IUTAM International Union of Theoretical and Applied Mechanics

UNIVERSITÄT SIEGEN

Innovative numerical approaches for materials and structures in multi-field and multi-scale problems

A symposium celebrating the 60th birthday of Michael Ortiz

September 1st-4th 2014 - Burg Schnellenberg, Attendorn, Germany

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Festkörpermechanik

WELCOME

During the past two decades research in the field of computational mechanics has progressed remarkably, mainly because of the development of a sound mathematical background and efficient computational strategies. Beyond the classical finite element method, several innovative techniques and novel approaches for the analysis of microstructural evolution, growth, damage, and structural failure in multi-field and multi-scale problems have emerged.

It is our pleasure to welcome a remarkable group of 50 scientists to this IUTAM symposium "Innovative numerical approaches for materials and structures in multi-field and multi-scale problems". Official host of the event is the University of Siegen, a modern institute of higher education with about 18.000 students located on the hills of the city of Siegen, North Rhine-Westphalia.

City of Siegen, you can guess the buildings of the university in the background

Our symposium especially celebrates the 60th birthday of Professor Michael Ortiz. Along his exceptional career, Professor Ortiz has been at the forefront of computational mechanics, his work being a constant source of inspiration for many. All participants of this symposium are grateful to Professor Ortiz for being an inspiring collaborator, a reliable colleague, an illuminating scientist, and a valuable friend. We all wish to convey him our brightest wishes for many enjoyable and productive further years!

The venue of this IUTAM symposium is the castle Burg Schnellenberg, a mighty fortress located north of Siegen, in the green heart of Westphalia. With its massive gateways, stone bridges, high vaulted ceilings, and tower rooms, the castle takes you back to medieval times. Once again, we welcome in Burg Schnellenberg all the attendees, wishing a symposium full of interesting presentations, fruitful conversations and inspiring discussions.

In the name of the organizers,
Kerstin Weinberg

	Monday, Sept. 1	Tuesday, Sept. 2	Wednesday, Sept. 3	Thursday, Sept. 4
till 9:00	*Breakfast*	*Breakfast*	*Breakfast*	*Breakfast*
9:15 - 9:45	Registration & get together	Alan Needleman	Sanjay Govindjee	Xanthippi Markenscoff
9:45 - 10:15		Jean-Francois Molinari	Adrian Lew	Ellen Kuhl
10:15 - 10:45		Fehmi Cirak	Sergio Conti	Pilar Ariza
10:45 - 11:15		*Coffee break*	*Coffee break*	*Coffee break*
11:15 - 11:45		Rena Yu	Irene Arias	Jaime Marian
11:45 - 12:15	12:00 Opening	Bo Li	Dennis Kochmann	Thomas Blesgen
12:15 - 12:45	*Lunch*	Malena Espanol	Julian Rimoli	Fernando Fraternali
12:45 - 13:45		*Lunch*	*Lunch*	*Lunch*
13:45 - 14:15	Richard James			
14:15 - 14:45	Alain Molinari	Christopher Larsen	Alexander Mielke	Closing remarks
14:45 - 15:15	Adriana Garroni	Houman Owhadi	Deborah Sulsky	
15:15 - 15:45	Sigrid Leyendecker	Marino Arroyo	Alberto Cuitino	
15:45 - 16:15	Matteo Negri	*Coffee break*	*Coffee break*	
16:15 - 16:45	*Coffee break*	Ignacio Romero	Antonio DeSimone	
16:45 - 17:15	Guruswami Ravichandran	Arash Yavari	Vikram Gavini	
17:15 - 17:45		Bernd Schmidt	Ercan Gürses	
19:00-20:00	*Dinner*	*Special event "Knight Meal"*	*Dinner*	
20:00-21:00	*Walk in the forest*			

Chairs

Monday early afternoon session	Kerstin Weinberg
Monday late afternoon session	Anna Pandolfi
Tuesday morning session	Curt Bronkhorst
Tuesday afternoon session	Alan Needleman
Wednesday morning session	Alain Molinari
Wednesday afternoon session	Sanjay Govindjee
Thursday morning session	Laurent Stainier

LIST OF SPEAKERS AND TITLES OF THE TALKS

Arias, Irene	A computational study of flexoelectricity in nanostructures
Ariza, Pilar	Engineered grapgene based devices
Arroyo, Marino	Mechanics of confined solid and fluid thin films: Graphene and lipid bilayers
Blesgen, Thomas	A Tucker Tensor approach for Kohn-Sham density functional theory
Cirak, Fehmi	Multiresolution subdivision surfaces in variational shape optimisation
Conti, Sergio	Folding patterns in partially delaminated thin films
Cuitino, Alberto	Non-local particle simulations reveal post-jamming response of highly confined granular solids
DeSimone, Antonio	Bio-inspired crawling motility across length scales: opportunities and challenges
Espanol, Malena	A Gamma-Convergence Analysis of the Quasicontinuum Method
Fraternali, Fernando	On the constitutive response and the wave dynamics of tensegrity lattices
Garroni, Adriana	Metastability and dynamics of screw discrete dislocations
Gavini, Vikram	Large-scale real-space Kohn-Sham density functional theory calculations
Govindjee, Sanjay	Variational upscaling in plasticity and viscoelasticity
Gürses, Ercan	Modeling of Spherulite Microstructure in Semicrystalline Polymers
Heyden, Stefanie	A micromechanical damage and fracture model for polymers based on fractional strain-gradient elasticity (poster)
James, Richard	How to find a better shape memory alloy than NiTi
Kochmann, Dennis	The Quasicontinuum Method Revisited: Recent Advances and Open Challenges
Kuhl, Ellen	A mechanical model explains brain development
Larsen, Christopher	Threshold formulations for material defects
Lew, Adrian	The simulation of brittle fracture problems with universal meshes
Leyendecker, Sigrid	Structure preserving multirate integration of constrained systems
Li, Bo	Dynamic inelasticity and failure in cryogenic ice under extreme loading conditions
Marian, Jaime	Atomistically-informed kinetic Monte Carlo simulations of Screw Dislocation Motion in Tungsten
Markenscoff, Xanthippi	Hadamard Instability Analysis for coupled thermo-mechanochemical Systems
Mielke, Alexander	Gradient structures and homogenization for thermomechanical systems
Molinari, Alain	A micro-mechanical approach for the dynamic fracture of ductile materials
Molinari, Jean Francois	A finite temperature atomistic/continuum coupled model for contact applications
Needleman, Alan	The Competition between Failure and Localization of Deformation in Progressively Softening Solids
Negri, Matteo	Quasi-static evolutions for a phase field model in fracture
Owhadi, Houman	Bayesian Numerical Homogenization
Rimoli, Julian	A Concurrent Multi-Scale Model for the Thermo-Mechanical Response of Materials
Romero, Ignacio	A fully Lagrangian method for fluid/solid interaction
Schmidt, Bernd	An analysis of crystal cleavage in the passage from atomistic models to continuum theory
Sulsky, Deborah	Convergence and Accuracy of the Material-Point Method
Yavari, Arash	Differential Complexes in Continuum Mechanics
Yu, Rena	Meshfree numerical schemes applied to unconfined seepage problems through earth dams

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MODELING AND SIMULATION OF FRACTURE IN FERROELECTRIC POLYCRYSTALS

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Ferroelectric materials are important to a broad range of applications, from common-rail fuel injection to medical ultrasound, structural health monitoring and prognosis. However, the reliability of these systems is still an important concern due to the inherent brittleness of ferroelectric ceramics, demanding investigations into their complex fracture behavior. Complexity stems mainly from the interactions between the cracks, material microstructure (both ferroelectric domains and polycrystalline grains), and localized stress and electric fields near crack tips. Domain switching (formation and evolution of ferroelectric twins and domains) has been reported near cracks, and it has been made responsible for changes in the fracture behavior of ferroelectric materials. We simulate the fracture processes of ferroelectric polycrystals in three dimensions using a phase-field model [1,2]. The grain boundaries, cracks and ferroelectric domain walls are represented in a diffuse way by three phase-fields [3]. We thereby avoid the difficulty of tracking the evolving interfaces in three dimensions. The simulation results show the effect of the polycrystalline and ferroelectric domain microstructures on the fracture response of the material. Crack deflection, crack bridging, crack branching and ferroelastic domain switching are observed to act as the main fracture toughening mechanisms in ferroelectric polycrystals. Our fully 3D simulations illustrate how the combination of these mechanisms enhances the fracture toughness of the material [4].

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ENGINEERED GRAPHENE BASED DEVICES

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In the field of electronics, due to its excellent mechanical and electrical properties, graphene has become the most promising material for the production of next generation thin and flexible graphene-based electronic components. Pristine defect-free graphene has no bandgap and is of limited use for semiconductor-based electronics. It was found experimentally that the Stone-Wales defects could change the local density of states, however, is not expected to introduce band gaps. Therefore, many attempts have been made to engineer band gaps in graphene. Among other mechanisms, it has been shown theoretically that grain boundaries might insert band gaps. In order to identify appropriate geometrical configurations, we have carried out an appraisal of the stability and dynamics of grain boundaries in graphene for different misorientation angles at finite temperature and up to extremely high temperatures. To this end, we have developed a simulation tool based on lattice harmonics and tight-binding potentials.

