupled micro-electro-mechanical systems (MEMS) or nano-electro-mechanical systems (NEMS) applications. It is necessary to investigate the mechanical behavior of functionally graded microporous plates under thermal mechanical loading. Kim and Reddy [1] developed a finite element model for functionally graded micro plates based on the GTPT and the modified couple stress theory [2] to capture the size dependency in small-scale structures. In the current study, a finite element analysis is conducted to study the effect of porosity distribution, material variation, and size of structures on the bending behavior of functionally graded micro porous plates under thermal-mechanical loading. A displacement-based weak-form Galerkin finite element model is developed using the principle of virtual work. The size dependency is captured using a length scale parameter via the modified couple stress theory. The variation of two-constituents and porosity distribution are assumed only through thickness direction according to a power-law distribution and a cosine distribution [3], respectively. Three different types of porosity distributions (one symmetrical and two asymmetrical distributions) are considered. Numerical results for static bending problems of rectangular plates with various boundary conditions are presented. The parametric effects of the power-law index, types of porosity distribution, and length scale parameter on the bending deflections are discussed. [1] J. Kim, J. N. Reddy, A general third-order theory of functionally graded plates with modified couple stress effect and the von Kármán nonlinearity: Theory and finite element analysis, Acta Mechanica 226 (9), 2973-2998, 2015 [2] F. Yang, A. C.M. Chong, D. C.C. Lam, and P. Tong. Couple stress based strain gradient theory for elasticity. International Journal of Solids and Structures, 39(10):2731-2743, 2002 [3] J. Kim, K. K. Zur, J. N. Reddy, Bending, free vibration, and buckling of modified couples stress-based functionally graded porous micro-plates, Composite Structures 209, 879-888, 2019

15th U.S. National Congress on Computational Mechanics
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Title: Technology Assessment of Patents and Proposal on the Utilization of 5G Technology in Extended CAE Region

Author(s): *Kenji Yasutake, *Asteroid Research Inc.*;

These days, the third generation AI (Artificial Intelligence), IoT (Internet of Things) and 5G (5th generation mobile networks) technology is developing rapidly and it is widely utilized in various industrial fields. Especially 5G will be important as a communication platform between AI and IoT. CAE (Computer Aided Engineering) technology has been quite important for the design and development of new products and ecosystems in the enterprises. However the AI, IoT and 5G technology is not yet widely available for the Working-Level design process in the manufacturing industry. In this paper, patent trends of 5G technology about "Extended CAE" are described. First, the patent trends of 5G technology about patent pool for manufacturing industry are summarized. Second, a concept of “Extended CAE” in the industrial manufacturing process is defined and the patent trends of 5G technology about the Extended CAE are mentioned. Finally, the future development plans of 5G technology using the Extended CAE about industrial manufacturing process in the enterprises are proposed. <References> [1] Kenji. Yasutake, Utilization of CAE technology and Patent Application Strategy in Manufacturing Process (In Japanese), JSME 27th Computational Mechanics Division Conference (CMD2014), 2014, F206. [2] Kenji. Yasutake, Utilization of CAE Technology for Patent Application Strategy of Innovative Design in the Enterprise, The 12th World Congress in Computational Mechanics (WCCM2016), 2016, MS915. [3] Kenji. Yasutake, Trend of Patents about Utilization of AI Technology in Extended Computer Aided Engineering Region ~ The Field of Application and the Proposal of Development Policy of AI Technology in Manufacturing Industry ~, The 13th World Congress in Computational Mechanics (WCCM2018), 2018, MS1314.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Nanomechanics on the Single-layer Molybdenum Disulfide (MoS2)

Author(s): *Hongfei Ye, *Dalian University of Technology*; Dong Li, *Dalian University of Technology*; Zhiqin Cai, *Dalian University of Technology*; Junfei Zhao, *Dalian University of Technology*; Yonggang Zheng, *Dalian University of Technology*; Hongwu Zhang, *Dalian University of Technology*; Zhen Chen, *Dalian University of Technology*;

In the recent years, the nanoscale two dimensional materials, such as graphene, black phosphorus, molybdenum disulfide, etc., have attracted considerable attention because of their potential applications in the nanoscale electric and cooling equipment. Understanding the mechanical property of the relevant materials would facilitate their design and application. In this work, the elastic properties including the elastic modulus, Poisson's ratio, shear modulus and bending modulus of the single-layer molybdenum disulfide (MoS2) are investigated based on the nanoscale computational methods. For the elastic modulus, Poisson's ratio and shear modulus, the analytical expressions are derived based on the molecular mechanics framework. Moreover, the molecular dynamics (MD) method is adopted to verify the obtained analytical results. The results indicate that the elastic property of the single-layer MoS2 exhibits pronounced chiral dependence and size effect: as the characteristic size increases, the elastic modulus for armchair direction and zigzag direction increases and decreases, respectively, and gradually approach the same value 178.9 GPa; the Poisson's ratio for two directions decrease monotonously and gradually approach the same value 0.22; the shear modulus increases monotonously and gradually approach the same value 73.32 GPa. As for the bending modulus, a skillful computational method for the nanoscale two dimensional materials is proposed on the basis of the MD simulation. Similarly, the bending modulus exhibits obvious size and chiral dependence. The present results on the mechanical property of MoS2 provide an important reference for the design of the nanoscale product on the basis of this material, and also have an insight into the researches on the mechanical property of the other two dimensional materials. The supports from NSFC (11672063, 11672062, 11772082, 11472117 and 11232003), Young Science and Technology Star Program of Dalian (2016RQ018) and Fundamental Research Funds for the Central Universities are gratefully acknowledged.

15th U.S. National Congress on Computational Mechanics
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Title: Multi-material Topology Optimization for Continuum Structure Based on Independent Continuous Mapping Method

Author(s): *Hongling Ye, *Beijing University of Technology*; Weiwei Wang, *Beijing University of Technology*; Qingsheng Yang, *Beijing University of Technology*; Yunkang Sui, *Beijing University of Technology*;

Multi-material Topology Optimization is a simulation technique based on the principle of the finite element method which is able to determine the optimal distribution of two or more different materials in combination under thermal and mechanical loads. The purpose of present work is to study the multi-material problem with continuum topology optimization design. A model of multi-material topology optimization is established based on independent, continuous and mapping (ICM) method, which is considering structural mass as object and displacements as constraints. Firstly, two types of independent topological design variables and filter functions are introduced to realize and recognize the interpolations of the element stiffness matrix, element mass matrix and element weight. Furthermore, the displacement constraints are approximately expressed as explicit functions with respect to the design variables by taking advantage of Moore theorem. Finally, the topological optimal model is solved by using Lagrangian multiplier method. The numerical examples have best performance on the view of iterative numbers and structural mass. The results show that the presented method based on Independent Continuous Mapping (ICM) method is feasibility and effectiveness for multi-material continuum topology optimization.

15th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Magnetically Actuated Self-Folding Origami Structures

Author(s): *Qian Ye, *Ph.D. Candidate*; Shikui Chen, *Assistant Professor*; Xianfeng David Gu, *Associate Professor*;

Origami, namely the art of paper folding, has inspired the engineering design of self-assemble and reconfigurable devices. Under certain crease pattern, a 2D flatten object can be transformed into a complex 3D structure. Especially, the self-folding origami structure which fabricated along with the active material, such as ferromagnetic material, light or heat reactive polymer, and dielectric elastomer, allows the automatic switching from original status to a target shape under the corresponding stimulating conditions. The type and placement of the active material can influence the folding capabilities of a self-folding origami significantly. Particularly, the magnetic actuation can offer a fast response with remote control. Ideally, with the proper active material distribution, the target shape can be achieved accurately with a minimum amount of active material. In this paper, we propose a method using topology optimization to design magnetically actuated self-folding origami structures. The origami structure with prescribed crease pattern is modeled as a kinematic system as shown in Figure 1. Each facet is considered as a rigid body, and the folding lines are regarded as rotational joints with additional geometric constraints such as the locking angles. The topology optimization problem is summarized as finding the optimal ferromagnetic material placement on the origami structure in order to fold/unfold to the target shape under predefined magnetic field. The extended level set method which leverages the conformal mapping theory is used in this work. The conformal mapping reveals the mathematical relation of origami structure between the flatten 2D and the folding 3D status which enable us to recast the 3D topology optimization problem into 2D. The magnetic material disposition is represented by the level set function defined on the unfolded 2D plane. Meanwhile, the corresponding material locations can be transferred to the 3D targeted shape by conformal mapping for the FEM simulation. In the future, the work can be improved to a systematic method of designing shape-programmable self-folding structure. For instance, by further considering the folding lines and stimuli (like a magnetic field) as design variables, one can simplify the crease pattern or designing pieces-wise self-folding origami which can morph between multi-shapes from 2D to 3D in order to satisfy different working scenarios.

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Title: The WG and The HDG Methods

Author(s): *Xu Ye, *University of Arkansas at Little Rock*;

In this presentation, basics of the weak Galerkin (WG) method will be introduced and relations with the HDG method will be discussed. We will demonstrate that the WG and the HDG methods are two different methods representing different methodologies.

15th U.S. National Congress on Computational Mechanics
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Title: Reduced Order Modeling of the Nonlinear Time-Dependent Thermal Radiative Transfer Problem

Author(s): *Ben Yee, *Lawrence Livermore National Laboratory*; Youngsoo Choi, *Lawrence Livermore National Laboratory*; Robert Anderson, *Lawrence Livermore National Laboratory*; Geoffrey Oxberry, *Lawrence Livermore National Laboratory*;

The thermal radiative transfer (TRT) consists of two partial differential equations, the Boltzmann transport equation and a material energy balance equation, which are solved for two unknown quantities of interest: the 7-dimensional specific angular intensity and the temperature. Because of its high dimensionality, the TRT problem is a computationally challenging task that constitutes a significant portion (if not most) of the computational effort required for applications of interest such as the simulation of astrophysical phenomena or Inertial Confinement Fusion (ICF). Moreover, the coefficients and sources of the system are dependent on temperature in a highly nonlinear manner (many quantities scale as the fourth power of temperature). Because of this nonlinearity, an explicit time-stepping scheme would require a prohibitively small time step. Semi-implicit or fully implicit time stepping schemes are needed as a result, further increasing the computational difficulty of solving the TRT problem. For a small number of simulations, the computational resources required for solving large systems such as the TRT problem may be tractable. However, many applications of interest (e.g., uncertainty quantification or design optimization) require a large number of simulations, making the computational cost prohibitively large. For such applications, reduced-order models (ROMs) are a practical option. Reduced-order modeling is a technique for reducing the dimensionality of the solution space by sampling solutions of the problem within a certain parameter space. For problems within this parameter space, ROMs can reduce runtimes by many orders of magnitude while still providing sufficiently accurate solutions. In our work, we apply a projection-based reduced order model to the TRT problem discretized spatially by discontinuous Galerkin finite elements. A projection-based reduced order model has been successfully applied to many physics simulations such as computational fluids, structural dynamics, and, recently, linear Boltzmann transport problems. However, to the best of our knowledge, ROMs have never been applied to TRT problems. In particular, recent developments have made it possible to extend ROMs to nonlinear dynamical systems and to reduce the temporal dimensionality. These two developments make ROM well-suited for application to the TRT problem. In this talk, we discuss the challenges of the TRT problem from the perspective of reduced-order modeling, and we present our findings on the potential benefits of using ROMs for TRT problems. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

