IP1

Diffusion Generated Motion for Large Scale Simulations of Grain Growth and Recrystallization

A polycrystalline material consists of many crystallites called grains that are differentiated by their varying orientation. These materials are very common, including most metals and ceramics. The properties of the network of grains making up these materials influence macroscale properties, such as strength and conductivity. Hence, understanding the statistics of the grain network and how it evolves is of great interest. We describe new, efficient numerical algorithms for simulating with high accuracy on uniform grids the motion of grain boundaries in polycrystals. These algorithms are related to the level set method, but generate the desired geometric motion of a network of curves or surfaces (along with the appropriate boundary conditions) by alternating two very simple operations for which fast algorithms already exist: Convolution with a kernel, and the construction of the signed distance function to a set. Motions that can be treated with these algorithms include grain growth under misorientation dependent surface energies, and various models of recrystallization. We will present simulations with hundreds of thousands of fully resolved grains in 3D. Joint work with Matt Elsey and Peter Smereka.

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IP2

Accurate and Efficient Atomistic-to-Continuum Coupling Methods

Many materials problems require the accuracy of atomistic modeling in small regions, such as the neighborhood of a crack tip. However, these localized defects typically interact with a much larger region through long-ranged elastic fields. These regions are too large to be computed atomistically. Materials scientists have proposed many methods to compute solutions to these multiscale problems by coupling atomistic models near a localized defect with continuum models where the deformation is nearly uniform. The development of coupling methods for crystalline materials that are reliable and accurate for configurations near the onset of lattice instabilities such as dislocation formation has been particularly challenging. I will present theory developed with Mathew Dobson and Christoph Ortner to assess currently utilized methods and to propose more reliable, accurate, and efficient methods.

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IP3

Approaches to Finite-strain Elastoplasticity

Elastoplastic material models involve a decomposition of the strain tensor into an elastic and a plastic part. The latter is driven by a nonsmooth evolution law, the flow rule. Small-strain elastoplasticity, which is based on the additive decomposition of the strain tensor, has developed significantly over the last decades, since techniques from convex analysis and variational inequalities are applicable. For finite-strain elastoplasticity, convexity is unacceptable because of physical requirements like objectivity and plastic indifference. The latter leads to the multiplicative decomposition of the strain tensor and asks to consider the plastic tensor as elements of multiplicative matrix group, which leads to strong geometric nonlinearities. We show how polyconvexity and time-incremental minimization can be used to establish global existence for elastoplastic evolutionary systems.

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IP4

Gels and Microfluidic Devices

Gels are materials that consist of a solid, crosslinked system in a fluid solvent. They are over-whelmingly present in biological systems and also occur in many aspects of materials applications. Some gels are mostly characterized by their mechanical properties whereas for the large class of *hydrogels*, the electric effect of ions is the signature feature. In the biomedical industry, mechanical properties of gels are relevant to the prediction of the life-cycle of body implantable devices such as pacemaker, bone-replacement systems and artifcial skin. Upon body implantation, devices swell due to the moisture of the environment, resulting in stress concentrations that may cause failure of the device. A main goal is to determine the time evolution of stresses at interfaces between different materials of the device, and controlability conditions that ensure that the stress values will remain below an allowed threshold. The proposed governing equations involve transport, diffusion, elasticity and dissipation. To study hydrogels, we explore the coupling of the mechanics of gels with the *Poisson-Nernst-Planck equations* governing the transport and diffusion of ions in the solvent, and in the presence of the electric potential of the system. We focus on two types of microuidic models that emerge from such a setting, cyclic drug-delivery devices and microvalves.