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MECHANICS OF CONFINED SOLID AND FLUID THIN FILMS: GRAPHENE AND LIPID BILAYERS

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Many natural and man-made systems consist of a thin elastic sheet coupled to a substrate. As the substrate undergoes compressive deformation, a variety of buckling responses can be observed. In this talk, I will discuss two particular instances of such systems, and how mathematical modeling and computational mechanics can help understand their complex behavior. Graphene is the ultimate thin elastic sheet, only one atom thick. Wrinkle networks are ubiquitous buckle-induced delaminations in supported graphene, which locally modify the electronic structure and degrade device performance. Through simulations, we understand how strain anisotropy, adhesion and friction govern spontaneous wrinkling [1]. We propose a strategy to delicately control the location of wrinkles through patterns of weaker adhesion, leading to a variety of network geometries and junction configurations, with the goal of assisting constructive use of strain-engineered wrinkle networks [2]. Lipid bilayers compartmentalize cells, and mediate in a large number of biological processes. They exhibit complex mechanics involving elasticity and hydrodynamics of two tightly coupled monolayers [3]. Bilayers are often confined by the extracellular matrix, the cortex or other membranes. By an integrated experimental and theoretical approach, we investigate the mechanics of confined membranes, including the influence of adhesion, strain, and osmotic pressure [4]. We find that supported lipid bilayers respond to stress by nucleating and evolving spherical and tubular protrusions. These responses are also observed in cells, playing a role in surface area regulation.

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A TUCKER TENSOR APPROACH FOR KOHN-SHAM DENSITY FUNCTIONAL THEORY

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Recent studies on a wide range of materials systems have demonstrated that the electronic structure admits a low-rank tensor structure approximation [1,2], in particular the Tucker tensor format. These investigations have shown that the computed electronic structure can be significantly compressed using the Tucker tensor approximation with a convergence of the approximation error that is exponential with the Tucker rank. Recently, it was also demonstrated that the Tucker tensor rank only exhibits a weak dependence on the system size [3], which presents significant promise for developing computationally efficient techniques for Kohn-Sham density functional theory (DFT) calculations based on tensor-structured approximations.

In this talk, we present the development of a new and efficient computational scheme for Kohn-Sham DFT calculations using a Tucker tensor basis. The Tucker tensor basis is constructed from the eigenfunctions of an additive separable approximation of the Kohn-Sham Hamiltonian in each iteration of the self-consistent field (SCF) approach. We present and contrast two approaches of constructing the additive separable approximation of the Hamiltonian: (i) from a constrained variational problem using a rank-one approximation of the wavefunctions; (ii) from a weighted residual minimization of the Kohn-Sham potential. While both approaches are applicable for local pseudopotential calculations, the former approach is a more natural choice for non-local pseudopotential computations. Upon construction of the Tucker tensor basis which is a globally adapted basis for the Hamiltonian at each SCF cycle, the Kohn-Sham Hamiltonian is projected into the Tucker tensor basis and the resulting eigenvalue problem is solved using Chebyshev acceleration techniques [4,5].

The efficiency and convergence properties of the new algorithm are analyzed for a range of materials systems including Aluminum clusters and Alkane chains of different sizes. Our studies indicate that a Tucker rank around 50 is sufficient to achieve chemical accuracy and is only weakly dependent on the system size. This weak dependence has important consequences on the computational complexity of the proposed method. In particular, if the Tucker rank is independent of the system size, the computational complexity of the algorithm scales linearly with

N, the number of electrons in the system, for all materials systems (insulating and metallic) providing an efficient approach for large-scale DFT calculations.

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MULTIRESOLUTION SUBDIVISION SURFACES IN VARIATIONAL SHAPE OPTIMISATION

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We consider the isogeometric shape optimisation of structures by combining multiresolution subdivision surfaces with immersed finite elements. The interoperability limitations of the current computer aided design (CAD) and finite element analysis (FEA) techniques are most evident in structural shape optimisation. Due to the lack of a bidirectional mapping between the CAD and FEA models usually the geometry of the finite element mesh is optimised. It is tedious or impossible to propagate these changes back to the CAD model, which is essential for continuing with the design process and for manufacturing purposes. Moreover, geometric design features are usually defined with respect to the CAD model and cannot be easily enforced on the finer finite element mesh.

For domain discretisation we use immersed, or embedded, boundary finite elements, which have clear advantages when applied to structural shape optimisation [5]. Most importantly, there is no need to maintain an analysis-suitable domain discretisation during the optimisation iterations. On the fixed non-boundary-conforming domain grid, we use tensor-product b-splines as basis functions and enforce the Dirichlet boundary conditions with the Nitsche technique. For gradient-based shape optimisation, the shape derivative of the cost functional with respect to geometry perturbations is needed. To this end, we use the adjoint approach and solve the primary and the adjoint boundary value problems with the immersed finite element method.

On the fixed volume grid we represent domain boundaries with subdivision surfaces. Specifically, we use either the Loop scheme based on triangular quartic box-splines or the Catmull-Clark scheme based on tensor-product cubic b-splines. In subdivision a limit surface is obtained through the repeated refinement of a coarse control mesh [3, 4]. The hierarchy of control meshes underlying a subdivision surface lends itself naturally to multiresolution editing. The coarse control mesh vertex positions are modified to perform large-scale editing and the fine control mesh vertex positions are modified to add localised changes. In multiresolution shape optimisation we use a fine control mesh for finite element discretisation and coarser control meshes for geometry modification [1, 2]. We start optimising with the coarsest control mesh and progress to optimise increasingly finer control meshes.

As will be demonstrated with a number of examples, the fine-grained geometry control provided by multiresolution optimisation leads in general to more optimal designs compared to traditional

approaches. In addition, any non-physical geometry oscillations and the occurrence of mesh pathologies, like inverted elements, are excluded from the onset.

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FOLDING PATTERNS IN PARTIALLY DELAMINATED THIN FILMS

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Elastic films deposited on a substrate are often subject, after thermal expansion, to compressive strains which are released by debonding and buckling, generating a variety of microstructures. The work of Michael Ortiz and Gustavo Gioia in the 90s [1,2] opened the way for the study of these structures with the tools of calculus of variations. One of their insights was that the key nonconvexity which originates to the microstructure can be understood in terms of the out-of-plane displacement alone, leading after some rescalings to the Eikonal functional,

$$E_\sigma[w] = \int_\Omega \Big(\big(|Dw|^2 - 1\big)^2 + \sigma^2 |D^2 w|^2 \Big)\, dx, \tag{1}$$

subject to $w = 0$ on $\partial\Omega$. Here $\Omega \subset \mathbb{R}^2$ represents the debonded region, $w : \Omega \to [0, \infty)$ the rescaled normal displacement, and σ is a small parameter related to the thickness of the film. This functional, despite a large mathematical effort, is not yet completely understood; it has been shown that the minimal energy is proportional to σ but the Γ-limit of $\sigma^{-1} E_\sigma[w]$ is not yet completely identified. The work of Ortiz and Gioia was then extended to related problems, showing for example that under anisotropic compression branching-type microstructures appear close to the boundary [3], or that in certain regimes telephone-cord blisters develop [4]. A finer analysis of the nonlinear elastic model which had led to (1) has shown that also in the case of isotropic compression the in-plane components exhibit fine-scale oscillations which refine close to the boundary [5,6].

Recently interest has been directed to controlling the microstructures by designing the geometry of the debonded region appropriately. The key idea is to introduce a sacrificial layer between film and substrate, and then to selectively etch away a part of it, so that the boundary of the debonded region is straight. The film then partially rebonds to the surface, leading to complex patterns of tunnels [7,8]. The patterns can be studied coupling the von-Kármán energy with a fracture model proportional to the debonded area,

$$E_{\sigma,\gamma}[u, w] = \int_\Omega \big(|Du + Du^T + Dw \otimes Dw - \mathrm{Id}|^2 + \sigma^2 |D^2 w|^2 \big)\, dx + \gamma |\{w > 0\}|. \tag{2}$$

Here $u : \Omega \to \mathbb{R}^2$ are the (scaled) tangential displacements and $\gamma > 0$ is the bonding energy (related with Griffith's fracture energy). The mathematical analysis of the energy (2) shows a rich phase-diagram, which contains four different regimes [9]. For large bonding energy

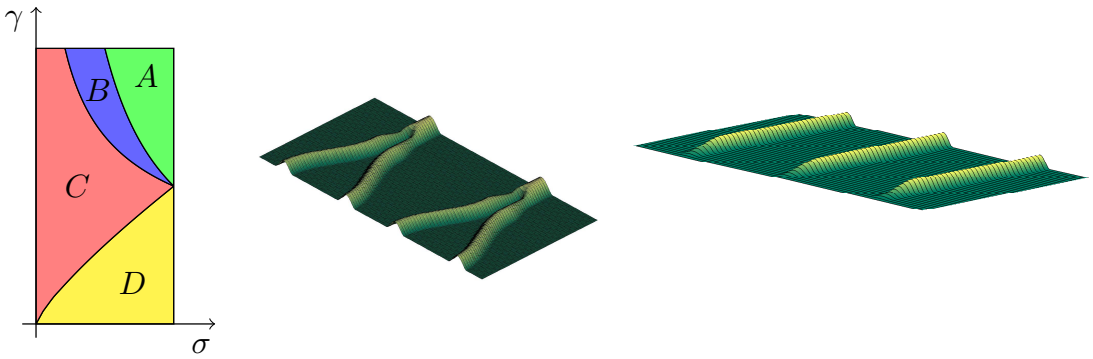

Figure 1: Phase diagram for $E_{\sigma,\gamma}[u,w]$ in the (σ,γ) plane, with a sketch of the tube branching (C) and the laminate (B) regime. From [9].