15th U.S. National Congress on Computational Mechanics
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Title: Entropy Stable Method for the Euler Equations Revisited: Central Differencing via Entropy Splitting and SBP

Author(s): *Helen C. Yee, *NASA Ames research center*;

The two decades old high order central differencing via entropy splitting and SBP (summation-by-parts) difference boundary closure of Olsson & Oliger (1994), Gerritsen & Olsson (1996), and Yee et al. (2000) is revisited. The entropy splitting is a form of skew-symmetric splitting of the nonlinear Euler flux derivatives. Central differencing applied to the entropy splitting form of the Euler flux derivatives together with SBP (summation-by-parts) difference boundary closure will, hereafter, be referred to as entropy split schemes. This study is prompted by the recent growing interest in numerical methods for which a discrete entropy conservation law holds, a discrete global entropy conservation can be proved and/or the numerical method possesses a stable entropy in the framework of SBP difference operators and L2-energy norm estimate. The objective of this paper is to recast the entropy split scheme as the recent definition of an entropy stable method for central differencing with SBP operators for both periodic and non-periodic boundary conditions for nonlinear Euler equations. Standard high order spatial central differencing as well as high order central spatial DRP (dispersion relation preserving) spatial differencing is part of the entropy stable methodology framework. Long time integration of 2D and 3D test cases is included to show the comparison of this efficient entropy stable method with the Tadmor-type of entropy conservative methods. Studies also include the comparison among the three skew-symmetric splittings. These are namely, entropy splitting, Ducros et al. splitting and the Kennedy & Grubber splitting.

15th U.S. National Congress on Computational Mechanics
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Title: CAD-compatible Structural Topology Optimisation

Author(s): *Ge Yin, *University of Cambridge*; Xiao Xiao, *University of Cambridge*; Fehmi Cirak, *University of Cambridge*;

We present a topology optimisation approach that is fully compatible with computer-aided design (CAD) representations used in industry. The availability of a CAD model is critical in all aspects of design, analysis and manufacturing. Topology optimisation, however, relies on a finite element analysis model to evaluate a given cost function and its derivatives with respect to some design parameters, i.e. design sensitivities. Consequently, optimisation is usually performed on a finite element analysis model, which is far from trivial to convert into a CAD model. In our approach, first a skeletonisation algorithm is used to extract the topology of the optimized structure from a finite element mesh. The obtained graph-like structural skeleton consists of edges and nodes, and is significantly easier to analyse and to manipulate than the voxel mesh. While the structural skeleton exactly encodes the topology of the optimized structure, it does not contain any thickness information and its geometry is usually not optimal. Therefore, we use the skeleton to define a spatial frame structure which is subsequently size and layout optimized. The optimized spatial frame is converted into a CAD model using Boolean combinations of a set of primitive solids, i.e. cylinders, cones and spheres.

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Title: Numerical Investigation on Flapping Aerodynamics of MAV with Active and Passive Pitch

Author(s): *Shinobu Yoshimura, *The University of Tokyo*; Giwon Hong, *The University of Tokyo*; Tomonori Yamada, *The University of Tokyo*; Naoto Mitsume, *The University of Tokyo*;

Flapping aerodynamics has been studies from a variety of perspectives in worldwide. Especially, micro air vehicles (MAVs) employing flapping wing motions have been developed in the field of engineering. There were tangible results as some prototypes of flapping wing MAVs flied up, but a number of parameters related to flapping kinematics and morphology still obscure finding out core parameters that contribute to flapping aerodynamics resulting in outstanding flight performance. In this study, taking an advantage of fluid-structure interaction simulations, we investigate flapping aerodynamics of active and passive pitch. Among various types of FSI simulations, we have been developing a parallel coupling method using partitioned coupling algorithms [1-3]. In the FSI analyses within the framework of partitioned coupling algorithms, we employ a parallel solid solver named ADVENTURE_Solid, a parallel LES-based flow solver named FrontFlow/blue (FFB), and a parallel coupling tool named ADVENTURE_Coupler for parallel data exchange and execution of partitioned coupling algorithms. In addition, we employ combined mesh controlling techniques to stabilize FSI simulations for a variety of large and complex movements of flapping wing. Pitch that is one of the rotational degrees of freedom in flapping kinematics has been reported to contribute to enhancing mean lift during strokes. However, its effect was not clearly investigated, so we set numerical experiments to evaluate the characteristics of active and passive pitch. We modeled flapping wing motions as simplifying the kinematics and morphology in consideration of the design by engineering approaches. Then, we analyzed flapping wing motions by varying the parameters related to active and passive pitch. Finally, we evaluated the aerodynamics and confirmed how active and passive pitch played to generate enough mean lift against the weight of the wing. References [1] T. Yamada, S. Yoshimura, (2008) Line search partitioned approach for fluid-structure interaction analysis of flapping wing. Computer Modeling in Engineering and Sciences, 24 (2008), 51-60. [2] S. Kataoka, S. Minami, H. Kawai, T. Yamada, S. Yoshimura, A parallel iterative partitioned coupling analysis system for large-scale acoustic fluid-structure interactions. Computational Mechanics, 53 (2014), 1299-1310. [3] T. Yamada, G.-W. Hong, S. Kataoka, S. Yoshimura, Parallel partitioned coupling analysis system for large-scale incompressible viscous fluid-structure interaction problems”, Computers and Fluids, 141 (2016), 259–268.

15th U.S. National Congress on Computational Mechanics
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Title: Data-driven Multiscale Clustering Analysis for Material Design

Author(s): *Cheng Yu, *Northwestern University*; Orion Kafka, *Northwestern University*; Hengyang Li, *Northwestern University*; Wing Kam Liu, *Northwestern University*;

Accurate prediction of material microstructure response and evolution is highly desirable for tasks such as topology optimization, material design, and manufacturing process control. However, direct representation of material microstructure in a macroscale simulation is prohibitively expensive with direct numerical simulation (DNS). To overcome this difficulty, a mechanistic data-driven framework is developed for fast multiscale analysis of material response and structure performance. The new capabilities of the proposed framework stem from three major factors: (1) the use of an unsupervised learning-based discretization method to achieve significant order reduction at both macroscale and microscale, resulting in clusters that each represents a carefully constructed region within the problem domain; (2) the generation of a database of interaction tensors among these clusters with only linear elastic analysis in the offline stage; (3) concurrent macroscale and microscale response prediction based on an efficient supervised learning algorithm to solve the mechanistic equations in the online stage. These three factors allow for an orders-of-magnitude decrease in the computational expense involved in predictions of multiscale mechanical response when compared to DNS or schemes such as FE^2 and FE-FFT. This method provides sufficiently high fidelity and speed to reasonably conduct inverse modeling for, e.g., material design and manufacturing process control.

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Title: An Asymptotically Compatible Framework for Local-nonlocal Coupling Problems

Author(s): *Yue Yu, *Lehigh University*; Huaiqian You, *Lehigh University*; Nathaniel Trask, *Sandia National Lab*; David Kamensky, *Brown University*;

In this work we consider 2D nonlocal models with a finite horizon parameter d which characterizes the range of nonlocal interactions, and its interaction with the local model. In the nonlocal differential equations the boundary conditions should be defined in a nonlocal way, namely, on a region with non-zero volume outside the surface, while in multiphysics coupling applications the physical boundary conditions are typically provided on a sharp co-dimension one surface. Therefore, a nonlocal constraint should be developed for the coupling framework, which is a proper nonlocal analogue to the local Neumann-type boundary conditions, so the formulation provides an approximation of physical boundary conditions on a sharp surface. Moreover, the asymptotic compatibility is desired in the coupling framework and the corresponding numerical solver, so the local-nonlocal coupling discretization is able to recover the classical model as both the horizon size d and a characteristic discretization lengthscale are reduced at the same rate. In this work we firstly develop a new nonlocal Neumann-type constraint as an analog to the traction load applied on a sharp interface. With rigorous mathematical analysis and numerical verifications, we show that the nonlocal model with this nonlocal constraint converges to the corresponding local problem with the local traction load as d-->0. Based on this new boundary condition, we develop the partitioned coupling methods between local and nonlocal models, and show that the coupling framework converges to the classical coupling problem as d-->0. As a numerical verification and application of the new coupling framework, we have implemented the nonlocal model in the context of an optimization based meshfree quadrature rule and couple it with a numerical solver based on finite element methods.

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Title: Mesh Optimization for Space–Time Isogeometric Analysis of Coronary Blood Flow with Vessel Wall Motion

Author(s): *Yuxuan Yu, *Carnegie Mellon University, USA*; Yongjie Zhang, *Carnegie Mellon University, USA*; Kenji Takizawa, *Waseda University, Japan*; Tayfun Tezduyar, *Rice University, USA*; Takafumi Sasaki, *Waseda University, Japan*;

Coronary blood flow simulation with vessel wall motion can provide valuable information for the physician to make treatment decisions. Reliable computational analysis requires robust and accurate mesh motion to match the boundary motion. Here, we focus on the spatial and temporal continuity property of the geometry and motion. The isogeometric discretization in space can increase the fluid mechanics accuracy by providing smoother representation of the wall geometry and more accuracy in the flow solution. Control mesh motion with temporal C^2-continuity is also needed in fluid mechanics computation. We present a new algorithm to convert temporally non-smooth motion extracted from time-varying medical images to high-order B-spline representation in time. Compared to least-squares projection, we introduce two penalty terms in the energy functional, which are associated with the first-order and second -order derivatives of the trajectory of each control point. The resulting temporally C^2-continuous mesh motion avoids wiggles (known as the Runge's phenomenon). The effectiveness of the proposed algorithm is demonstrated on space–time isogeometric analysis of coronary blood flow with vessel wall motion. REFERENCES [1] Y. Yu, Y. J. Zhang, K. Takizawa, T. E. Tezduyar, and T. Sasaki. Mesh Optimization for Space–Time Coronary Blood Flow Simulation with Vessel Wall Motion. In Preparation. [2] K. Takizawa, B. Henicke, A. Puntel, T. Spielman, and T. E. Tezduyar. Space–time computational techniques for the aerodynamics of flapping wings. Journal of Applied Mechanics, 79, 010903, 2012. [3] P. H. C. Eilers and B. D. Marx. Flexible smoothing with B-splines and penalties, Statistical science, 11(2), 89-102, 1996.