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IP5

Predictive Atomistic and Coarse-Grained Modeling of Epitaxial Thin Film Growth

Thin film deposition provides a pathway to create a variety of complex surface nanostructures with diverse functionality. Atomistic modeling of homoepitaxial film growth (A on A) on single-crystal surfaces, when combined with kinetic Monte Carlo (KMC) simulation, has achieved remarkable predictive accuracy in describing far-from-equilibrium evolution*. This includes both initial submonolayer 2D island formation and subsequent multilayer growth and kinetic roughening (i.e., formation of 3D mound-like stacks of 2D islands). Less progress has been made for heteroepitaxy on single-element substrates (A on B) or on alloys (A on BC), where strain and quantum size effects can be significant. As an alternative to atomistic treatments, coarse-grained modeling is appealing from the perspective of algorithmic efficiency, and also to provide deeper insight into fundamental issues such as development 2D island distributions or 3D mound coarsening dynamics. We review recent successes and open challenges for modeling. *Evans et al.,

Surf. Sci. Rep. 61 (2006) 1-128.

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IP6

Symmetries Broken by Electrostatics in Nanoscale Ionic Assemblies

Electrostatic interactions are essential in the structure and function of biological assemblies since most biomolecules are charged. Oppositely charged molecules often co-assemble into units with some inherent asymmetry that renders functionality. Symmetric electrostatic interactions alone are shown to spontaneously break symmetries at the nanometer scale, such as the formation of helical ionic patterns on fibers and the buckling of ionic shells into icosahedra. Through varying the strength of the electrostatic interactions we control the pitch of the helical patterns of the surface of virus-like fibers or of aqueous channels. In ionic spheres, correlations may lead to faceting into icosahedra without rotational symmetry. This buckling appears on vesicles of cationic-anionic molecules, as well as on co-adsorbed charged molecules that form ionic rafts.

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IP7

Polycrystalline Materials: Greater Than the Sum of Their Crystals

Polycrystalline materials are pervasive in nature and engineering, and have long been studied as a collection of individual crystalline grains. Mathematical tools to represent the statistics of many individual grains and to more intuitively visualize the grain structure were developed long ago, and have greatly facilitated advances in understanding and designing these materials. However, it is not the crystals themselves, but the boundaries between crystals, that frequently dominate the properties of polycrystalline materials. Unfortunately, the population of these boundaries is more difficult to measure, visualize, and represent statistically. This talk will highlight our recent work towards quantitatively understanding the population of grain boundaries in materials. Beginning from an understanding of the topology of the group space for grain misorientations, we develop new methods of mapping and visualizing boundary character, representing their statistics with continuous functions, and understanding the rules that govern their connectivity as a network.

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IP8

Failure of Polymer Gum Gels Close to their Critical Strain

Polymer gels prepared from synergistic blends of xanthan and konjac gums exhibit remarkable flow characteristics. Creep measurements indicate that when the applied stress results in a deformation of the gel in excess of the critical strain, the gel rapidly fails and flows; when the applied stress results in a deformation far less than the critical strain, the gel only slowly creeps. Remarkably, when the applied stress results in a deformation close to the critical strain, the gel slowly creeps for an extended incubation time at which point it catastrophically fails and flows. In fact, there is a power-law relationship between the applied stress and the incubation time. Although similar behavior is reported in materials ranging from ketchup to waxy crude oil, surprisingly little is understood about the creeping behavior of materials close to their critical strain. We have looked to structural kinetic models, which balance the rate of structure formation and stress-induced structure break down, as a way to generalize the problem. These approaches should have broad application to a variety of industries and technologies.

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IP9

Mathematical Modelling of Hydrogen Fuel Cells

Hydrogen Fuel Cells can efficiently convert Hydrogen fuel and air to electrical power with zero emissions. This talk concerns Polymer Electrolyte Membrane Fuel Cells (PEMFC). A general overview of how these devices are constructed and how they work is given. PEMFCs are fundamentally multi-scale. The central component of a PEMFC (the Membrane Electrode Assembly or MEA) has micron scale. The MEA is made of composite layers which must facilitate selective multiphase transport of reactants to and products from catalyst sites. The need for composite materials with these selective transport properties is a recurring theme in energy conversion and storage applications. MEAs are built into unit cells which are then arranged in stacks. The micro-components have behaviour determined by their structure on the nano-scale. Modelling stack level behaviour from component models and components from their nano-scale structure are both of interest and are illustrated with examples.