γ the film is completely bound to the substrate, for very small γ it is completely detached. For intermediate values debonded channels are formed, which separate wider bonded regions. Depending on the relative value of the film thickness and the bonding energy, the tubes are either parallel (a pattern similar to a laminate) or form a branched structure (as in the fully debonded case), see Figure 1.

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NON-LOCAL PARTICLE SIMULATIONS REVEAL POST-JAMMING RESPONSE OF HIGHLY CONFINED GRANULAR SOLIDS

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Predictive multi-scale modeling and simulation of microstructure evolution during compaction of granular solids requires research efforts in two main fronts. First, the development of predictive constitutive models of inter-particle interactions that account for high levels of confinement and a variety of physical mechanisms; and second, the development of concurrent multi-scale strategies that combine a detailed description of the granular scale with the computational efficiency typical of continuum-level models. The outline of this work is then twofold: (i) we present a new 'nonlocal contact formulation' [1] that overcomes the typical, but unrealistic, assumption that contacts are independent regardless the confinement of the granular system, (ii) we describe a fully-discrete model which concurrently solves for contact forces at the granular scale, for nonlocal deformations at the mesoscale, and for static equilibrium at the macroscale.

This non-local particle mechanics simulation framework allows to investigate the response of granular media under large level of confinements. The numerical experimentation reveals a distinctive behavior between the initial stages of consolidation characterized by a well-know process of jamming, and the subsequent regime or *post-jamming* response where non-local particle interactions play a significant role. One of the key observations from the numerical studies is that the force network distribution evolves differently in the interior and the boundary of the granular solid as confinement is increased. The implications of these predictions are expected to play pivotal role in manufacturing by powder compaction, where the competition between developing bonding among particles and particle sticking to tooling defines the quality of consolidated materials.

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BIO-INSPIRED CRAWLING MOTILITY ACROSS LENGTH SCALES: OPPORTUNITIES AND CHALLENGES

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We present some of the first results obtained in the laboratory for Sensing and Moving Bioinspired Artifacts (SAMBA), an experimental facility recently established at Sissa, Trieste. The goal of the laboratory is to work at the triple point between theoretical, computational, and experimental mechanics in order to distill the 'secrets' of biological locomotion at small scales, and to reproduce them in the conceptual design of working self-propelled prototypes.

One of our current research topics is limbless locomotion on solid substrates. Limbless locomotion is the self-propulsion strategy of choice for several simple, invertebrate organisms (e.g., snails, earthworms), but also for unicellular organisms (amoeboid motion) and single cells (crawling motility). In fact, limbless locomotion scales well across sizes, from the micron scale of single motile cells to the meter scale of snakes. It is also very versatile: it allows organisms to move across very irregular and uneven terrains, or even inside biological tissues, as in the case of single crawling cells. For these reasons, it is attracting increasing attention as a possible paradigm for motility at microscopic scales and for the engineering of biomedical devices capable of navigating inside the human body for diagnostic or therapeutic purposes.

We will present some of our recent results on slender crawlers, modelled as one-dimensional systems capable of freely actuating their shape in order to control their position. Depending on the details of the frictional interaction between the crawler and the substrate, several motility strategies are feasible, which differ dramatically from the point of view of performance and energetic efficiency. Self-propulsion is possible even with a simple, linear relationship between frictional force and sliding velocity (Newtonian). The nonlinearities necessary to obtain net displacements (hence, non-periodic position histories) from periodic shape histories arise from the fact that frictional forces are distributed over deforming contact areas. Nonlinearities on the force-velocity relationship, such as the presence of a yield force for sliding (Bingham), allow for more effective propulsion, with stick and slip in selected portions of the contact interface [1]. Finally, directional surfaces, which have the property that the force-velocity relation is not even odd, allow for self-propulsion even when crawlers are only capable of reciprocal shape changes [2]. These *breathing modes* are particularly relevant, because they are the simplest

shape changes that can be excited with a time-periodic stimulus. Our results shows that the so-called *scallop theorem* of low Reynolds number hydrodynamics [5] is no longer valid in the context of crawling motility.

We are currently working on the actual implementation of these concepts in actual working prototypes [4,5], exploiting smart materials for actuation purposes, with the aim of producing a *dictionary* of elementary motility mechanisms.

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A Γ-CONVERGENCE ANALYSIS OF THE QUASICONTINUUM METHOD

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Continuum mechanics models of solids have certain limitations as the length scale of interest approaches the atomistic scale, for instance when studying defects. A possible solution in such situations is to use a pure atomistic model. However, this approach could be computational prohibited as we are dealing with millions of atoms. The quasicontinuum (QC) method [1] is a computational technique that reduces the atomic degrees of freedom. In this talk, we review two foundational steps of QC: interpolation schemes and summation rules. Using the tools of Γ-convergence (a variational notion of convergence which, in particular, implies convergence of energy minimizers), we identify sufficient conditions on the interpolation and on the summation rules for the sequence of approximating energies to be convergent in the case of harmonic lattices [2]. Numerical convergence studies on three-dimensional BCC crystals governed by empirical potentials are presented. The convergence properties of the numerical model bear out the results of the Γ-convergence analysis.

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ON THE CONSTITUTIVE RESPONSE AND THE WAVE DYNAMICS OF TENSEGRITY LATTICES

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The talk presents theoretical and numerical results on the wave dynamics of periodic lattices composed of lumped masses and tensegrity prisms under impact loading. Theoretical results and numerical simulations show that such systems can be tuned into an elastic softening regime by adjusting local and global prestress variables. The geometrically nonlinear response of the examined lattices results in an acoustic behavior supporting the formation of either compressive or rarefaction solitary waves under impulsive initially compressive loading. Numerical examples highlight that the amplitude of the leading rarefaction wave can be adjusted by local and global prestress.

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METASTABILITY AND DYNAMICS OF SCREW DISCRETE DISLOCATIONS

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Dislocations are defects in crystal and are considered the main mechanism for plasticity. Effective model for plasticity should then account for interaction and motion of dislocation which are affected by the crystalline structure. It is understood that such models should be obtained via a multi-scale analysis, from micro to macro scale, in a passage from discrete to continuum. A major difficulty in this program is the formulation of a good discrete model, able to encode all the crystallographic informations. Indeed the presence of the defects makes the use of a reference configuration not clear.

In the case of anti-plane elasticity and straight screw dislocations the use of a reference configuration is still possible (this being the projection of the defected crystal along the anti-plane direction). We consider a two-dimensional scaled Bravais lattice $\varepsilon\mathcal{L}$ and a periodic potential f acting on nearest neighbors. The interaction energy is then

$$E_\varepsilon(u) = \sum_{i,j\in\varepsilon\mathcal{L}\cap\Omega\ ,\ |i-j|=\varepsilon} f(u(i)-u(j)), \tag{1}$$

where $\Omega\subset\mathbf{R}^2$ and $u:\varepsilon\mathcal{L}\cap\Omega\to\mathbf{R}$ is the vertical rescaled displacement. A prototype example is the case corresponding to a piece-wise quadratic 1-periodic potential (see [4]). This model can be also obtained as a special case of a more general discrete model (fully three-dimensional) proposed by Ariza and Ortiz in [2]. Following the approach of [2] it is possible to define the plastic and the elastic discrete strain and, in a very natural way, to introduce the notion of discrete circulation in order to detect the presence of dislocations.

For this model it is possible to perform a complete multi-scale analysis, from the static and the dynamic point of view.

In [1], by means of an asymptotic expansion in terms of Γ-convergence, as the lattice spacing ε tends to zero, we can prove the existence of many local minima for the energy E_ε (see also [5] for a similar result with different techniques) and hence we deduce that the motion of dislocations is pinned by the discrete structure.

We then construct a limit evolution of point defects using a discrete scheme in time in the spirit of Minimizing Movements. From the definition of an appropriate crystalline dissipation in the

passage from discrete to continuum we obtain a limiting dynamics that accounts for the glide directions of the crystal (see also [3]).

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LARGE-SCALE REAL-SPACE KOHN-SHAM DENSITY FUNCTIONAL THEORY CALCULATIONS

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Quantum-mechanical calculations based on Kohn-Sham density functional theory (DFT) have played a significant role in accurately predicting various aspects of materials behavior over the past decade. The enormous computational effort associated with Kohn-Sham DFT calculations has restricted most investigations to computational domains containing at most a thousand atoms. The plane-wave basis has been a popular discretization technique for DFT calculations, especially for bulk materials properties, owing to the systematic and spectral convergence afforded by the basis. However, a plane-wave discretization restricts investigations to periodic geometries and boundary conditions that are not well-suited, or, not appropriate, for crystalline materials systems containing extended defects, finite-dimensional materials systems with nanoscale dimensions, and non-crystalline materials systems. The other widely adopted basis functions in DFT calculations comprises of atomic-orbital type basis sets that are well-suited for isolated systems, but can not easily handle other boundary conditions. Further, an atomic-orbital type basis does not offer systematic convergence in ground-state energies. Also, the parallel scalability is significantly affected beyond a few hundred processors, for both plane-wave and atomic-orbital basis, due to the non-locality of basis functions. This limits the accessible systems sizes even with the use of high performance computing resources. Thus, there has been an increasing thrust on systematically improvable and scalable real-space techniques for electronic-structure calculations over the past decade. Among the real-space techniques, the finite-element (FE) discretization of Kohn-Sham DFT presents some unique advantages. In particular, it allows for the consideration of complex geometries and boundary conditions, is amenable to unstructured coarse-graining, and, due to the locality in the basis functions, is better suited for an efficient parallel implementation. Following this line of thought, we developed computationally efficient and robust parallel algorithms to conduct large-scale real-space Kohn-Sham DFT calculations using the FE basis. In particular, we demonstrate pseudopotential DFT calculations on materials systems containing $\sim$ 8,000 atoms and all-electron calculations on materials systems with $\sim$ 4000 electrons.