15th U.S. National Congress on Computational Mechanics
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Title: Optimum First Failure Load for Single-core and Two-core Rectangular Sandwich Plates under Blast Loads

Author(s): *Lisha Yuan, *Virginia Polytechnic Institute and State University*; Romesh C. Batra, *Virginia Polytechnic Institute and State University*;

We assume that the face sheets of a sandwich plate are made of unidirectional fiber-reinforced composite with fibers being either the glass, or carbon or aramid and the core made of balsa wood. A typical blast pressure [1], represented by the product of a function of time and two in-plane coordinates, is applied on the plate top surface. Two functional representations in time and space are envisaged. By assuming that the areal density is fixed and not considering delamination between adjacent layers, we use the Nest-Site Selection (NeSS) optimization algorithm [2], a third-order shear and normal deformable plate theory (TSNDT) [3], a one-step stress recovery scheme (SRS) and the Tsai-Wu failure criterion to find the face sheet materials and their fiber orientation angles so that the first failure load is the maximum. It is found that the optimal single-core sandwich designs are symmetric about the mid-surface with thick facesheets and the optimal two-core sandwich designs have a thin middle facesheet and thick top and bottom facesheets. The first failure load of the optimal clamped single-core (two-core) design is approximately 20% (30%) more than that of the corresponding simply-supported plate. For simply-supported (clamped) sandwich structures, the failure initiates at the centroid (center of the clamped edge) of either the top or the bottom surfaces. It is also found that the first failure occurs in a facesheet (core) due to the in-plane transverse axial stress (transverse shear stress) exceeding its critical value. Reference: [1] R. C. Batra, N. M. Hassan, Blast resistance of unidirectional fiber reinforced composites, Composites: Part B, 39 (2008) 513-536. [2] U. Taetragool, B. Sirinaovakul, T. Achalakul, NeSS: A modified artificial bee colony approach based on nest site selection behavior, Applied Soft Computing, 71 (2018) 659-671. [3] P. Shah, R. Batra, Through-the-thickness stress distributions near edges of composite laminates using stress recovery scheme and third order shear and normal deformable theory, Composite Structures, 131 (2015) 397-413.

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Title: Large-deformation Elastic-plastic Analysis of a Structure with Local Features Using Coupling-matrix-free Iterative S-version FEM

Author(s): *Yasunori Yusa, *Tokyo University of Science*; Daiji Toyama, *Tokyo University of Science*; Kazuma Ohashi, *Tokyo University of Science*; Hiroshi Okada, *Tokyo University of Science*;

The s-version FEM [1] was proposed to tractably analyze a structure with local features such as holes, cracks and inclusions. In the s-version FEM, local meshes representing the local features are superposed on a global mesh of the structure. The global and local meshes are solved monolithically with a single linear system of equations. However, the s-version FEM has a significant difficulty with the treatment of the coupling effect between the global and local meshes. Generating a coupling stiffness matrix between partly overlapping finite elements requires a very sophisticated numerical integration method that is specific to the s-version FEM. To overcome this difficulty, the authors proposed a modified version of the s-version FEM, namely the coupling-matrix-free iterative s-version FEM [2, 3]. In this method, the coupling effect is considered by the transfers of stresses between the meshes. The transferred stresses is dealt with as initial stresses. Ordinary finite element analyses with initial stresses are performed alternately for each mesh until convergence. This approach enables us to use existing FEM programs. Recently, we are developing a nonlinear version of the coupling-matrix-free iterative s-version FEM. The resulting algorithm is very different from that of nonlinear analysis with the original s-version FEM. In our method, ordinary nonlinear finite element analyses with Newton-Raphson iteration are performed alternately. Existing nonlinear FEM programs can be used. In the presentation, methodology of the nonlinear version of the coupling-matrix-free iterative s-version FEM for both total and updated Lagrangian methods are explained, followed by some numerical examples including a large-deformation elastic-plastic problem. [1] Fish, J. The s-version of the finite element method. Comput. Struct., 43 (3), 539-547, 1992. [2] Yumoto, Y., Yusa, Y., Okada, H. An s-version finite element method without generation of coupling stiffness matrix by using iterative technique. Mech. Eng. J., 3 (5), 16-00001, 2016. [3] Yusa, Y., Okada, H., Yumoto, Y. Three-dimensional elastic analysis of a structure with holes using accelerated coupling-matrix-free iterative s-version FEM. Int. J. Comput. Methods, 15 (5), 1850036, 2018.

15th U.S. National Congress on Computational Mechanics
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Title: The Data-driven Multiscale Multigrid

Author(s): *Dewen Yushu, *University of Notre Dame*; Kevin Deweese, *University of Washington*; Karel Matouš, *University of Notre Dame*;

In the recent years, the development of fast numerical methods and high performance computational platforms has enabled detailed numerical simulations in numerous scientific and engineering fields. However, direct numerical modeling still requires large computing resources and novel numerical approaches are needed to make a leap to next generation exascale platforms. Therefore, multiscale modeling gains popularity because of its capability of balancing between capturing detailed features and reducing the underlying computational complexities. Similar challenges also exist in computer graphics for rendering complex geometries while maintaining the real-time rendering rate. One of the typical approaches targeting this problem is the level of detail. Based on this idea, an image-based mutiscale modeling technique (i.e., the sharp volumetric billboard based modeling) has been developed, which manages to preserve microstructural characteristics with high degrees of data compression. As one of the multiscale approaches, multigrid has high algorithmic efficiency and offers the possibility of solving a system of algebraic equations with optimal operation counts and storage. However, for heterogeneous media where material properties are fluctuating, the multigrid performance becomes fragile. Therefore, we propose a novel data-driven multiscale multigrid approach to address the numerical complexity associated with data heterogeneity. In this talk, we will present a novel image-based multiscale multigrid solver (MGs) which is developed based on an image-based, multi-resolution paradigm that enables reliable data flow between computational grids and provides large data compression. A set of inter-grid operators is developed via incorporating the microstructural information from the multi-resolution image model. Moreover, the integration of the MGs into the Trilinos package and its parallel scaling properties will also be highlighted. As an illustration, a steady-state heat conduction equation is solved in a complex domain obtained from high energy ball milled Ni/Al composites. We solve this problem using various coefficient contrasts and different number of grid levels. It is shown that MGs is robust at high coefficient contrast and has a near optimal convergence rate. The weak scaling performance of the parallelized MGs also shows a significant speedup with increased core number compared with other multigrid methods, such as the black box multigrid and the smoothed aggregation. This work opens a new possibility for solving a system of linear equations associated with data heterogeneity, which is a fundamental problem in a large array of engineering and science disciplines.

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Title: An Optimization-Based Approach for the Reduction of Conservation Laws with Parametrized Discontinuities

Author(s): *Matthew Zahr, *University of Notre Dame*;

We introduce an optimization-based model reduction framework to solve steady conservation laws with parametrized, discontinuous solution features such as shock waves. The main idea behind the proposed reduction framework is to align discontinuities in the reduced basis with discontinuities in the solution. This is accomplished using an Arbitrary Lagrangian-Eulerian (ALE) formulation where the conservation law and its solution are transformed to a fixed reference domain and the mapping from the reference to physical domain is encoded in the flux of the transformed conservation law. Snapshots for the solution and ALE domain mapping (mesh deformation at the discrete level) will be generated using the discontinuity-tracking method proposed in [1], whereby the domain is deformed such that element faces of the mesh align with discontinuities in the solution, and compressed to form reduced-order bases. We require the same element faces lie on the discontinuity surface across all snapshots to guarantee the discontinuities in all snapshots perfectly align in the reference domain. This implies the snapshots can be effectively compressed into a reduced basis because discontinuities are hidden since there is no mixing between smooth and discontinuous regions. The reduced-order model is formulated as an optimization problem that simultaneously seeks the reduced coordinates of the solution and the deformation of the underlying mesh (ALE mapping) that minimize the full-order residual. Even though we restrict solutions in the reference domain to lie in a linear subspace using the traditional model reduction ansatz, the deformation of the underlying mesh implies the solution in the physical domain lies on a relevant nonlinear manifold. We demonstrate the merit of the framework with one- and two-dimensional test cases from computational fluid dynamics. References: [1] M.J. Zahr and P.-O. Persson. An optimization-based approach for high-order accurate discretization of conservation laws with discontinuous solutions. Journal of Computational Physics, 365:105 – 134, 2018.

15th U.S. National Congress on Computational Mechanics
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Title: Shape Optimization Using Density-based Topology Optimization

Author(s): *Tomas Zegard, *Pontificia Universidad Catolica de Chile (PUC Chile)*; Diego Salinas, *Pontificia Universidad Catolica de Chile (PUC Chile)*; Emilio Silva, *Universidade de São Paulo (USP)*;

Shape optimization is a technique often used in mechanical design where the boundary of some component is fine-tuned for better performance based on some specific measure (objective). The traditional approach involves subdividing the solid boundary into curves, which are in turn defined by "control points". The location of these control points can be optimized, which translates into an optimization of the shape of the boundary. The approach is typically Lagrangian in nature, and thus the solid must be re-meshed with every design variation. This technique is quite robust, and mature, but it depends on relatively sophisticated meshing algorithms and is constrained to a design space indirectly defined by the (typically few) control points. This work presents an new Eulerian approach for shape optimization. In this method there is no need to predefine control points nor subdivide the boundary into curves. The method is based on density-based topology optimization, which traditionally is used to generate (quasi) optimal shapes based on some specific measure. However, as the name implies, the topology can change during the optimization process which is not a desirable feature in shape optimization. Thus, the method is based on a topologically-constrained version of the traditional density-based topology optimization method. The algorithm is gradient based, and thus rapid convergence and local optimality can be guaranteed. Advantages and shortcomings of the formulation are discussed, and a few examples are shown to validate and benchmark the proposed method.

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Title: Development, Enhancement and Evaluation of a Mid-Sized Male Thorax and Upper Extremity Finite Element Model

Author(s): *Wei Zeng, *University of Virginia*; Sayak Mukherjee, *University of Virginia*; Adrian Caudillo, *University of Virginia*; J. Sebastian Giudice, *University of Virginia*; Matthew Panzer, *University of Virginia*;

In automobile crashes, thoracic and upper extremity injuries are two of the most prevalent body injury regions, and ranks second only to head injury with reference to the number of fatalities and serious injury outcomes. To design better safety systems, engineers perform many iterations of simulated crash testing and injury analysis to determine a set of parameters optimized for reducing injurious outcomes. Human body finite element models are a powerful and versatile tool that can accurately describe the human anatomy, biomechanics, and variability for injury risk predictions and vehicle safety systems development. Ensuring the biofidelity of these models, particularly in the thorax, is important for the utility of the tool for predicting injury to the ribcage and to the organs inside thoracic cavity. In this study, a state-of-the-art 50th-percentile male thorax finite element model (GHBMC M50 v5) was enhanced to improve the biofidelity of the organs and their boundary conditions. Organs within the thoracic cavity were improved by incorporating a novel sliding interface between the tissues to represent the action of the pleural space. This prevented voids from forming inside ribcage during impact. The aorta was improved through mesh enhancements and material updates to better represent aortic laceration injuries. The thoracic musculoskeletal system was enhanced by adding fracture features to the clavicles, sternum and costal cartilage. Component level validation tests were implemented to assess appropriate material parameters. To evaluate the impact of model updates, body regional level or full torso level validation tests were conducted under various thoracic loading environments. These tests contained point loading of the eviscerated ribcage, vertical loading trial, frontal pendulum impacts, shoulder pendulum impact and table-top belt loading tests. The biomechanical response of the thorax was overall deemed biofidelic and the model was found to be in good agreement with the experimental data using both qualitatively and quantitative assessments. This model will serve as a valuable tool for safety researchers and automobile designers to predict, prevent, and mitigate thoracic and upper extremity injuries due to vehicle crashes. In addition, this study provides a framework to evaluate and enhance the biofidelity of future computational human body models for injury risk prediction and prevention.