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IP10

Nonlinear Mechanics of Elastic Plates

The mechanics of thin elastic or viscous objects is critical to our understanding of e.g. the buckling of engineering structures, the spinning of polymer fibers, or the crumpling of plates and shells. During the past decade, the mathematics, mechanics and physics communities have witnessed an upsurge of interest in those issues. Yet, fundamental questions are still open. For example, the exact nature of the singularities in crumpled plates remains a topic of passionate debate. My talk will address this problem, focussing specifically on the internal structure of conical singularities. I will propose an explicit construction which is amenable to analytical calculations, and is at odds with scaling arguments usually assumed in the literature.

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IP11

Modeling the Plastic Deformation of Crystals and Glasses with Colloids

Dense colloidal systems form crystalline, liquid and glassy phases similar to those observed in simple atomic systems. Confocal microscope makes it possible to track the individual particles in space and time, which allows a unique look at the mechanisms of deformation on the particle level. Dislocations in colloidal crystals can also be visualized by laser diffraction microscopy. Measurements of the geometry and dynamics of these dislocations agree remarkably well with the classical predictions for atomic-scale crystals. In glasses, the technique has allowed direct measurments of the size, strain and concentration of the local shear transformations that govern the macroscopic flow.

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CP1

Higher Order Phase Field Equation for Direct Calculation of Surface Tension Anisotropy

Recently, it was shown [Caginalp and Esenturk, accepted in DCDS] that for interfaces of symmetric microscopic interactions (4-fold or higher), one needs to go to higher orders (in derivatives) in the phase field equation to capture the anisotropy of the surface tension. For a given type of molecular interactions one can find a explicit formula for the surface tension in terms of the phase field. As an example we will start with an an anisotropic interaction potential, seek numerical solutions to the differential equation and calculate the surface tension anisotropy.

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CP1

Diffusion and Homogenization Approximation for Semiconductor Gaz Sensor Boltzmann Equation

The aim of this work is to derive, from a kinetic discription, a drift-diffusion model for electron transport in semiconductor gaz sensor, by using diffusion and homogenization approximation. An homoenized absorption term appears in the fluid model. In the presence of a self-consistent spatially oscillating electrostatic potential, the right hand side of the Boltzmann equation presents, an absorption term added to the electron-phonon operator collision. This absorption term has the periodicity of the oscillating electrostatic potential.

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CP1

Finite Element Simulations for Active Acoustic Cloaking Devices

We investigate a class of active acoustic cloaking devices where the device and the cloaked region can be mapped into two nested balls. Finite energy solutions for these cloaking devices are studied in weighted Sobolev spaces with singular weights. We describe the behavior of the finite energy solution in the cloaking medium, in the cloaked region, and at the interface between the two regions. A special finite element method is proposed for simulating these devices.

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CP1

A Long Wave Approximation for a Model Describing the Self-Assembly of Quantum Dots

Evolution equations for the self-assembly and coarsening of nano-crystals are of growing interest since two decades and in particular heteroepitaxial systems leading to quantum dot growth have been considered in many works. We extend a model that captures the effects of surface diffusion, elasticity, wetting and isotropic surface energy to one that additionally reflects preferred orientations as minima in the surface energy. A long wave reduction allows to simplify the equation such that it can be simulated efficiently by a pseudospectral method on large domains. The evolving dots indeed show faceting and an Ostwald ripening process can be observed. The island density obeys a power law and the ripening is accelerated in comparison to the isotropic case. A linear stability analysis shows that the anisotropy destabilizes flat films and that above a critical number all wave numbers are unstable.

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CP1

Computations of Asymptotic Scaling for the Kohn-Müller and Aviles-Giga Functionals

We report on computations using spectral methods which capture asymptotic behavior for the Kohn-Müller model for branching in martensitic materials and on the Aviles-Giga functional. The simulation results show that by solving evolutionary partial differential equations, it is feasible to explore the energy landscape of these non-convex model energies and to provide conjectures for the behavior of the global energy minimising solutions as the parameters in the models are changed.