The key ideas involved in this work [1] include: (i) employing higher-order spectral FE basis functions, (ii) developing *a-priori* mesh adaption technique to construct close to optimal FE discretization of the problem, (iii) employing Chebyshev acceleration strategies to compute the solution of the Kohn-Sham eigenvalue problem. Our numerical studies show staggering computational savings of the order 1000-fold by using higher-order FE discretization, in comparison

to linear finite-elements employed in prior studies. A comparative study of the computational efficiency of higher-order spectral FE discretization shows that the performance of FE basis is competing with commercial codes using plane-wave discretization for non-periodic pseudopotential calculations, and compares well with Gaussian basis for all-electron calculations. Using these ideas, electronic structure calculations have been demonstrated on a few thousand atoms using using modest computational resources, and good scalability of the implementation with over 90% efficiency has been observed on up to 200 processors.

The conventional approach of solving the Kohn-Sham problem involves the diagonalization of the Hamiltonian to compute the lowest eigenvalues and eigenstates corresponding to the number of electrons N_e. The computational complexity of the solution of the Kohn-Sham problem, thus, scales as $O(N_e^3)$, which becomes prohibitively expensive for large scale electronic structure calculations. To this end, we further build on our developments to formulate a sub-quadratic scaling subspace projection technique. The framework extends ideas in [2] to metallic systems and treats metallic and insulating systems on the same footing. The key ideas involved in the approach are: (i) employing the Chebyshev filtering approach to compute the eigensubspace corresponding to lowest N_e eigenstates of the Hamiltonian, (ii) construct non-orthogonal localized wavefunctions spanning the eigensubspace by employing a localization procedure, (iii) compute the density matrix by employing a Chebyshev-polynomial expansion of the projected Hamiltonian expressed in the basis comprising of the non-orthogonal localized wavefunctions. We employ an adaptive truncation procedure to achieve a compact support for the localized wavefunctions, where the truncation tolerances progressively become tighter as the self-consistent field iteration of the Kohn-Sham problem proceeds towards convergence. The accuracy and sub-quadratic scaling of the algorithm are demonstrated on representative benchmark atomic systems involving pseudopotential calculations on varying sizes of metallic aluminium face-centered-cubic nano-clusters up to 3430 atoms, insulating alkane chains up to 8000 atoms, and semi-conducting silicon nano-clusters (all-electron calculations) up to 3920 electrons [3].

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VARIATIONAL UPSCALING IN PLASTICITY AND VISCOELASTICITY

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Given an inelastic material model, a structural geometry, and a set of boundary conditions, one can in principle always solve the governing equations to determine the system's mechanical response. However, for large inelastic systems this procedure can quickly become computationally overwhelming, especially in three-dimensions and when the material is locally complex. In such settings multiscale modeling offers a route to a more efficient model by holding out the promise of a framework with fewer degrees of freedom which at the same time faithfully represents up to a certain scale the behavior of the system.

In this talk, we present a scheme that produces such models upon the basis of a variational scheme. The essence of the scheme is the construction of a variational statement for the strain energy as well as the dissipation potential for a coarse scale model in terms of the strain energy and dissipation of fine scale model. From the coarse scale energy and dissipation we can then generate coarse scale material models that are computationally far more efficient than either directly solving the fine scale model or by resorting to FE^2 type modeling. An essential feature for such schemes is the proper definition of the coarse scale inelastic variables. By way of concrete examples, we illustrate the needed features to generate successful models. The final validity of the the developed models is demonstrated by comparison to brute force fine scale simulations. As illustrative examples, we consider the conceptually simple problem of determining the torque to twist-rate relation for an elastically perfectly-plastic circular bar, the effective pressure to radial motion relation for a thick-walled cylinder, and lastly we apply our framework for the derivation of fully variationally consistent micro-sphere models with viscoelasticity – i.e. to non-gradient homogenization.

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MODELING OF SPHERULITE MICROSTRUCTURE IN SEMICRYSTALLINE POLYMERS

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Polymers, being the typical constituent of plastics in industry, have wide range of application areas in modern life. Among polymers, semicrystalline polymers (SCP) form a subset with a significant interest; owing to their remarkable deformability and toughness, good impact strength, very low gas-permeability, superior wear resistance. With notable examples of high-density polyethylene (HDPE), Nylon-6, poly(ethylene terephthalate) (PET), isotactic polypropylene (iPP); semicrystalline polymers have been used in applications such as electrical insulation systems and substrates for flexible electronic devices to plastic bags, piping systems, liquid and gas containers. Semicrystalline polymers are composed of crystalline structures and amorphous polymer chain networks and therefore they exhibit deformation mechanisms of both crystalline materials and amorphous polymers. They can be considered as two-phase materials consisting of a soft amorph phase and a hard crystalline phase, where percentage of crystalline phase can normally vary from 10% to 80%. One of the most common microstructures observed in melt crystallized semicrystalline polymers is the spherulite microstructure. In a spherulite microstructure, crystalline lamellae are embedded in a matrix of amorphous material and grow out from a common central nucleus in radial directions. The crystalline lamellae are 3 to 20 nm thick, whereas spherulite diameters are normally in the range of 2 to 100 microns. Complicated and hierarchical microstructure of semicrystalline polymers, results in deformation mechanisms that involve complex and multistage processes.

In this work, mechanical behavior of semicrystalline polymers is studied by direct finite element modeling of a spherulite microstructure under different loading conditions. Finite element meshes of idealized spherulite microstructures are constructed where different constitutive models are assigned to crystalline phase and amorphous polymer phase regions. A crystal plasticity model, which takes into account the crystalline slip constraints induced by covalently bonded strong polymer chains is used for the crystalline phase, while elastic microsphere model is employed for the amorphous phase. Effects of several parameters, such as spherulite size and degree of crystallinity, on the mechanical behavior are studied. Furthermore, it is shown that the model captures the evolution of inhomogeneous plastic deformation activity in spherulite microstructure reported in the literature

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A MICROMECHANICAL DAMAGE AND FRACTURE MODEL FOR POLYMERS BASED ON FRACTIONAL STRAIN-GRADIENT ELASTICITY

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We formulate a simple one-parameter macroscopic model of distributed damage and fracture of polymers that is amenable to a straightforward and efficient numerical implementation. We show that the macroscopic model can be rigorously derived, in the sense of optimal scaling, from a micromechanical model of chain elasticity and failure regularized by means of fractional strain-gradient elasticity. In particular, we derive optimal scaling laws that supply a link between the single parameter of the macroscopic model, namely, the critical energy-release rate of the material, and micromechanical parameters pertaining to the elasticity and strength of the polymer chains and to the strain-gradient elasticity regularization. We show how the critical energy-release rate of specific materials can be determined from test data. Finally, we demonstrate the scope and fidelity of the model by means of an example of application, namely, Taylor-impact experiments of polyurea 1000 rods.

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HOW TO FIND A BETTER SHAPE MEMORY ALLOY THAN NiTi

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In recent years desirable features of phase transformations such as low hysteresis and reversibility have been linked to "supercompatibility" conditions between phases [1,2]. We review these conditions and propose a route to highly reversible shape memory alloys. Interestingly, NiTi does not satisfy any of these conditions of compatibility; it is not even close. We suggest a highly speculative, as yet unconfirmed, idea on why NiTi has nevertheless emerged as the most popular shape memory alloy.

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THE QUASICONTINUUM METHOD REVISITED: RECENT ADVANCES AND OPEN CHALLENGES

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The quasicontinuum (QC) method [1] was introduced to efficiently coarse-grain crystalline atomistic ensembles in order to bridge the scales from individual atoms to the micro- and mesoscales. Various flavors of the QC method have been reported which differ by their local vs. nonlocal thermodynamic formulation, their approximation of the total Hamiltonian [2] or of the interatomic forces [3], their interpolation schemes, and their model adaption techniques, to name but a few. Within the family of energy-based QC methods (whose Γ-convergence was shown in [4]) we recently introduced a new sampling scheme in three dimensions which is fully-nonlocal and thus does not conceptually differentiate between atomistic and coarse-grained domains [5,6]. The underlying optimal energy-based summation rules are based on a set of sampling atoms different from the representative atoms and whose locations are determined to optimally approximate the total Hamiltonian.