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Title: Computational Modeling of Force Driven Epithelial Wound Healing

Author(s): *Xiaowei Zeng, *University of Texas at San Antonio*; Jie Bai, *University of Texas at San Antonio*; Liqiang Lin, *University of Texas at San Antonio*;

Wound healing is a complex, evolutionarily conserved, multi-cellular process aimed toward epithelium restoration after injury. Epithelial repair is achieved through the collective movement of wound-bordering cells into the wound bed. In the past two decades, the epithelialization phase of wound healing has been broadly studied in the laboratory, using a variety of in vitro models. However, this complex process has not been fully elucidated, e.g. how the wound healing efficiency is related to the mechanical forces (the magnitude of motility forces, the cell-cell interactions within the monolayer sheet, the interactions between cell and substrate etc.). Wound healing remains a challenging clinical problem in which correct and efficient wound management is essential. In this presentation, we shall present our latest results on epithelial wound healing process computational modeling and simulation. In the simulation model, an epithelial monolayer sheet with a wound region was generated. The macroscale cell is modeled as soft materials, and cell-cell/subtract interactions are governed by a recently developed interfacial zone model. The polygonal shape of epithelial cells is generated using Voronoi tessellation techniques. We have developed and implemented the related computational algorithms into simulation code for the described simulation model. The simulation shows that the wound healing process depends on cell growth and division rate, and cell-cell adhesion strength.

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Title: Experimental and Numerical Study on High-Speed Impact Damage Behavior of Triaxially Braided Composite

Author(s): *Chao Zhang, *Northwestern Polytechnical University*; Zhenqiang Zhao, *Northwestern Polytechnical University*; Yulong Li, *Northwestern Polytechnical University*;

Abstract: Fiber reinforced composite materials are widely used in various manufacturing such as aerospace, automotive, marine and exercise equipment due to their outstanding physical, mechanical and thermal properties. Particularly, textile/braided composites have emerged as leading contenders in industrial sectors because of the more excellent properties than traditional laminated structures in terms of damage tolerance and energy absorption [1]. Thus, engine manufactures try to fabricate new engine fan cases by employing textile composites, to contain the blade and fragments during the rotor failure event. For instance, the two-dimension triaxially braided composite (2DTBC) has been used as the engine casing material of GEnx. The penetration resistance and impact damage behavior of the 2DTBC is investigated by conducting the ballistic experiments on the single-stage gas gun. Meanwhile, a multi-scale modeling framework is established for impact damage simulation of the 8-layer 2DTBC panel, which compound by T700 carbon fiber fabric and 3266 epoxy resin. The experimental results show that the quasi-isotropic braided architecture of 2DTBC which exhibits equal mechanical properties in-plane efficiently enhances the energy absorption of the composite panel. And the complicated braided structure can arrest the crack in nature to avoid the damage propagation along a single path, as a result, localized damage region has inspected and detected in the panel after impact. Apart from these, the numerical predicted failure patterns from the multi-scale simulation approach matched very well with the experimental results, and the influence of impact attitude on damage behavior of the target is further examined using the numerical simulation method. References [1] Song, S., Waas, A. M., Shahwan, K. W., Faruque, O., & Xiao, X “Compression response of 2d braided textile composites: single cell and multiple cell micromechanics based strength predictions”. Journal of Composite Materials, 42(23), 2461-2482, 2008. [2] Zhao, Z., Dang, H., Zhang, C., Yun, G. J., & Li, Y. “A multi-scale modeling framework for impact damage simulation of triaxially braided composites”. Composites Part A Applied Science & Manufacturing, 110, 113-125, 2018.

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Title: Sweeping Wave Impact Calculated Using Multivelocity Dual Domain Material Point Method

Author(s): *Duan Zhang, *Los Alamos National Laboratory*; Christopher Long, *Los Alamos National Laboratory*;

We use the ensemble phase averaged equations [1] to study sweeping wave impact on a tantalum plate. The sweeping wave is generated by detonation of high explosives. The gaseous reaction product is modeled using the Jones-Wilkins-Lee (JWL) equation of state and is represented using Eulerian description in the calculation. To model large material deformation and pore growth in the metal, tensile plasticity (TEPLA) model is used [2], in which the porosity growth is considered as a part of plastic deformation. To compute large deformation of the metal, while accurately tracking the material deformation history, Dual Domain Material Point (DDMP) method is employed. The DDMP method is a reliable numerical method using both Eulerian and Lagrangian descriptions. In this work, we use the Eulerian velocity to describe the large deformation of the solid caused by the sweeping shock wave and the Lagrangian capability to track history dependent plastic deformation and pore growth. The Lagrangian capability of the DDMP method is used to accurately calculate the large plastic deformation without the difficulties associated with mesh distortion and numerical diffusion. To ensure numerical stability, plastic deformation is solved implicitly. Similar to the computation of multiphase flows, the material pressures are determined using continuity condition, which requires summation of volume fractions be unity. In our combined Eulerian-DDMP calculations, the gas phase and solid phase are discretized differently, leading to incompatible volume fractions. Direct enforcement of the continuity condition leads to erroneous results. A weak solution approach is then employed [3] to derive equivalent continuity condition accommodating the discretization differences. Material pressures are then solved by enforcing this equivalent continuity condition. Several numerical results from such calculations are compared with the experiments. [1] D. Z. Zhang, W. B. VanderHeyden, Q. Zou, N. T. Padial-Collins, Pressure calculations in disperse and continuous multiphase flows, Journal of Multiphase Flow 33 (2007) 86–100. [2] J. Johnson, F. Addessio, Tensile plasticity and ductile fracture, J. Appl. Phys. 64 (12) (1988) 6699–6712. [3] Zhang, D. Z., Zou, Q., VanderHeyden, W. B. & Ma, X. 2008, Material point method applied to multiphase flows. Journal of Computational Physics. 227, pp. 3159-3173

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Title: Design of Dissipative Metamaterials via Topology Optimization and Nonlinear Homogenization

Author(s): *Guodong Zhang, *University of Notre Dame*; Kapil Khandelwal, *University of Notre Dame*;

Materials with intrinsic damping is of great importance in engineering practice for vibration control, noise attenuation, and energy dissipation. Studies have shown that combining soft viscoelastic phase with stiff elastic phase can greatly improve both damping and stiffness properties of the resulting composite system [1]. However, design of such metamaterials with optimal damping and stiffness characteristics is not trivial. In the past, efforts have been made towards designing microstructures for maximizing damping under small strain assumptions in the frequency domain [2]. Although promising results were achieved, the optimality of such designs can be degraded when arbitrary time-dependent loading is considered. Moreover, since viscoelastic materials usually exhibits viscous damping effects under large deformations, the results obtained from small strain theories can be misleading. To bridge these gaps, a novel computational framework is presented for designing dissipative metamaterials with tailored damping and stiffness properties, under arbitrary time-dependent loading conditions while considering finite deformations. In this approach, a density-based topology optimization method is integrated with nonlinear homogenization for designing such metamaterials. Challenges pertaining to consistent path/time-dependent sensitivity analysis, incorporation of nonlinear homogenization and construction of appropriate material interpolation schemes are addressed. Various new dissipative metamaterials with tailored damping properties are obtained with different periodicities and stiffness constraints. Keywords: Metamaterials Design; Energy Dissipation; Finite Strain; Topology Optimization; Nonlinear Homogenization. References: [1] Treviso A., Van Genechten B., Mundo D., & Tournour M. (2015), “Damping in composite materials: Properties and models”, Composites Part B: Engineering, Volume 78, 2015, Pages 144-152, doi:10.1016/j.compositesb.2015.03.081. [2] Huang X., Zhou S., Sun G., Li G., & Xie Y.M. (2015). “Topology optimization for microstructures of viscoelastic composite materials”. Computer Methods in Applied Mechanics and Engineering, Vol 283, Pages 503-516, doi:10.1016/j.cma.2014.10.007.

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Title: A Practical Unstructured Spline Modeling Platform for Isogeometric Analysis Applications

Author(s): *Jessica Zhang, *Carnegie Mellon University*;

As a new advancement of traditional finite element method, isogeometric analysis (IGA) adopts the same set of basis functions to represent both the geometry and the solution space, integrating design with analysis seamlessly. In this talk, I will present a practical unstructured spline modeling platform that allows IGA to be incorporated into existing commercial software such as Abaqus and LS-DYNA, heading one step further to bridge the gap between design and analysis. The platform includes all the necessary modules of the design-through-analysis pipeline: pre-processing, surface and volumetric spline construction, analysis and post-processing. Taking IGES files from commercial computer aided design packages, Rhino specific files and mesh data, the platform provides several control mesh generation techniques, such as converting any unstructured quadrilateral/hexahedral meshes to T-splines, frame field based quadrilateral meshing, and polycube method. Truncated T-splines, hierarchical B-splines and subdivision basis functions are supported with local refinement and sharp feature preservation. To ensure analysis suitability, partition of unity, linear independence and optimal convergence rate of these basis functions are also studied in our research. In the end, several practical application problems are presented to demonstrate the capability of our software platform. References: [1] Y. Lai, Y. J. Zhang, L. Liu, X. Wei, E. Fang, J. Lua. Integrating CAD with Abaqus: A Practical Isogeometric Analysis Software Platform for Industrial Applications. A Special Issue of HOFEIM 2016 in Computers and Mathematics with Applications, 74(7):1648-1660, 2017. [2] X. Wei, Y. J. Zhang, D. Toshniwal, H. Speleers, X. Li, C. Manni, J. Evans, T. J. R. Hughes. Blended B-Spline Construction on Unstructured Quadrilateral and Hexahedral Meshes with Optimal Convergence Rates in Isogeometric Analysis. Computer Methods in Applied Mechanics and Engineering, 341:609-639, 2018. [3] X. Wei, Y. J. Zhang, L. Liu, T. J. R. Hughes. Truncated T-splines: Fundamentals and Methods. Computer Methods in Applied Mechanics and Engineering Special Issue on Isogeometric Analysis, 316:349-372, 2017.

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Title: Deep Learning Method to Accelerate Monte Carlo Simulation in Spin Configuration Models

Author(s): *Jiaxin Zhang, *Oak Ridge National Laboratory*; Markus Eisenbach, *Oak Ridge National Laboratory*;

Monte Carlo methods are some of the most effective methods for computational statistical mechanics in many systems, but it is often too expensive for large-scale materials simulations to directly calculate energies using first principle calculation, such as density functional theory. It therefore motivates us to integrate a machine learning model with Monte Carlo calculations. Here we propose an efficient workflow for accelerating stochastic sampling and predicting thermodynamic quantities by combined supervised learning and unsupervised learning methods. First, a convolutional neural network (CNN) is used to train a data-driven surrogate model for the energy instead of the expensive first principle calculation. Generative adversarial networks (GAN) are then trained to learn the feature in the configurations generated from stochastic sampling in the previous step. The trained GAN model is able to generate more spin states for which I compare thermodynamic observables to those computed by direct Markov Chain Monte Carlo sampling. The results demonstrate that the GAN model can faithfully reproduce the observables of the physical systems. Moreover, only one batch of training datasets are required, and these data can be utilized for both supervised learning (CNN) and unsupervised learning (GAN). Here, we employ classical models to demonstrate the workflow and the proposed method can be widely extended to various many-body configuration problems (e.g. alloy model).