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CP1

Design of the Potential in a Parametrically Forced Schroedinger Equation to Minimize Radiative Loss

We consider a micro-cavity governed by the Schroedinger equation with a potential. When the system is parametrically forced, the eigenfunction becomes a resonant state and decays according to Fermi's Golden Rule. We pose the Design Problem: what potential maximizes the lifetime of this resonant state? This is formulated and studied as a constrained optimization problem. Optimal potentials emerge which are periodic with a localized defect. Quality factors improve from $O(10^2)$ to $O(10^9)$.

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CP2

Convective Instabilities During the Solidification of An Ideal Ternary Alloy in a Mushy Layer

We consider a model for the solidification of an ideal ternary alloy in a mushy layer that incorporates the effects of thermal and solutal diffusion, convection and solidification. Our results reveal that the system admits double-diffusive modes of instability. Additionally, modes of instability exist even in situations in which the thermal and solute fields are each individually stable from a static point of view. We show both numerical and analytical solutions.

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CP2

Controlling Nonlinear Dynamics in Continuous Crystallizers

Crystallization is a process widely used in industry for the production of many particle products. Continuous crystallizers typically exhibit oscillatory dynamics. We are addressing the suppression of oscillatory behavior in continuous crystallizers via a feedback control approach. Two controllers are applied and compared, a control based on modeling error compensation ideas, and high-order sliding mode control. Numerical simulations on a dynamical model described by integro-differential equations are used to illustrate the control performance.

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CP2

The Rapid Advance and Slow Retreat of a Mushy Zone

Mushy zones are regions of intermixed liquid and solid which result from instability due to the build-up of solute during solidification of multispecies materials. If solute diffusion is ignored there is a steady-state mushy zone representative of what is observed over typical laboratory time scales, but even a small amount of diffusion dramatically alters the eventual steady state. We discuss the evolution of a mushy zone where diffusion of the solute is not ignored.

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CP2

Molecular-Dynamics Calculation of Thermodynamic Melting Point

We tried to bring closer mechanical melting to thermodynamic melting by incorporating an extra energy constant corresponding to thermodynamics energy gap into the Tight-Binding potential of Molecular Dynamic (MD) simulation. The calculated melting point of single elements was 0.5 to 9.8% deviated from the experimental ones instead of 20 to 30% in conventional simulation. The method works especially well for elements with a low ratio between Debye temperature and melting temperature.

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CP2

Nonlinear Convection in a Mushy Layer: Chimney Spacing and Optimal Solute Fluxes

The rapid solidification of any binary alloy leads to the formation of a chemically reactive porous medium, or mushy layer. Convection and dissolution generate drainage channels devoid of solid, or chimneys, with a spacing that evolves over time. We consider a numerical model of nonlinear convection within a mushy layer and investigate the spacing mechanism for fully developed chimneys. This yields insight into the evolution of solute fluxes and composition in growing mushy layers.

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CP3

Euler-Poisson System for Leo Spacecraft Charging

Not available at time of publication.

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CP3

New Augmented Primal-Mixed Finite Element Methods in Elasticity

We introduce a new augmented variational formulation for the linear elasticity problem based on the Hu-Washizu method. The resulting problem is well posed for appropriate values of a stabilization parameter. We establish sufficient conditions for the well posedness of the corresponding Galerkin scheme and give concrete examples of discrete spaces satisfying these conditions. Error estimates are also provided. The application of the method to the case when the stress-strain relation is given by a nonlinear or semilinear operator is also discussed.

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CP3

An Unbiased Method for Estimating Stationary Transition Rates of Markov Processes

The dynamics of phenomena such as nucleation, diffusion, or coarsening may be modeled as Markov processes if the transition rates between states are known theoretically or empirically. These transition rates can be estimated from simulation or experiment results via a formula proposed by Reiss et al. We show that Reiss' formula gives a biased estimate and propose an unbiased alternative. We demonstrate an efficient implementation of our formula for molecular dynamics simulation of nucleation.