We show that the new optimal scheme results in minimal approximation errors and thus marginal residual and spurious force artifacts. The new summation rule, similar in spirit to quadrature rules [7], allows for automatic model adaption and guarantees no force artifacts in the limits of full atomistic resolution as well as in large elements. Approximation errors and force artifacts in the intermediate regime are small compared to previous schemes of comparable efficiency. Furthermore, we use a new adaptation scheme which locally re-maps atomic neighborhoods so that the QC model can accurately represent large atomistic motion. We also review our recent

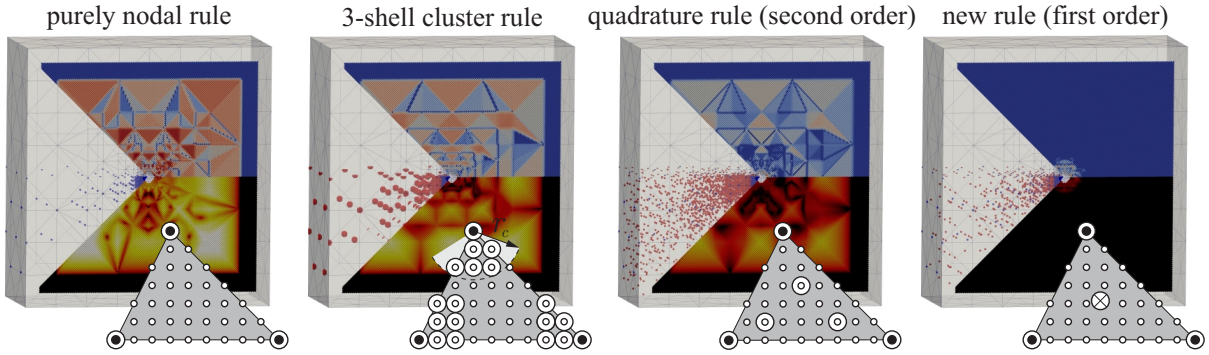

Figure 1: The evolution of summation and sampling rules for the QC method: from nodal to cluster summation rules, to quadrature-based rules and to the new optimal schemes that offer a compromise between the traditional local/nonlocal QC method [1] and more recent energy-based QC flavors [2,4].

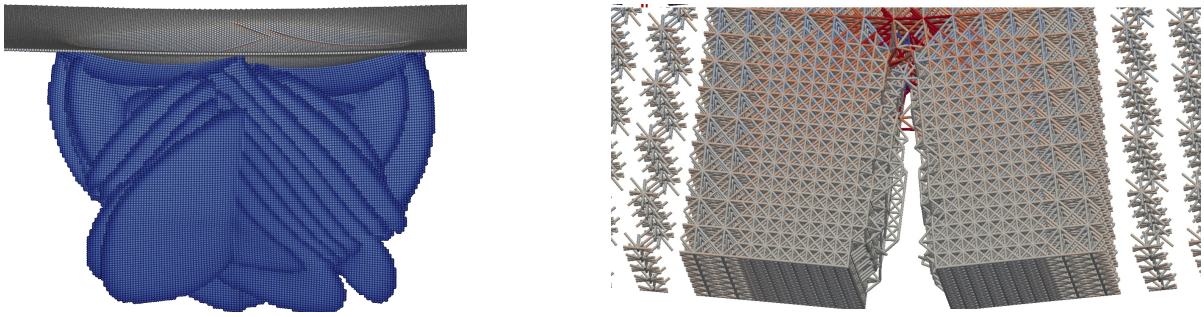

Figure 2: Example applications of the new QC framework: nano-indentation into a single-crystal modeled by the QC method, and small-scale periodic truss structures coarse-grained by an extension of the QC methodology.

meshless extension of the QC method [8] which employs local maximum-entropy interpolation schemes [9]. We present selected examples of small-scale deformation and failure mechanisms investigated by the new computational QC framework. These include micro-indentation, nano-void growth and coalescence, and small-scale truss structures.

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A MECHANICAL MODEL EXPLAINS BRAIN DEVELOPMENT

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Convolutions are a classical hallmark of most mammalian brains, see Figure 1, left. Brain surface morphology is often associated with intelligence and closely correlated to neurological dysfunction. Yet, we know surprisingly little about the underlying mechanisms of cortical folding. Here we show that mechanics plays a major role in regulating brain development [1]. To establish analytical estimates for the critical wavelength at the onset of folding, we model cortical folding as the instability problem of a confined layered medium under growth-induced compression using the Föppl-von-Kármán plate theory. To predict realistic surface morphologies in the post-critical regime, we establish a computational model using the continuum theory of finite growth, Figure 1 right. A better understanding the mechanisms that drive brain folding may have direct implications on the diagnostics - and possibly treatment - of neurological disorders including epilepsy, schizophrenia, and autism.

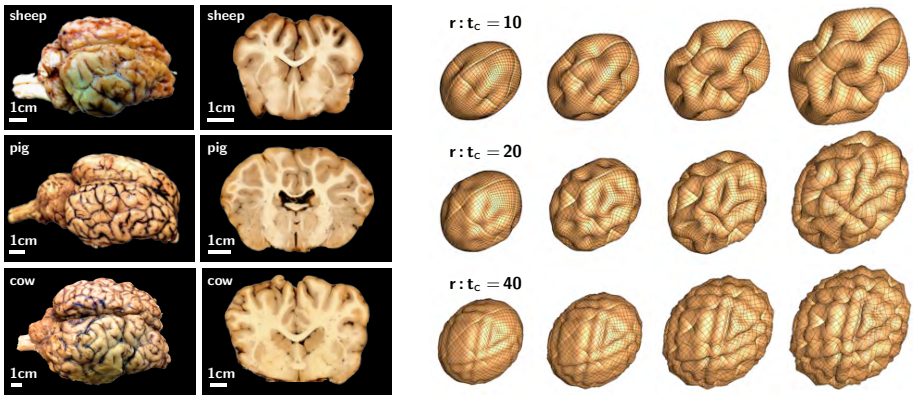

Figure 1: Surface morphology of the mammalian brain. Larger mammals tend to have larger and more folded brains, left. The model predicts that the number of folds increases with increasing radius-to-thickness ratio, right.

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THRESHOLD FORMULATIONS FOR MATERIAL DEFECTS

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We describe models for quasi-static damage evolution, quasi-static cohesive fracture evolution, and dynamic cohesive fracture, based on strain thresholds for defects, rather than energy minimization. Aside from being more physically motivated, advantages of this approach include clarification of the role of irreversibility of defects, and existence of solutions for a broader range of defect energies.

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THE SIMULATION OF BRITTLE FRACTURE PROBLEMS WITH UNIVERSAL MESHES

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We describe our approach to simulating curvilinear brittle fractures in two-dimensions based on the use of Universal Meshes. A Universal Mesh is one that can be used to mesh a class of geometries by slightly perturbing some nodes in the mesh, and hence the name universal. In this way, as the crack evolves, the Universal Mesh is always deformed so as to exactly mesh the crack surface. The advantages of such an approach are: (a) the crack faces are exactly meshed with a conforming mesh at all times, and the quality of the surface mesh is guaranteed to be good, (b) apart from duplicating degrees of freedom when the crack grows, the connectivity of the mesh and the sparsity of the associated stiffness matrix remains unaltered; this has the positive effect of enabling efficient iteration over the crack geometry, needed for the satisfaction of Griffith's criterion at the crack tip.

In the presentation I will introduce the notion of a Universal Mesh, illustrate the progress we have made so far with some examples, and then focus on the simulation of curvilinear fractures, and in particular, show examples in which the computed crack path converge to the exact crack path, regardless of the mesh. If time permits, simulation of thermally induced fracture and hydraulic fractures will be discussed.

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STRUCTURE PRESERVING MULTIRATE INTEGRATION OF CONSTRAINED SYSTEMS

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Mechanical systems with dynamics on varying time scales, e.g. including highly oscillatory motion, impose challenging questions for numerical integration schemes. Tiny step sizes are required to guarantee a stable integration of the fast frequencies. However, for the simulation of the slow dynamics, integration with a larger time step is accurate enough. Here, small time steps increase integration times unnecessarily, especially for costly function evaluations. For systems comprising fast and slow dynamics, multirate methods integrate the slow part of the system with a relatively large step size while the fast part is integrated with a small time step [1,2]. A particular challenge is the treatment of the coupling between slow and fast dynamics, e.g. via potentials or holonomic constraints. In this work, a multirate integrator is derived in closed form via a discrete variational principle, resulting in a symplectic and momentum preserving multirate scheme [3]. Depending on the discrete approximations for the Lagrangian function, one obtains different integrators with varying convergence properties, e.g. purely implicit second order or purely explicit first order schemes, or methods that treat the fast and slow parts in different ways.

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DYNAMIC INELASTICITY AND FAILURE IN CRYOGENIC ICE UNDER EXTREME LOADING CONDITIONS

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A mission to the Jupiters moon, Europa, to search for life in its ice-covered oceans will provide a unique opportunity to place scientific instruments onto the surface of Europa and get a close glimpse into some of the mysteries of this moon. Many fundamental questions about the preservation of Europas evolutionary history in the ice, ice/ocean chemical properties, and possibility of finding life can be best examined by performing in-situ analysis of both the ice and ocean. One of the most important challenges to be faced in the mission is the deep penetration of the ice crust of Europa to deliver the scientific instruments for in-situ analysis into the subsurface layers. The further development of advanced technologies for deep penetration of icy moons necessitates a better understanding of the basic physics of impact into cryogenic ice. The fundamental thermomechanical properties of the target ice determine the boundary conditions applied to the projectile and significantly affect the stress state, peak loads and accelerations, and penetration depth of the deep penetrator. As the temperature at the surface of Europa ranges from 50K to 140K, our recent in-house experiments have indicated that the dynamic strength and inelastic behavior including failure of ice are very different at these very low temperatures and exhibit strong strain rate and temperature dependence [1]. In this work, a micromechanics-based constitutive model of cryogenic ice that incorporates microstructure and is amenable to large-scale dynamic structural computations will be developed to bypass the limited phenomenological evolution laws for the prediction of the dynamic response of ice at high strain rate and various temperatures. An incremental variational formulation based on thermodynamic approach is implemented to predict the deformation, temperature and evolution of the microstructure of ice [2, 3]. In addition, the polycrystalline structure of ice is explicitly accounted for simply by assigning different crystal orientations to each material point in the discretization of the OTM method [4].