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Title: Simulations of Shock-induced Blast on Structure Failure Using Immersed Non-intrusive Coupling of Particle-based Structure Dynamics in a Shock Environment

Author(s): *Lucy Zhang, *Rensselaer Polytechnic Institute*; Jie Cheng, *Rensselaer Polytechnic Institute*;

In this talk, we will show the developed framework that simulates shock-induced blast and its effect on structural and material failure using non-intrusively coupled continuum fluid solver and particle-based structure dynamics solver. Existing simulators focus either on the shocks and shock wave propagation or on structural damage and failure. The coupled fluid-structure response requires the integration of both physics. In this project, we propose to adopt an “immersed” framework that couples a shock simulator (Eulerian) with a RKPM structural dynamics solver (Lagrangian) to simulate a coupled shock-induced blast on structure failure. The immersed framework allows the co-existence of independent meshes/particles for the fluid and the structure without the expensive or prohibitive cost of re-meshing. RKPM allows realistic representation of structural damage that involve large deformation and bombardment of fragments. Such an immersed particle framework yields efficient and accurate prediction of shock-induced structural damage in an extreme environmentß.

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Title: Coupled Peridynamics/Finite Element Method for Multiscale Fracture Simulations

Author(s): *Rui Zhang, *The University of Texas at Dallas*; Shogo Wada, *Bridgestone Corporation*; Clint Nicely, *Raytheon Airborne and Space Systems*; Dong Qian, *The University of Texas at Dallas*;

We present a concurrently coupled multiscale approach that integrates non-ordinary state-based peridynamics (NOPD) with finite element method (FEM). Peridynamics is a reformulation of the classical continuum mechanics theory based on an integro-differential governing equation. Numerical discretization of peridynamics leads to meshfree representation of the continuum. There is an increasing interest in applying peridynamics for fracture modeling. However, due to its non-local formulation peridynamics generally leads to high computational cost. To accelerate fracture simulations, we propose a coupled NOPD/FEM multiscale approach. FEM is applied in the coarse scale and extended by using discontinuous enrichment that represents the physics in fracture problems [1-2]. NOPD is introduced to capture cracks initiation and propagation in the fine scale and limited to local region around crack tips. A multiscale projection approach is developed to realize a concurrent coupling between the two numerical methods. To accommodate the evolving nature of the dynamic fracture, an adaptive scheme is established so that the NOPD simulation is dynamically prescribed to trace the propagating crack and potentially events such as branching. The main challenge in this approach is to eliminate artificial wave reflections at the numerical interface between NOPD and FEM. A class of nonlocal matching boundary condition (NMBC) is developed to realize non-reflective interfaces [3]. The effectiveness and robustness of the proposed multiscale approach is demonstrated by comparisons with full NOPD simulations on benchmark examples that involve brittle failure. References: [1] Y Yang, S Chirputkar, DN Alpert, T Eason, S Spottswood, and D Qian, “Enriched space-time finite element method: a new paradigm for multiscaling from elastodynamics to molecular dynamics,” International Journal for Numerical Methods in Engineering, 92, pp. 115-140, 2012. [2] S Wada, R Zhang, SR Mannava, VK Vasudevan, and D Qian, “Simulation-based prediction of cyclic failure in rubbery materials using nonlinear space-time finite element method coupled with continuum damage mechanics,” Finite Elements in Analysis and Design, 138, pp. 21-30, 2018. [3] C Nicely, S Tang, and D Qian, “Nonlocal matching boundary conditions for non-ordinary peridynamics with correspondence material model”, Computer Methods in Applied Mechanics and Engineering 338, pp. 463-490, 2018.

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Title: A Phase Field Model of Crack Propagation in Anisotropic Brittle Materials

Author(s): *Shuaifang Zhang, *University of Florida*; Wen Jiang, *Idaho National Lab*; Dong-Uk Kim, *University of Florida*; Michael Tonks, *University of Florida*;

The phase field method is a powerful approach for the numerical simulation of crack propagation since it does not require tracking of the fracture surfaces. We present a phase field fracture model that includes both an anisotropic elasticity tensor, which can include the impact of elastic anisotropy on stress strain curves, and anisotropic fracture energy, which can show the impact on crack paths. Also, our model excludes the contributions of compressive stress on driving crack propagation. In this work, we will show our model works well in both Mode I and II fracture simulations. Then Mode I fracture simulations are conducted to investigate the impact of grain orientation on the fracture. Finally, a polycrystal structure with different crystal orientations that impact the elasticity and crack path is shown to demonstrate the capacity of our model.

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Title: Explicit Structural Topology Optimization based on Boundary Element Method

Author(s): *Weisheng Zhang, *Dalian University of Technology*; Qingqing Jiang, *Dalian University of Technology*; Xu Guo, *Dalian University of Technology*;

Traditionally, structural topology optimization problems are often solved by adopting implicit geometry representation model and finite element method (FEM) on fixed mesh. This may lead to some disadvantages such as the inherent inconsistency existing between the geometrical representation model and the finite element analysis model (especially in level set method, LSM), the lack of accurate geometry information, high computational cost involved, and possible destroying of the optimality of optimization results due to inevitable post-processing. In order to resolve the aforementioned issues straightforwardly, in the present work, we propose an explicit structural topology optimization approach integrating the Moving Morphable Void (MMV)-based topology optimization method and Boundary Element Method (BEM) seamlessly. With the use of the proposed approach, it is not only possible to describe the geometry of structural boundaries explicitly, but also to generate precise boundary element-based structural analysis model. Numerical examples provided demonstrate the effectiveness of the proposed approach. [1] X. Guo, W.S. Zhang, W.L. Zhong, Doing topology optimization explicitly and geometrically—a new moving morphable components based framework, Trans. ASME J. Appl. Mech. 81 (2014) 081009-1–081009-12. [2] W.S. Zhang, J. Yuan, J. Zhang, X. Guo, A new topology optimization approach based on Moving Morphable Components (MMC) and the ersatz material model, Struct. Multidiscip. Optim. 53 (2016) 1243–1260. [3] W.S. Zhang, W.Y. Yang, J.H. Zhou, D. Li, X. Guo, Structural topology optimization through explicit boundary evolution, ASME J. Appl. Mech. 84 (2017) 011011-1–011011-10.

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Title: A Machine Learning Model for Heart Valve Remodeling

Author(s): *Wenbo Zhang, *University of Texas at Austin*; Tan Bui-Thanh, *University of Texas at Austin*; Michael Sacks, *University of Texas at Austin*;

When complex mechanical behaviors are involved, the high-fidelity mesoscale/multiscale methods for soft tissue constitutive models are attractive and predictive but are also computationally very demanding. Traditional phenomenological models have simple forms based on physical insight, but they often lack the ability to be predictive. For example, for remodeling of the bioprosthetic heart valve (BHV), predictive structural constitutive models have been developed for time independent and time evolving properties of exogenously crosslinked collagenous soft tissues under cyclic loading [1,2]. To simulate novel BHV designs or further identify underlying mechanism, efficient computational methods are crucial. Neural networks approaches are an attractive alternative attention because of their high representation capability, flexible designs, and high speed when properly designed. To this end, we investigated possible approaches to build a neural network (NN) model that can replicate the responses of detailed structural models for soft tissue with manageable computational costs. The fact that the NN model was trained on analytical model instead of experimental data helped to implicitly impose proper regularization so that the fitting problem was well-defined. In this work, we considered a particular analytical model, i.e. a recently developed full structural model for cross-linked soft tissue [1]. We have for the first time examined building a NN model as a surrogate constitutive model for a high-fidelity but computationally costly soft tissue model. We show that the results for the NN model fits the data, i.e., the strain-to-stress mapping, and it has reasonable convergence. The present NN with only 21 neurons can serves as an efficient surrogate model for detailed structural model. Therefore, the present work serves as a proof-of-concept for the use of neural networks in replicating the same response as the predictive structural model with improved efficiency. Thanks to the flexibility of the NN model, it paves the way for applying machine learning methods for simulation of soft tissues and identification its mechanical properties to much broader applications. We are currently extending it to time dependent models that include fatigue and growth for simulating the long-term behavior of soft tissues. [1] M.S. Sacks, W. Zhang, S. Wognum, A novel fibre-ensemble level constitutive model for exogenous cross-linked collagenous tissues, Interface Focus. 6 (2016) 20150090. doi:10.1098/rsfs.2015.0090. [2] W. Zhang, M.S. Sacks, Modeling the response of exogenously crosslinked tissue to cyclic loading: The effects of permanent set., J. Mech. Behav. Biomed. Mater. 75 (2017) 336–350. doi:10.1016/j.jmbbm.2017.07.013.

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Title: State of the Art Simulation of the Early Stages of Bioprosthetic Heart Valve Fatigue

Author(s): *Will Zhang, *University of Texas at Austin*; Michael Sacks, *University of Texas at Austin*;

INTRODUCTION - The most popular heart valve replacements continue to be bioprosthetic heart valves (BHV) fabricated from xenograft biomaterials. However, failure due to structural deterioration continues to be the central issue plaguing the current designs. Despite decades of usage, evaluating their durability remain very empirical, and the mechanisms underlying their failure remains poorly understood. Thus, there is a profound need for the development of novel simulation technologies to better understand and predict the changes in the mechanical properties of BHVs. METHODS - In this work, we developed a numerical framework for simulating the intact BHVs based on the constitutive model we previously developed for permanent set, which is the process that dominates initial stages of cyclic loading [1]. Permanent set is due to the use of glutaraldehyde to suppress the immunogenic response, but the crosslinks formed are reversible at body temperature and allows the microstructure and stress-free geometry to gradually change. The effects of permanent set at the material level are determined from this structural model based on the results of the quasi-static simulation at each time step, whereas we utilized an effective model to homogenizes the response of the structural model for efficient simulations [2] and a growth stress approach for updating the intact geometry. RESULTS - BHVs undergo significant changes in geometry, especially in the first 25 million cycles. This process gradually stops after 40-50 million cycles. The regions that undergo most permanent set are the belly region, the center of the free edge, and the regions near the commissures, the most common regions of failure in BHVs. We were also able to predict the change in the collagen fiber architecture, where the recruitment of collagen fibers causes permanent set to seize. DISCUSSION & CONCLUSION - We have shown that permanent set can be used to predict the evolving geometry, microstructural and material property changes in the first 50-70 million cycles of loading. This framework opens the possibility of optimizing the initial BHV design to the final geometry after permanent set has seized, where it will operate for its remaining 9- to 14-year lifespan. Thus, accounting for permanent set is especially important in the design of BHVs. REFERENCES [1] Zhang, W., et al. J Mech Behav Biomed Mater. 75:336-50, 2017. [2] Zhang, W., et al. J Mech Behav Biomed Mater. 89:168-98, 2019.

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Title: Modeling and Design of a New Printing Process for 3D Freeform Polymer Components based on Frontal Polymerization

Author(s): *Xiang Zhang Zhang, *University of Illinois at Urbana-Champaign*; Jia Aw, *University of Illinois at Urbana-Champaign*; Leon Dean, *University of Illinois at Urbana-Champaign*; Nancy Sottos, *University of Illinois at Urbana-Champaign*; Jeffrey Moore, *University of Illinois at Urbana-Champaign*; Philippe Geubelle, *University of Illinois at Urbana-Champaign*;

A rapid and energy-efficient manufacturing process for polymer and polymer composites called frontal polymerization (FP) was recently developed [1]. In FP-based manufacturing, only an initial local heat stimulus is required to activate the polymerization, upon which the heat from the exothermic polymerization of the monomer creates a self-propagating polymerization front that transforms the monomers into fully cured polymers. A 3D printing technique that uses FP to simultaneously cure the printed material as it is deposited has also been recently introduced for free-standing polymer components. During this printing process, the polymerizing front follows the printing nozzle and rapidly transforms the viscoelastic filament into a stiff thermoset, thereby eliminating the need for support structures and post curing process and providing high printing accuracy compared to traditional direct ink writing. In this presentation, we start by introducing a coupled thermo-chemo-mechanical model specially developed to model the evolution of temperature, degree of cure, and strain fields during the FP process. The model is first validated against experimental measurements and then used to probe the front characteristics under different experimental settings. We then focus on the development of a design diagram for FP-based 3D printing to maximize the printing efficiency (i.e., maximum printing velocity) while maintaining the desired printing accuracy (i.e., limited deformation of the printed filament). The design space contains parameters that characterize the settings of the printer (e.g., ink temperature, extruding pressure, length and diameter of the nozzle), the nature of the ink (e.g., initial degree of cure and cure kinetics associated with the chosen ink composition), and the printing environment (e.g., ambient temperature and air flow rate). The constraints are associated with equilibrated printing for which the front velocity equals the printing speed, the printing accuracy achieved by limiting the deflection of the deposited filament, the capability of the printer, and non-blocking of the nozzle by a threshold depositing temperature. References [1] I. D. Robertson, M. Yourdkhani, P. J. Centellas, J. E. Aw, D. G. Ivanoff, E. Goli, E. M. Lloyd, L. M. Dean, N. R. Sottos, P. H. Geubelle, J. S. Moore, and S. R. White. Rapid energy-efficient manufacturing of polymers and composites via frontal polymerization. Nature, 557:223–227, 2018.

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Title: Adaptive Multi-Material Topology Optimization with Many Constraints: A Novel Approach with Material and Geometric Nonlinearities

Author(s): *Xiaojia Shelly Zhang, *University of Illinois at Urbana-Champaign*; Heng Chi, *Georgia Tech*; Glaucio Paulino, *Georgia Tech*;

Multi-material topology optimization is a practical tool that allows for improved structural designs. Most work in this field has been restricted to linear material behavior with limited constraint settings. To address these issues, we propose a general multi-material topology optimization formulation considering material and geometric nonlinearities. The proposed formulation handles an arbitrary number of candidate materials with flexible material properties and features a generalized setting of local and global volume constraints. To efficiently handle such arbitrary volume constraints, we employ the ZPR (Zhang-Paulino-Ramos) design variable update algorithm [1], which is based upon the separability of the dual objective function of the convex subproblem with respect to Lagrange multipliers. We tailor the ZPR update for the proposed formulation. The tailored ZPR update performs robust updates of the design variables associated with each volume constraint independently in parallel. From the perspective of computational efficiency, a major challenge associated with topology optimization considering nonlinearities is the high computational cost. To efficiently solve the nonlinear state equations resulting from material and geometric nonlinearities, we introduced the Virtual Element Method (VEM) [2] in conjunction with an adaptive meshing scheme, which greatly improves the convergence speed of the nonlinear structural analysis. Through examples in two and three dimensions, using combinations of various types of nonlinear materials, we demonstrate that the proposed multi-material topology optimization framework, with VEM and mesh adaptivity, leads to a practical design tool that not only finds the optimal topology but also selects the proper type and local distribution of materials efficiently and effectively.

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Title: Robust Topology Optimization of Phononic Crystals Considering Manufacture Uncertainty

Author(s): *Xiaopeng Zhang, *Dalian Univerisity of Technology*; Zhan Kang, *Dalian Univerisity of Technology*; Akihiro Takezawa, *Hiroshima University*;

The uncertainty of the material properties can remarkably affect the band gap characteristics of phononic crystals (PnCs). In practical applications, however, PnCs usually exhibit a random distribution of material properties resulting from manufacturing processes. It has been found that the band gap properties of photonic/phononic materials are sensitive to the microstructure configuration and material properties Thus, it is necessary to consider this issue when designing and manufacturing the PnCs materials/structures. This paper investigates a robusttopology optimization method in designing the microstructures of PnCs by considering stochastic material properties. Herein, the random material properties fields are firstly represented and discretized into several uncorrelated stochastics variables with the Expansion Optimal Linear Estimation (EOLE) method, then the stochastics band gap analysis is implemented with the Polynomial Chaos expansion (PCE). Further, a robust topology optimization formulation of PnCs is proposed based on the relative elemental density based approach, where has a weighted objective function that handles the balance of the mean value and corresponding standard deviation of the PnCs band gap. The band gap response analysis is performed with finite element method (FEM) at each sample of the PCE. In this context, the sensitivities for stochastic band gap response to the design variables are also derived. Numerical examples demonstrate that the proposed method can generate meaningful optimal topologies of PnCs with a relative wide-width and less sensitive band gap. Also, the influences of the weight factors and the variation coefficient of material properties in the objective function on the optimal solutions are discussed. References [1] Zhang, X., He, J., Takezawa, A., & Kang, Z. (2018). Robust topology optimization of phononic crystals with random field uncertainty. International Journal for Numerical Methods in Engineering, 115(9), 1154-1173. [2] Lazarov, B. S., Schevenels, M., & Sigmund, O. (2012). Topology optimization considering material and geometric uncertainties using stochastic collocation methods. Structural and Multidisciplinary optimization, 46(4), 597-612. [3] Keshavarzzadeh, V., Meidani, H., & Tortorelli, D. A. (2016). Gradient based design optimization under uncertainty via stochastic expansion methods. Computer Methods in Applied Mechanics and Engineering, 306, 47-76.

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Title: Machine Learning Material Physics: A Data-driven Approach for Predicting Effective Material Properties in Multi-component Crystalline Solids

Author(s): *Xiaoxuan Zhang, *Department of Mechanical Engineering, University of Michigan*; Krishna Garikipati, *Department of Mechanical Engineering, and Mathematics, University of Michigan*;

Many important multi-component crystalline solids undergo mechano-chemical phase transformations, in which the compositional redistribution is coupled with a crystal structural change. Capable of rapidly calculating the macroscopic behavior of this class of material based on their detailed microscopic structures is of paramount importance for accelerating new material design and discovery. However, evaluation of macroscopic material properties purely based on direct numerical simulation (DNS) is computationally very expensive and thus impractical for material design when a large number of microstructures need to be tested. To address this challenge, we present a data-driven approach, which combines deep neural networks (DNNs) with DNS, to predict the effective elastic material properties of a family of 3D multi-component crystalline solids, whose microstructures are numerically generated by solving a coupled, higher-order diffusion and nonlinear strain gradient elasticity problem. DNNs are trained with these synthetically generated data to reduce the dimensionality of the problem. Numerical examples, including studies on hyperparameters, accuracy, and convergence, are presented to demonstrate the effectiveness of our approach.

15th U.S. National Congress on Computational Mechanics
July 28 - August 1, 2019, Austin, Texas, USA

Title: Sensitivity Analysis and Variability Assessment of the Dynamic Response of Polycrystalline Energetic Materials subjected to Impact Loading

Author(s): *Xiaoyu Zhang, *Vanderbilt University*; Caglar Oskay, *Vanderbilt University*;

Accurate assessment and control of the variability in the response of energetic materials are extremely important for their safe and effective use of the existing stockpiles, as well as the design of new energetic formulations with improved properties and performance. While a significant body of work exists on numerical modeling and experimental characterization of various failure mechanisms (e.g., pore collapse, inter-granular friction, particle fracture, dislocation pile-ups), the systematic assessment of the variability associated with these failure mechanisms, and understanding of which of these failure mechanisms ultimately control detonation characteristics are relatively scarce. In this work, we propose a global sensitivity analysis framework for sensitivity analysis and variability assessment of the dynamic response of polycrystalline ?-HMX subjected to impact loading. The particular focus is on understanding sensitivities of the response to the elasticity constants associated with the monoclinic lattice, as well as to delineate the mechanisms that contribute to the nonlinear response of the polycrystalline energetic particle. The sensitivities of material properties and interactions between different deformation mechanisms are quantified using the Sobol Indices. The evaluation of these indices is assisted and accelerated by the Gaussian Process surrogate model in information collection of material response over the entire parameter space. The plastic response of ?-HMX is modeled using a crystal plasticity finite element model incorporating the slip mechanisms of thermal activation and phonon drag driven by the evolution of dislocation generation and annihilation. The results show that the anisotropic elasticity coefficients in the monoclinic crystalline have a modest effect on the energy dissipation and temperature rise dominated by sensitivities of a few coefficients. Among the two primary slip mechanisms, phonon drag appears dominant within the load rate and amplitude regimes considered in this study.

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Title: A New Wave Based Heat Source Model and Coupling Analysis of Temperature-microstructure Relations in Laser Additive Manufacturing

Author(s): *Zhao Zhang, *Dalian University of Technology, China*; Peng Ge, *Dalian University of Technology, China*; XinXin Yao, *Dalian University of Technology, China*; Tao Li, *Dalian University of Technology, China*; Weiwei Liu, *Dalian University of Technology, China*;

Laser-particle interaction is a very interesting topic in laser additive manufacturing due to the fact that the final product quality produced by LAM can be determined by the selection of power particles. However, the mechanism on controlling of powder particles in LAM remains ambiguous in theory. So, it is necessary to consider the laser-particle interaction and link the selection of power particles with microstructures in LAM. In current work, laser beam is expressed by high frequency electromagnetic wave form. Then, the heating of spatially distributed powder particles can be modeled by coupled electromagnetic wave conduction-heat transfer method. The effects of powder particle sizes and particle distributions are studied. The calculated heat power is then combined with double ellipsoid heat source in finite element model. The CO2 laser with a power of 1000W with wavelength of 900-1070nm is used in the experiment. Infrared radiation thermometer is used to measure the temperature of deposition layers. The temperature field predicted by finite element model is compared with experimental data to validate the proposed models. The predicted temperature is then linked with phase field model and Monte Carlo model for analysis for solidification in laser additive manufacturing. When the powder flow rate and velocity are increased, the average temperature of powder particles inside the laser beam is increased. With increase of average powder radius, the heating of smaller powder particles is intensified. The effects of temperature changes caused by powders on microstructures are then revealed.