The presented model for cryogenic ice incorporates three principal deformation mechanisms: (i) nonlinear elasticity involving multiphase equation of state, anisotropic deviatoric elastic response and temperature-dependent viscosity [5, 6]; (ii) microcrack extension modeled explicitly by the variational material point EigenErosion algorithm using a temperature-dependent critical energy release rate [7, 8]; and (iii) granular flow of densely-packed comminuted particles simulated by a Drucker-Prager plasticity law, with transitions between these mechanisms determined by the state of stress, temperature and the extent of comminution by microcrack extension. Furthermore, the model can be calibrated through a series of physical experiments measuring the

fundamental properties of ice such as hardness, fracture toughness, grain size and orientations, friction coefficient, etc. Validation tests are performed by direct comparisons of the OTM simulations of high speed impact of steel projectile on cryogenic ice target against experimental results, shown in Figure 1. It is evident that the size of the crater and penetration depth calculated in the OTM simulations are in good agreement with experimental measurements as well as the failure mechanisms of the cryogenic ice targets.

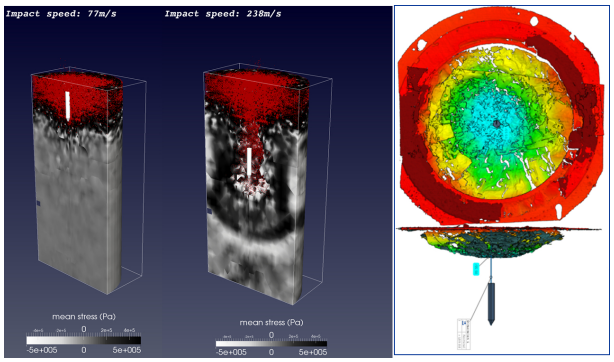

Figure 1: OTM model validation simulations of steel projectile impact into ice at 100K. Simulation results (left) are in good agreement with experimental results (right).

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ATOMISTICALLY-INFORMED KINETIC MONTE CARLO SIMULATIONS OF SCREW DISLOCATION MOTION IN TUNGSTEN

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Thermally-activated glide of screw dislocations is the controlling plastic process at low temperatures in bcc metals. Dislocation motion physically links the atomistic dislocation core with the surrounding medium, and its study thus requires methods capable of atomistic resolution. However, the thermally activated nature of screw dislocation glide precludes the use of direct molecular dynamics due to the impossibility to resolve the relevant time scale. Here we present kinetic Monte Carlo simulations of screw dislocation motion in tungsten to capture thermally-activated glide into time and length scales that resemble those observed experimentally. Our method is parameterized solely with tailored atomistic calculations, so that the connection with the underlying atomistic structure is ensured. To reflect the asymmetries of the bcc lattice, we study the deviation of the critical stress from Schmid's law to captures the twinning/anti-twinning asymmetry. KMC affords a computational speedup that allows us to explore the relevant parametric space much more efficiently than with atomistic simulations. We present results of dislocation velocity as a function of stress, dislocation length, temperature, and loading orientation.

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HADAMARD INSTABILITY ANALYSIS FOR COUPLED THERMO-MECHANOCHEMICAL SYSTEMS

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A Hadamard instabiblity analysis of the system of partial differential equations governing a coupled thermo-mechano-chemical system provides a unified analysis of both spinodal type Larche-Cahn instabilities[1] and "negative creep" ones [2], by balancing different order terms in the eigenvalue equation.

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GRADIENT STRUCTURES AND HOMOGENIZATION FOR THERMOMECHANICAL SYSTEMS

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We consider closed thermomechanical systems involving elastic deformations via displacement u, internal variables z (plastic strain or phase indicators), and the scalar field r for temperature dependence, namely either the temperature θ, the internal energy e, or the entropy s.

1 A gradient structure for thermomechanics

Following [Mie11a, Mie11b, Mie13] we show that such systems can be written as a formal gradient system, where the total energy $\mathcal{E}$ is a conserved quantity, while the total entropy $\mathcal{S}$ acts as the driving functional. The derivation starts from the GENERIC form, which reduces in the quasistatic setting to a system for the unknown $q = (u, z, r)$ given in terms of $\mathcal{E}$, $\mathcal{S}$, and a dual entropy-production potential $\mathcal{R}^*$. The latter is given defined in terms of the thermodynamically conjugate variables ξ_z and ξ_r for the dissipative variables z and r, respectively, and takes the form

$$\mathcal{R}^*(u,z,r;\xi_z,\xi_r) = \mathcal{R}_{\text{int}}\big(z,r;\ \xi_z - \tfrac{\xi_r}{\mathrm{D}_r\mathcal{E}(u,z,r)} * \mathrm{D}_z\mathcal{S}(u,z,r)\big) + \mathcal{R}_{\text{heat}}\big(z,r;\ \tfrac{\xi_r}{\mathrm{D}_r\mathcal{E}(u,z,r)}\big).$$

The typical choice $\mathcal{R}^*_{\text{heat}}(z,r;\mu_r) = \int_\Omega \frac{\kappa(z,r)}{2}|\nabla\mu_r|^2\,\mathrm{d}x$ leads to the heat equation. The choices

$$\text{(a)}\ \ \mathcal{R}_{\text{int}}(z,r;\mu_r) = \int_\Omega \frac{1}{2\nu}\mathrm{dist}(\mu_z,K^*)^2\,\mathrm{d}x,$$

$$\text{(b)}\ \ \mathcal{R}_{\text{int}}(z,r;\mu_r) = \int_\Omega \frac{m}{2}|\mu_z|^2\,\mathrm{d}x, \qquad \text{(c)}\ \ \mathcal{R}_{\text{int}}(z,r;\mu_r) = \int_\Omega \frac{M}{2}|\nabla\mu_z|^2\,\mathrm{d}x$$

corresponds (a) to viscoplasticity (where $z \in \mathbb{R}^{d\times d}_{\text{sym},0}$ and K^* is the elastic domain), (b) to Allen-Cahn type mobility, and (c) to Cahn-Hilliard type mobility.

The full coupled system with quasistatic elasticity now takes the form

$$0 = \mathrm{D}_u\mathcal{F}(u,z,r) = \mathrm{D}_u\mathcal{E}(u,z,r) - \Theta(u,z,r) * \mathrm{D}_u\mathcal{S}(u,z,r), \tag{1a}$$

$$\dot z = \partial_{\xi_z}\mathcal{R}^*\big(u,z,r;\ \mathrm{D}_z\mathcal{S}(u,z,r),\mathrm{D}_r\mathcal{S}(u,r,z)\big), \tag{1b}$$

$$\dot r = -\tfrac{\Delta S(u,z,r)[\dot u]}{\mathrm{D}_r\mathcal{S}(u,z,r)} + \partial_{\xi_r}\mathcal{R}^*\big(u,z,r;\ \mathrm{D}_z\mathcal{S}(u,z,r),\mathrm{D}_r\mathcal{S}(u,r,z)\big), \tag{1c}$$

where $r \in \{\theta, e, s\}$ is still arbitrary and $\theta = \Theta(u,z,r) = \frac{\mathrm{D}_r \mathcal{S}(u,z,r)}{\mathrm{D}_r \mathcal{E}(u,z,r)}$, by Gibbs' relation.

Following [Mie11a, Mie11b] we eliminate u in the form $u = U(z,r)$ and define the reduced energy and entropy functionals $\widehat{\mathcal{E}}(z,r) = \mathcal{E}(U(z,r),z,r)$ and $\widehat{\mathcal{S}}(z,r) = \mathcal{S}(U(z,r),z,r)$ and find, after some lengthy calculations, that the remaining system is the gradient system

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} z \\ r \end{pmatrix} = \partial_{\xi_z,\xi_r} \widehat{\mathcal{R}}^*\big(z, r; \mathrm{D}_{z,r}\widehat{\mathcal{S}}(z,r)\big) \quad \text{with the conserved energy } \widehat{\mathcal{E}}.$$

2 Homogenization of thermomechanical systems

In [MiS14] We consider the Penrose-Fife system for the scalar phase-filed variable z and the internal energy e, such that the conserved total energy is $\mathcal{E}(z,e) = \int_\Omega e(t,x)\,\mathrm{d}x$. The total entropy takes the form

$$\mathcal{S}(z,e) = \int_\Omega S(\frac{1}{\varepsilon}x, z, e) - \frac{1}{2}\alpha(\frac{1}{\varepsilon}x)|\nabla z|^2\,\mathrm{d}x,$$

where S satisfies $\partial_e S > 0$, $\partial_e^2 S < 0$, and $\mathrm{D}_{z,e} S \le \lambda I_{2\times 2}$ for some $\lambda \in \mathbb{R}$. and the dual dissipation potential is the state-independent quadratic form

$$\mathcal{R}^*(\xi_z, \xi_e) = \frac{1}{2}\int_\Omega m(\frac{1}{\varepsilon}x)\xi_z(x)^2 + \kappa(\frac{1}{\varepsilon})|\nabla \xi_e(x)|^2\,\mathrm{d}x.$$

Using the homogenization theory via evolutionary variational estimates developed in [Mie14], we show convergence to an effective Penrose-Fife system, where m_{eff}, κ_{eff}, α_{eff}, and S_{eff} can be characterized. It is interesting to note that homogenizing the entropy as a function of the internal energy e is equivalent to averaging the free energy as a function of θ.