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Title: Machine Learning in Optimizing Supersonic Nozzle and Process Parameters in Metal Cold Spray Additive Manufacturing Process

Author(s): *Zhi-Qian Zhang, *Institute of High Performance Computing, A*STAR, Singapore, 138632*; Sridhar Narayanaswamy, *Institute of High Performance Computing, A*STAR, Singapore, 138632*;

Cold Spray (CS) has been attracting increasing interest as a powder-based Additive Manufacturing (AM) process, in repairing and re-manufacturing of damaged components, building free-form structures and creating functional coatings. In metal CS process, metal powder particles are accelerated by pre-heated high pressure supersonic gas flow to the desired critical velocity for bonding. The critical velocity for bonding differs for different powder-particle material combinations, powder particle geometry, powder feed rate, residual stress of substrate, pre-heated temperature of powder and substrate, nozzle impingement angle and etc. In CS facility, the converging-diverging nozzle is the one of the key components to control the process parameters and deliver the powder particles with the desired in-flight velocity. The internal contour of the nozzle controls the powder particle velocity distribution and spatial distribution, consequently, influences deposition feasibility, deposition efficiency, coating material property, product quality, process parameters and production cost. To investigate the characteristics and performance of the CS nozzle, a computational model based on a multiphase CFD model is employed to characterise supersonic gas flow and the trajectory of the powder particles in the CS process. The model is validated by comparing the experimental data for CS processes with different nozzles, and is used to generate simulation data sets correlating the in-flight powder particle dynamic data to the parameterized nozzle geometry and process parameter input. These data sets serve as the input for a machine learning toolbox to develop a data-driven model for nozzle performance prediction. Experimental data is also generated at select data points to validate the prediction and to characterize the uncertainty of the virtual engine. The data-driven model presented here provides a tool to seek the optimal nozzle geometry for altering and improving the deposition profile, elevating production efficiency and reducing production cost.

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Title: Topology Optimization Considering the von Mises and the Drucker–Prager Criteria by Means of a Surrogate Nonlinear Elastic Constitutive Model

Author(s): *Tuo Zhao, *Georgia Institute of Technology*; Eduardo Lages, *Federal University of Alagoas*; Adeildo Ramos Jr., *Federal University of Alagoas*; Glaucio Paulino, *Georgia Institute of Technology*;

We address material nonlinear topology optimization problems considering the von Mises and the Drucker–Prager criteria by means of a surrogate nonlinear elastic model. The nonlinear material model is based on a generalized J2 deformation theory of plasticity. From an algorithmic viewpoint, we consider the topology optimization problem subjected to prescribed energy, which leads to robust convergence in nonlinear problems. The objective function of the optimization problem consists of maximizing the strain energy of the system in equilibrium subjected to a volume constraint. The sensitivity analysis is quite effective and efficient in the sense that there is no extra adjoint equation. In addition, the nonlinear structural equilibrium problem is solved by means of direct minimization of the potential energy using Newton’s method with an inexact line search strategy. Numerical examples demonstrate features of the proposed nonlinear topology optimization framework considering the von Mises and the Drucker–Prager criteria.

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Title: A Multi-Layered Model of Human Skin Reveals Mechanisms of Wrinkling in the Forehead

Author(s): *Yunmei Zhao, *University of Connecticut, Storrs, CT*; Bin Feng, *University of Connecticut, Storrs, CT*; Jian-Ming Lee, *Unilever, Trumbull, CT*; Nandou Lu, *Unilever, Trumbull, CT*; David Pierce, *University of Connecticut, Storrs, CT*;

Wrinkling in human skin is an important outward sign of aging, but the underlying mechanisms of wrinkle formation remain unclear. Wrinkles in the face are among the first noticeable, and facial expressions frequently highlight wrinkles occurring at sun-exposed areas, such as the forehead, corners of the eyes, and the cheeks. These wrinkles tend to develop perpendicular to the direction of contraction of the underlying muscles; consider, for example, the horizontal wrinkles of the forehead. Temporary wrinkles can form in the forehead by local buckling of the skin due to contraction of underlying facial muscles; then static wrinkles form due to reductions in skin elasticity and decreases in the thicknesses of skin layers, e.g. atrophy of epidermis and dermis in photo-aged skin. Wrinkles in the forehead are usually shallow furrows with depths reaching through the epidermis into the dermis, but not into the hypodermis. Understanding the mechanisms of wrinkle formation in the forehead is vital for identifying treatment targets for rejuvenation of facial skin. Researchers have proposed that permanent wrinkle lines first appear as early wrinkles due to repetitive muscle contraction, and that these wrinkles gradually become permanent due to the effects of aging. However, mechanistic numerical simulations based on experimental data have not yet tested these hypotheses. In this study, we (1) establish a 3-D layered model of human skin by incorporating the morphological and biomechanical data of layered human skin, and (2) investigate the potential mechanisms of wrinkle formation in the forehead. We incorporate both short-term muscle contraction and long-term aging in our simulations and study three potential wrinkle-forming mechanisms: (a) pure muscle contraction; (b) pure volume loss due to aging; and (c) combined effect of muscle contraction and volume loss. Numerical results indicate that: (1) our model recapitulates the biomechanical behaviors of both normal and aged human skins; (2) the material parameters considered significantly impact wrinkle morphology. Specifically, wrinkles increase in both width and depth as the stratum corneum stiffens, and wrinkles prominently increase in depth with progressive aging (the dermis/hypodermis border curves when suffering severe loss of hypodermis). Our parametric model can naturally extend to other types of wrinkles in human skin, e.g. “crow’s feet” in the corners of the eyes.

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Title: An Implicit Generalized Interpolation Material Point Method for Coupled Thermomechanics in Cosserat Continuum

Author(s): *Yonggang Zheng, *Dalian University of Technology*; Jun Tao, *Dalian University of Technology*; Hongwu Zhang, *Dalian University of Technology*; Zhen Chen, *Dalian University of Technology and University of Missouri*;

Based on the conservation laws of mass, momentum and energy, we have developed the unified generalized interpolation material point (GIMP) methods for coupled thermomechanical problems. However, these explicit GIMP approaches exhibit numerical limitations in special circumstances, such as the long-time simulation, conditional time step and error control. To further simulate the thermal induced strain localization phenomena, an effort is being made to develop the implicit formulation of the coupled thermomechanical GIMP method with the Cosserat micro-polar continuum theory. The heat conduction matrix and the global stiffness matrix are respectively constructed on the background grid assembled from each material point, based on the weak formulations of heat conduction equation and the equilibrium equation in Cosserat continuum within the framework of GIMP method. The discrete coupled equations are then solved on the grid nodes using a staggered incremental procedure with the Newton-Raphson iterative algorithm. Various numerical examples are carried out to demonstrate the accuracy and efficiency of the proposed method. The effects of different particle distributions and the convergence behavior are particularly discussed in the implicit thermal analyses. The influences of constitutive parameters in the Cosserat continuum model and background cell sizes on the strain localization band are also studied specifically in the simulations for thermal softening. Supports from NSFC (11672062 and 11772082) are gratefully acknowledged.

15th U.S. National Congress on Computational Mechanics
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Title: Development of a Three-dimensional EMPS-FEM Method for Tire Hydroplaning Analysis

Author(s): *Zumei Zheng, *The University of Tokyo*; Naoto Mitsume, *The University of Tokyo*; Guangtao Duan, *The University of Tokyo*; Shunhua Chen, *The University of Tokyo*; Tomonori Yamada, *The University of Tokyo*; Shinobu Yoshimura, *The University of Tokyo*;

The tire hydroplaning is a complicated fluid-structure interaction (FSI) phenomenon, which, however, is of prime importance for driving safety. In this work, we advocate the coupled explicit moving particle simulation method and the finite element method (EMPS-FEM) to solve this problem, where the EMPS is used to describe the fluid flow and the FEM is for structural deformation. In the existing EMPS-FEM, the interface interaction between the fluid and the structure is solved by an explicitly represented polygon (ERP) wall boundary model. For the situations with complicated solid structures, e.g. angled edges, the ERP model attempts to address the particle leakage problem by adding repulsive forces to the ghost particle model. However, numerical inaccuracy and instability may arise in this model, because only the repulsive force contributed by the nearest polygon is considered for each particle undergoing leakage. The purpose of this work is to develop a robust and accurate EMPS-FEM coupling approach based on the ERP wall boundary model. Special attention is paid to the interaction situations with complicated solid structures. Numerical examples are performed to validate the capacity of the proposed algorithm in the tire hydroplaning analysis.

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Title: Bending Behavior of Hybrid Sandwich Panels with 3D Printed Polymer Lattice Cores

Author(s): *Xia Zhou, *Dalian University of Technology, China*; Wenming Bu, *Dalian University of Technology, China*; Guohui Qu, *Dalian Xinzhong Group Co., LTD., China*; Xiaorun Huang, *Dalian University of Technology, China*;

Hybrid composite sandwich panels are widely used due to their lightweight structures which provide high in-plane and flexural stiffness [1]. These structures consist of solid face sheets and low-density cellular core structures, which are often based upon honeycomb topologies. The recent progress of 3D printing processes has allowed lattice configurations and hybrid sandwich panel structures to be designed with improved mechanical properties. In the present paper, the bending behavior of the hybrid composite sandwich panels with 3D printed polymer cores and AZ31 magnesium skins were systematically studied, which was funded by the National Natural Science Foundation of China (grant number 11672055). To capture the differences in bending properties, two different polymer lattice configurations including the BCC and BCCAV structures were first fabricated by additive manufacturing, and then two composite sandwich panels formed by the resin boning and curing process were investigated under 3-point bending loads by finite element and experiment testing methods. A reliable numerical model for the simulation of the sandwich panels under 3-point bending loads was built. An explicit finite element analysis using ABAQUS/Explicit with a user-defined subroutine was carried out, looking for a detailed model which permitted to understand the influence of each component of the sandwich at failure; importance to the modeling of the interface between the core and the magnesium alloy sheet and the failure criterion was given for good results. In addition, the 3-point bending tests for the sandwich panels were done to validate the results obtained in the FEA. To obtain a validated numerical model for the damage behavior of the hybrid sandwich panels under bending loads, a comparison between the FEA and the experimental results was done. The results of the comparison showed a good agreement between the FEA model and the experimental tests. Compared to the BCC sandwich structures with magnesium metal faces, the sandwich structure with BCCAV cores has the better bending bearing capacity. This is attributed to the increasement of the overall stiffness of the BCCAV core structures. Based on the model and experiments, the failure mechanisms have been identified as four modes: face buckling, core yielding, core collapse and adhesive damage initiation. Keywords: Hybrid sandwich panels, 3D printed lattice cores, bending strength, failure modes, VUMAT subroutine [1] Victor Birman, George A. Kardomateas. Review of current trends in research and applications of sandwich structures [J]. Composites Part B, 2018, 142: 221-240.

15th U.S. National Congress on Computational Mechanics
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Title: A Multi-layer Based Overhang Constraint in Topology Optimization for Additive Manufacturing

Author(s): *Hongyu Zhu, *United Technologies Research Center*; Grum Ngatu, *Collins Aerospace*; Matt Lynch, *United Technologies Research Center*;

Additive manufacturing (AM) allows the creation of components in a layer-by-layer, additive fashion, which offers enormous geometrical freedom compared to conventional manufacturing technologies. It is widely recognized that topology optimization is essential to exploit the design space AM allows. However, overhang limitation in additive manufacturing prevents the direct production of topology optimized parts. Post-processing is generally need. Lately, a layerwise filter has been incorporated in density-based topology optimization on uniform structured meshes for print-ready designs. The limitation of this technique is that the minimum allowable overhang angle (the angle a down-facing surface has with the base plate) is restricted to 45 degree. In practice, smaller overhang angles cause more roughness. At times, a greater overhang angle is desired due to the smoothness requirement. In this work, we present a multi-layer based overhang constraint that allows minimum overhang angle greater than 45 degree without changing the element aspect ratio of the mesh. The newly developed constraint is demonstrated on 2D examples while it can be extended to 3D.

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Title: A Background Mesh Approach for Fluid-Structure Interaction Simulation of Tsunami Debris Using PFEM

Author(s): *Minjie Zhu, *Oregon State University*; Michael Scott, *Oregon State University*;

Tsunami borne debris can cause significant damage to coastal structures. Numerical simulation to consider the debris impact loading is challenging due to the complexity of the analysis and the implementation (Riggs et al. 2014). The difficulty arises from various interactions between fluid, debris, and structures. Although solid debris can be modeled as a structure, it still does not solve the problem of impact and contact between debris and structures and it is difficult to combine all interactions in a single analysis. To this end, a background mesh approach was extended to include debris in FSI simulation. By using the Particle Finite Element Method (PFEM), the background mesh that combines fixed and moving meshes was used by Zhu et al. (2018) to handle FSI analysis of tsunami wave impacting a wide range of structural types. The majority of the fluid domain uses the high quality fixed mesh, which is based on the fluid particles, but in the FSI domain around the structure, Delaunay Triangulation (Watson 1981) is used to generate a moving mesh between the fluid nodes and the structural nodes. Therefore, both the mesh quality and flexibility are preserved for FSI simulation. To incorporate debris in the simulation, debris particles are employed to generate the fixed solid mesh which is updated in every time step as the fixed fluid mesh. The fluid-debris interaction is naturally considered in the fixed mesh domain. Then a moving mesh is generated between the fluid, debris, and structural nodes to account for the fluid-structure and the debris-structure interactions. An additional advantage of the background mesh approach is a coupled system of FSI and debris simulation, which is an accurate approximation for large debris, such as shipping containers and vehicles. Riggs, H. R., Cox, D. T., Naito, C. J., Kobayashi, M. H., Aghl, P. P., Ko, H. T.-S., 1and Khowitar, E. (2014). “Experimental and analytical study of water-driven debris impact forces on structures.” Journal of Offshore Mechanics and Arctic Engineering, 136(4), 041603–041603–8. Watson, D. (1981). “Computing the n-dimensional delaunay tessellation with application to voronoi polytopes.” The Computer Journal, 24(2), 167–172. Zhu, M., Elkhetali, I., and Scott, M. (2018). “Validation of opensees for tsunami loading on bridge superstructures..” Journal of Bridge Engineering, 23(4), 04018015.

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Title: Isogeometric Reissner-Mindlin Shell Based on Mixed Formulation

Author(s): *Zhihui Zou, *Brigham Young University, USA*; Michael Scott, *Brigham Young University, USA*; Derek Thomas, *Coreform LLC, USA*; Bastian Oesterle, *University of Stuttgart, Germany*; Manfred Bischoff, *University of Stuttgart, Germany*; Walfgang Dornisch, *Technische Universität Kaiserslautern, Germany*; Thomas Hughes, *The University of Texas at Austin, USA*;

In this talk we present an isogeometric Reissner-Mindlin shell element for the analysis of thin-walled structures. The variational formulation is based on the Hellinger-Reissner variational principle with independent displacement, membrane and shear strain as the unknown fields. Two types of function spaces are specified to interpolate the strain variables, which helps to overcome the deleterious effects of shear and membrane locking and avoid stress oscillations. The proposed formulation is general and applicable to any mesh topologies, i.e., structured and unstructured meshes. Additionally, it offers an insight into how to deal with the constraints on auxiliary variables in the so-called mixed displacement method, essentially a special case of the proposed mixed formulation. The presented formulation also allows us to explore the effects on the accuracy of the continuous and discrete rotation of the director vector without the pollution of locking. We demonstrate the utility of the formulation on several challenging benchmark problems.

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Title: Spline-based Methods for Inverse Design in Injection Molding

Author(s): *Florian Zwicke, *Chair for Computational Analysis of Technical Systems, RWTH Aachen University, Germany*; Stefanie Elgeti, *Chair for Computational Analysis of Technical Systems, RWTH Aachen University, Germany*;

Spline-based methods play an important role in shape optimization. Since any type of mathematical optimization benefits from a small dimension of the search space, it is important that even complex shapes can be described using a small number of parameters. In contrast to, e.g., finite element simulation meshes with linear interpolation spaces, splines (such as B-Splines or NURBS) of second or higher order have the advantageous property of being able to describe even curved and smooth sections of a shape's boundary using a very limited number of parameters. We develop shape optimization techniques for the specific application of injection molding. In this manufacturing process, a hot polymer melt is injected into a cavity and subsequently cooled down until it solidifies. Due to the cooling and also the solidification, the material shrinks and changes its shape. The resulting defects in the molding shape, when compared to the shape of the cavity, cannot be entirely avoided by adjusting the process. Therefore we wish to create a method that allows us to determine a suitable cavity shape, such that the shape of the finished molding will be as close as possible to the desired result. Since the injection molding process involves both fluid and solid states of the material, we also need to consider both flow and structural simulations. Depending on the type of simulation, several approaches for inverse design are available. For parts of the process, we apply truly inverse methods, where isogeometric analysis helps us obtain smooth shapes. However, we also apply methods of mathematical optimization. In these cases, a spline-based parameterization of the cavity shape, while also providing a smooth surface, provides a low number of design parameters and thus an efficient optimization method. We will present and compare both the inverse and the optimization method based on application-motivated test cases.

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Title: Crisp-boundary Design of Phononic Crystals Using an Interface-enriched Level-set Optimization

Author(s): *Sanne J. van den Boom, *Delft University of Technology, Delft, The Netherlands*; Alejandro M. Aragón, *Delft University of Technology, Delft, The Netherlands*; Fred van Keulen, *Delft University of Technology, Delft, The Netherlands*;

Phononic crystals (PnCs)—periodically arranged materials—have increasingly gained interest due to their remarkable impact on traveling waves. Due to Bragg scattering, they may exhibit bandgaps, i.e., ranges of frequencies for which waves cannot propagate. This effect has potential applications in many fields of engineering, provided that the design of the PnC is appropriately tailored. Therefore, accurate modeling and numerical design approaches are required. Topology optimization (TO) is a numerical design tool that can be used for systematic design of periodic unit cells (PUC) for phononic crystals targeted for specific functionality, for instance, bandgap maximization. Most commonly, a density-based method, where a continuous design variable is assigned to each element of the discretization, is employed for PnC design. However, density-based methods have a major disadvantage: the boundary description is directly coupled to the—usually structured—mesh, which results in a staircased description of the boundary. For Bragg scattering, which is dominated by material interfaces, this non-smooth boundary description is detrimental to the accuracy of the solution. Refining the mesh helps in getting a higher resolution for the boundary description, but a finer mesh inevitably leads to higher computational cost. The latter is undesirable, especially in an optimization setting. Moreover, in density-based topology optimization, the number of design variables is directly linked to the number of elements in the mesh, thus, increasing the computational costs even more. Level-set-based topology optimization, combined with an enriched finite element formulation, provides a crisp description of the boundary, partially alleviating the need for a very fine mesh. In this work, the Interface-enriched Generalized Finite Element Method (IGFEM)[1] is used to completely decouple the interface from the discretization mesh. Previously, IGFEM has been applied to the mesh-independent analysis of phononic crystals[2]. Here, we use IGFEM for the design of PnCs using level-set based topology optimization. Results are compared to those of a density-based mapping approach. References [1] Soghrati, S., Aragón, A. M., Armando Duarte, C., Geubelle, P. H. (2012). An interface?enriched generalized FEM for problems with discontinuous gradient fields. International Journal for Numerical Methods in Engineering, 89(8), 991-1008. [2] van den Boom, S.J., van Keulen, F., Aragón, A.M. (2019). Mesh-independent analysis of Phononic Crystals using an Immersed Discontinuity-Enriched Finite Element Method with Bloch-Floquet periodicity, in preparation.

15th U.S. National Congress on Computational Mechanics
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Title: Efficient Transient Linear Thermo-Mechanical Analysis Using Eigenmode-based Reduction and Analytical Enrichments

Author(s): *Max van der Kolk, *Delft University of Technology*; Matthijs Langelaar, *Delft University of Technology*; Fred van Keulen, *Delft University of Technology*;

Transient thermal behaviour is often encountered for processes such as energy conversion, manufacturing, and for precision instrumentation applications. Specifically, it is critical to understand these transient – and often multi-physical – responses, to design next generation high precision instrumentation, e.g., (aero)space and semiconductor applications. To accu- rately capture these responses, high-fidelity, three-dimensional models are required. How- ever, the resulting finely discretised geometries, result in large system matrices, and hence, long computation times. To alleviate this computational burden, attempts have been made to substitute the full order models by approximate, Reduced Order Models (ROMs) [1]. In this work, we propose an alternative ROM by extension of the Dynamic Correction Method (DCM) [2] with a Modal Truncation Augmentation (MTA) based enrichment [3]. For the first time, DCM is considered for the approx- imation of transient thermal systems. Here, the proposed ROM is constructed by combining particular and homogeneous solutions of the discretised heat equation. The particular solu- tions are obtained in an exact manner for a broad class of thermal excitations, while modal reduction is introduced for the homogeneous solution. Additional, we propose to improve the representation of the reduced homogeneous solution by an MTA-based enrichment. As a result, fast, initial transient responses are considerably better approximated compared to the original DCM. Moreover, the proposed MTA-based enrichment is computationally inex- pensive, especially in contrast with solving additional eigensolutions to enrich the truncated basis. Using both one- and three-dimensional numerical experiments, we illustrate the rela- tive performance of traditional ROMs, compared to our proposed extension of DCM. In the context of transient thermal analysis, the proposed method shows an equal or improved rep- resentation of the full order model, with lower point-wise errors as well as improved converge with respect to the size of the considered, reduced basis. [1] Besselink, B., Tabak, U., Lutowska, A., van de Wouw, N., Nijmeijer, H., Rixen, D. J., Hochstenbach, M. E., and Schilders, W. H. A. (2013). A comparison of model reduction techniques from structural dynamics, numerical mathematics and systems and control. Journal of Sound and Vibration, 332(19):4403–4422. [2] Borino, G. and Muscolino, G. (1986). Mode-superposition methods in dynamic analysis of classically and non-classically damped linear systems. Earthquake Engineering & Structural Dynamics, 14(5):705–717. [3] Dickens, J. M., Nakagawa, J. M., and Wittbrodt, M. J. (1997). A critique of mode acceleration and modal truncation augmentation methods for modal response analysis. Computers & Structures, 62(6):985–998.