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A MICRO-MECHANICAL APPROACH FOR THE DYNAMIC FRACTURE OF DUCTILE MATERIALS

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An important literature has been devoted to the failure of ductile materials by nucleation, growth and coalescence of micro-voids. Micromechanical models have been developed to describe the overall response of voided viscoplastic materials, [1], [11]. These models assume that the loading is quasistatic at the microscopic level or cell level (hollow sphere model for the Gurson approach, [5]). However, this hypothesis must be revisited when dynamic conditions are considered. Indeed, at the vicinity of a void under rapid expansion, the acceleration of material particles (with respect to a frame located at the void center) may induce inertia forces that highly influence the microscopic stress field, [2]

Thus, micro-inertia effects cannot be ignored when considering the homogenized response of voided materials subjected to high strain rates, [3], [7], [9], [12]. We present here a dynamic homogenization framework for porous viscoplastic materials that extends the classical GTN model in two aspects: (i) by accounting for micro-inertia effects, (ii) by considering the void-shape effect, [10]. These features are described by analytical means. When neglecting micro-inertia effects, the quasistatic model of [4] with spheroidal voids is retrieved. For spherical voids and quasisatitic loading , the GTN approach [11] is returned.

A multiscale approach is developed and embedded in a finite element code to solve structural problems. Applications to high strain rate processes are considered, especially for spalling, [3] and dynamic crack propagation, [6].

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A FINITE TEMPERATURE ATOMISTIC/CONTINUUM COUPLED MODEL FOR CONTACT APPLICATIONS

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Multiscale models, which couple an atomistic domain (to capture realistic physical mechanisms) to a continuum region (to reduce computational cost), are today applied to a variety of physical problems including crack nucleation and propagation, frictional contact and indentation [1]. However, most of these applications are limited to zero Kelvin. In this presentation, we begin with the application of one of the existing multiscale model known as the Bridging Domain method [2] to a normal contact problem at finite temperatures. We present a new multiscale model [3] to couple molecular dynamics with finite elements at finite temperatures using spatial filters. The need of spatial filters is demonstrated by simulating a one-dimensional model at constant finite temperature. The mismatch in the dispersion relations between continuum and atomistic models leads, at finite temperature, to unwanted mesh vibrations, which are illustrated using a standard least square coupling formulation. We propose the use of spatial filters with the least square minimization to selectively damp the unwanted mesh vibrations. The restitution force from the generalized Langevin equation is modified to perform a two-way thermal coupling between the two models. Several numerical examples, including a dynamic impact test, are shown to validate the proposed coupling formulation in two-dimensional space. In particular, our reduced-model calculations match accurately full-MD simulations, and the total energy of the system is preserved at all times. We also discuss the stability of coupling methods that do not use a well-defined energy functional. We show that generally these suffer from a dynamic instability. Remedies to this instability are proposed [4].

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THE COMPETITION BETWEEN FAILURE AND LOCALIZATION OF DEFORMATION IN PROGRESSIVELY SOFTENING SOLIDS

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A progressive softening solid is one for which the constitutive relation permits the stress to decrease monotonically to zero after the attainment of a maximum. For such a solid, failure in the sense of a complete loss of stress carrying capacity is inevitable. However, it is also possible for localization of deformation to precede failure. Quasi-static shearing of a planar block comprised of a rate dependent progressively softening solid is used to illustrate, in a simple context, circumstances where one or the other of these outcomes is favored. The role of various material properties and of the band thickness on affecting the outcome of this competition is explored.

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QUASI-STATIC EVOLUTIONS FOR A PHASE FIELD MODEL IN FRACTURE

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We consider a phase-field description for brittle fracture provided by a separately quadratic energy of Ambrosio-Tortorelli type. We study a couple of different quasi-static evolutions [1] [2], both obtained by sequences of time-discrete incremental minimization problems.

The first is a local minimizing movement in the phase field variable (with respect to the H^1 or L^2 norm). The second is instead obtained by the alternate minimization scheme. Our goals are the characterization of their time-continuous limits in terms of parametrized BV-evolutions and the thermodynamic consistence of the irreversibility constraint.

In the first case, the limit of the discrete evolutions satisfies a phase-field representation of Griffith's criterion, in the stable paths, together with an autonomous gradient flow in the phase-field variable (with respect to the H^1 or L^2 norm) along the unstable paths, i.e. where Griffith's criterion is not met. This type of evolution can be obtained also by means of a constrained forward Euler scheme.

In the second case, the limit evolutions provided by the alternate minimization scheme enjoy again equilibrium, in the stable regimes, together with a coupled system of evolutions equations in the unstable regimes: roughly speaking a gradient flow for the field variable together with a "visco-elastic" equation for the displacement field. It is interesting to note that the alternate minimization scheme does not require any "user-supplied" norm; the scheme itself and the separate quadratic energy induces a "family of intrinsic norms" which in particular appear in the unstable regimes.

In general both the evolutions are thermodynamically consistent, as far as the irreversibility constraint, only in the stable regimes of propagation.

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BAYESIAN NUMERICAL HOMOGENIZATION

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Numerical homogenization, i.e. the finite-dimensional approximation of solution spaces of PDEs with arbitrary rough coefficients, requires the identification of accurate basis elements. These basis elements are oftentimes found after a laborious process of scientific investigation and plain guesswork. Can this identification problem be facilitated? Is there a general recipe/decision framework for guiding the design of basis elements? We suggest that the answer to the above questions could be positive based on the reformulation of numerical homogenization as a Bayesian Inference problem in which a given PDE with rough coefficients (or multi-scale operator) is excited with noise (random right hand side/source term) and one tries to estimate the value of the solution at a given point based on a finite number of observations [1]. We apply this reformulation to the identification of bases for the numerical homogenization of arbitrary integro-differential equations and show that these bases have optimal recovery properties. In particular we show how Rough Polyharmonic Splines [2] can be re-discovered as the optimal solution of a Gaussian filtering problem. We also show how the decision framework solving this identification problem corresponds to a generalization of the Optimal Uncertainty Quantification framework [3] to the Scientific Computation of Optimal Statistical Estimators.

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A CONCURRENT MULTI-SCALE MODEL FOR THE THERMO-MECHANICAL RESPONSE OF MATERIALS

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By proper selection of chemical composition and microstructural arrangements, materials can be tailored to exhibit desired thermal and mechanical properties. The need to push for higher performance in engineering systems leads to the exposure of materials to increasingly demanding conditions, including high temperatures and mechanical loads. Predicting the response of materials under such conditions is critical for assessing the performance and life of components that utilize them, as well as for designing novel materials that can better resist these unusual performance demands.

Novel manufacturing and material synthesis techniques allow the manipulation of characteristic material length scales, e.g., grain size and grain size distribution. As the characteristic length scale of the material is reduced, e.g. due to the presence of microstructural interfaces, its effective thermal conductivity decreases drastically. In materials where heat conduction is mediated mainly by phonons, for example ceramics, this reduction is primarily due to the shortening of the bulk phonon mean free paths as a result of scattering at the interfaces. Even though homogenized material properties could be adopted to predict the macroscopic thermomechanical response of a given material, they would not account for the non-uniform temperature fields resulting from internally varying characteristic length scales. This variation would most likely be responsible for generating the concentration of thermal stresses, which in term could drive the localized failure of the material. In addition, by grading the characteristic size of the material, the macroscopic temperature field could be manipulated affecting the resulting thermoleastic stresses.

Even though extensive research has been conducted on the impact of length scale on thermal and mechanical properties of materials, little is known about the impact that length scale could have on their combined thermomechanical response. In fact, models able to predict such complex interactions are not readily available in the literature. We present a concurrent multi-scale model able to capture local variations on thermal conductivity, the resulting variations on the temperature field, and the consequent impact on thermal stresses. Our model consists of: (i) a sub-micron scale model for the thermal conductivity based on the Boltzmann transport equation under the relaxation time approximation, (ii) a Fourier heat transport model at the mesoscale, and (iii) a continuum model of mechanical deformation that explicitly resolves the microscopic geometric features of the material. The model is schematically depicted in Figure 1.

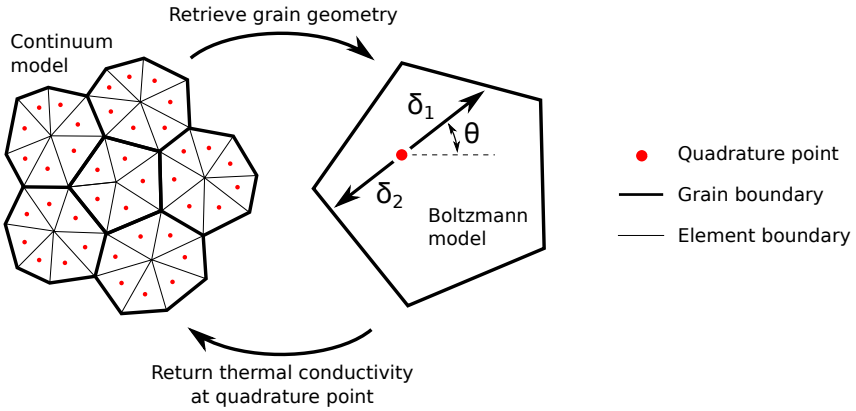

Figure 1: Schematics of multiscale model

Studies on reduced thermal conductivity available on the literature focus on structures of very specific shapes such as thin-films or nanowires. In addition, they assume the thermal gradient is kept constant along a particular direction, e.g. the in-plane, the cross-plane or the axial direction. That is, they focus on obtaining the thermal conductivity of the material in a single direction and for very simple configurations. We extend those formulations by accounting arbitrary size and shape of the intrinsic geometric features of the material, and by sweeping the direction of the thermal gradient in order to compute the full thermal conductivity tensor.

More precisely, to account for arbitrary geometric features within the material, we adopt a ray-tracing technique to calculate the distances between the point of interest within the material and the boundaries of the geometric feature. In this way, the thermal conductivity within the material depends on the location of the point of interest and the nearby geometric features of the material. As this procedure can be repeated for different directions of the thermal gradient, our formulation extends previous studies by computing the thermal conductivity for all directions thermal gradient. In this way, we can recover the fully anisotropic thermal conductivity tensor at every quadrature point of the material, which can then be included into the continuum model.

Our model is demonstrated through several key examples, including the computation of in-plane and cross-plane thermal conductivity in thin films, the anisotropic thermal conductivity on a silicon micro-grain, and the generation of thermal stresses in graded polycrystals.

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A FULLY LAGRANGIAN METHOD FOR FLUID/SOLID INTERACTION

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Fluids are most easily simulated numerically by employing Eulerian formulations, whereas solids, on their part, are most naturally described by Lagrangian numerical methods. To simulate problems in which fluids and solids strongly interact, one can employ Arbitrary Lagrangian-Eulerian methods, purely Eulerian formulations with embedded interfaces, or purely Lagrangian schemes. The latter has the advantage that keeping track of free surfaces is a trivial task, but invariably suffer from severe mesh distortions due to the large displacements in the fluid flow [1].

Purely Lagrangian formulations of fluid/solid interaction often resort to remeshing to alleviate mesh distortion [2, 3]. Alternatively, one might consider meshfree methods, where mesh entanglement and distortion is not an issue and fluid motion can be more easily tracked, but where additional difficulties arise in the approximation of the fluid and solid subdomains.

In this work show recent work on meshfree fluid/solid interaction based on a purely Lagrangian description of all the interacting bodies. The meshfree approach is based on a material point method with local maximum-entropy approximation functions [4]. For both the fluid and solid parts, the balance equations are expressed in a Lagrangian form, the only difference between them being that the fluid is constrained to be incompressible. This single constraint makes the corresponding Galerkin discretization unstable, as similar finite element formulations with equal order interpolations for the velocity and pressure fields. For that reason, a stabilized method is proposed following the ideas of [5]. We are able to show that the fluid formulation is stable both for the stationary case and the transient one, if a backward Euler integrator is employed.

In addition to describing the method formulation and showing the most relevant aspects of its numerical analysis, simulations will be presented to illustrate the possibilities of the proposed approach.

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AN ANALYSIS OF CRYSTAL CLEAVAGE IN THE PASSAGE FROM ATOMISTIC MODELS TO CONTINUUM THEORY

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We study the behavior of atomistic models in general dimensions under uniaxial tension and investigate the system for critical fracture loads. We rigorously prove that in the discrete-to-continuum limit the minimal energy satisfies a particular cleavage law with quadratic response to small boundary displacements followed by a sharp constant cut-off beyond some critical value. Moreover, we show that the minimal energy is attained by homogeneous elastic configurations in the subcritical case and that beyond critical loading cleavage along specific crystallographic hyperplanes is energetically favorable. For a two dimensional model problem we also provide a complete characterization of the energy minimizing configurations.

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CONVERGENCE AND ACCURACY OF THE MATERIAL-POINT METHOD

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The material-point method (MPM) was introduced about 20 years ago and is a versatile method for solving problems in continuum mechanics. The flexibility of the method is achieved by combining two discretizations of the material. One is a Lagrangian description based on representing the continuum by a set of material points that are followed throughout the calculation. The second is a background grid that is used to solve the continuum equations efficiently. There are four steps in the algorithm: (i) choose a convenient computational grid; (ii) map information from the material points to the grid; (iii) solve the field equations on the grid; and (iv) update the material points based on the grid solution.

In its original form, many applications of the method appeared to be second order accurate for small deformations, but lost accuracy for problems involving large deformations. This talk will provide analysis of the order of accuracy of MPM to shed light on these observations. Moreover, the analysis suggests modifications to the algorithm to achieve higher order accuracy. Each of the steps in the algorithm contributes to the overall accuracy and modifications must be made consistently to obtain a desired accuracy. The analysis also points to connections between MPM, OTM and other meshfree methods

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DIFFERENTIAL COMPLEXES IN CONTINUUM MECHANICS

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We present differential complexes for continuum mechanics, and in particular nonlinear elasticity, that involve both symmetric and non-symmetric second-order tensors. We show that the tensorial analogue of the standard grad-curl-div complex can simultaneously describe the kinematics and the kinetics of motions of a continuum when formulated in terms of the first Piola-Kirchhoff stress and the deformation gradient. The relation between this complex and the de Rham complex allows one to derive the necessary and sufficient conditions for the compatibility of the displacement gradient and the existence of stress functions on non-contractible bodies. We discuss similar complexes for Cauchy stress and the second Piola-Kirchhoff stress. We also derive the local compatibility equations in terms of the Green deformation tensor for motions of 2D and 3D bodies, and shells in curved ambient spaces with constant curvatures.

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MESHFREE NUMERICAL SCHEMES APPLIED TO UNCONFINED SEEPAGE PROBLEMS THROUGH EARTH DAMS

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Modelling seepage along with the mechanical responses of deformable Earth Dams under transient conditions is a challenging task, since both coupling between different phases, and computation of free-surface variables are involved. In the present work, we take on the meshfree numerical schemes to establish a framework for solving coupled, steady and transient problems for unconfined seepage through Earth Dams. The equations of Biot [1] are formulated in the displacement (or $u - w$) framework [2] assuming an elastic solid skeleton. Consequently, the impervious boundary conditions are naturally imposed as essential ones, the complexities in imposing such conditions in a $u - p_w$ formulation are eluded all together. The free surface location and its evolution in time, are obtained by interpolation of pore water pressures throughout the domain.

Shape functions based on the principle of Local Maximum Entropy [3] are chosen for the meshfree approximation schemes. In order to avoid the locking involved in the fluid phase, a B-Bar based algorithm is devised to compute the volumetric strain average in a patch composed of various material points. The idea behind the patch is analogous to that of the Diamond elements developed by Hauret, Kuhl and Ortiz [4]. The efficiency of such an implementation is shown through the Benchmark problem, Cook's Membrane loaded by a distributive shear load, see Fig. 1.

The proposed methodology is applied to various classical examples in unconfined seepage problems through Earth Dams, the obtained free surface locations are compared with available ones in the literature. See Fig. 2, for instance, for the case of a seepage problem through a heterogenous dam. The results obtained for steady seepage problems seem promising and testify to the feasibility of the proposed method in solving coupled problems in porous media.

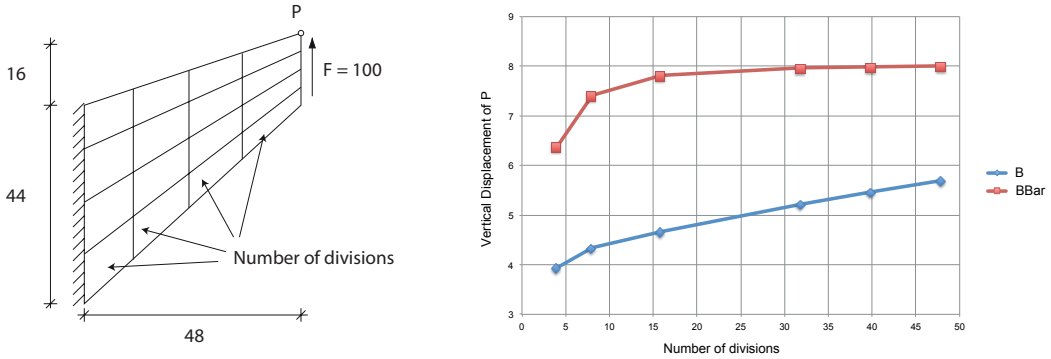

Figure 1: Geometry of the Cook's Membrane problem and the vertical displacement obtained with and without the B-Bar implementation.

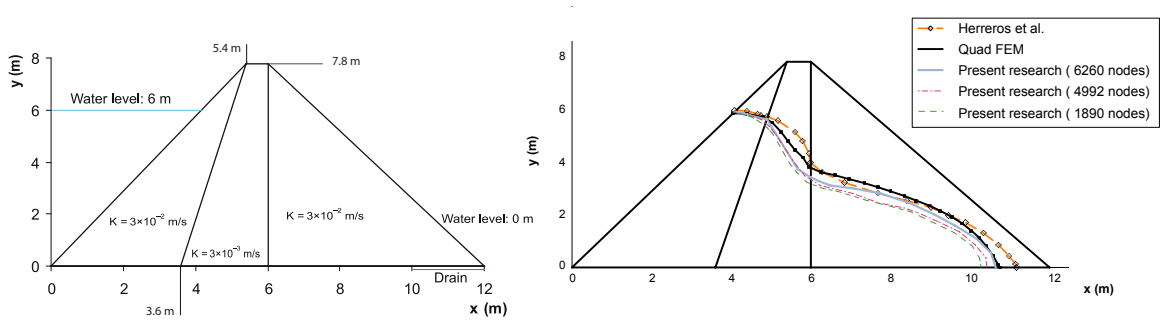

Figure 2: Geometry and permeability of a heterogeneous dam and the obtained free surface profile contrasted with that of Hererros, Mabssout and Pastor [5], and that of Navas and López-Querol [2] using quadratic finite elements.

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