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CP3

Nonlinear and Fractal Analysis of Electrochemical Noise Time Series in the Corrosion of 304 Steel with Heat Treatment

Electrochemical noise (EN) signals are widely used to characterize corrosion parameters and mechanisms of corroding materials. The highly irregular behavior of EN motivates the application of time series analyses that derive from statistical physics. In this work we have applied three fractal methods to EN data of 304 steel discs with different heat treatment in presence of NaCl. For completeness, standard non-linear analysis, such as delayed phase-plane reconstruction and lyapunov exponents, is also performed.

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CP3

Upscaling Multiscale Flows in Highly Porous Media

An iterative two-scale ?nite element method for solving Brinkmans equations is presented. These equations model ?uid ?ow in highly porous media. The method uses a DGFEM for Stokes equations by Wang and Ye and the concept of subgrid approximation developed by Arbogast for Darcys equations. The method is put in the framework of alternating Schwarz iterations to reduce boundary layer errors and to ensure convergence to the global ?ne solution.

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CP3

A Robust, Practical, and General Method for Coupled Iterations of Black Box Nonlinear Solvers by An Approximate Block Newton Method

We have developed an approximate block Newton-Krylov method to couple arbitrary black box nonlinear solvers. The ABN method preserves the quadratic approximation properties of exact Newton iteration. The notion of a solver is completely abstract, encompassing any interpolations or other transformations of data exchanged between solvers. We demonstrate the method on a modular coupling of the radiation heat transfer code CrysMAS to our multi-physics CFD code Cats3D. Application to other problem types will also be discussed.

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CP4

Effect of Stress on the Growth of Concentric Grains and Pores Embedded in a Matrix

The isothermal growth of a spherical grain from its melt filling a spherical pore embedded in a binary alloy matrix under stress is theoretically investigated as well as the dissolution of the matrix, assuming solute diffusion only proceeds in the liquid phase. The stress has been found to be responsible for the destabilization of both fronts leading in particular to the development of a delayed roughness on the stress-free grain interface.

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CP4

Continuum Simulations of Lipid Membranes Using a Phase-Field Method Coupling Composition with Membrane Mechanical Properties

Ternary lipid membranes are used extensively as a model for the plasma membrane of biological cells. They contain phase-separated domains and exhibit deformation. The morphologies of these systems provide information about the thermodynamics and kinetics of multicomponent membranes. We examine the formation and evolution of domains in lipid vesicles using a phase-field model coupling composition with deformation, and find that the compositional and shape evolutions are significantly altered when this coupling is present.

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CP4

Effects of Wetting and Anisotropy on Stability and Morphological Evolution of Ultrathin Solid Films

The combined effects of stress, two-layer wetting potential and strong surface energy anisotropy on linear stability of wetting epitaxial thin film on elastic substrate are analyzed within the framework of longwave approximation. The impacts of perturbation wavenumber, strain, film thickness, shear modulus ratio, and anisotropy strength are studied. Detailed stability diagrams are plotted, revealing some surprising linear responses of the film which were not previously noted in the studies of film stability. In the nonwetting, stress-free situation which may be appropriate for surface-energy driven dewetting of silicon-on-insulator, besides linear stability, the fully nonlinear evolution of an anisotropic surface pit in the attractive field of the substrate is studied numerically.

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CP4

Dislocation Propagation in Phase Field Dislocation Dynamics

We find analytical solutions of the Guinzburg Landau equation describing the evolution of dislocations in a single crystal. The solutions include estimations of the yield stress and stacking fault energy relations as well as the critical source size. For the dynamical solutions we are able to compute the dependency of the velocity on the applied stress with very good agreement with molecular dynamics simulations

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CP4

Mathematical Modeling of Fluid Flow Through a Porous Deformable Arterial Wall

We model a problem of fluid flow interactions within a deformable arterial wall. We have used mixture theory to compute both the structural displacement of the solid and fluid motion. The coupled system of equations is solved numerically. We compare the mixture theory model to a hierarchy of models including simple spring models as well as elastic deformation models. The applications of the model are to understand the deformation of the wall as a function of its material properties and the relation of this deformation to the growth and rupture of aneurysms.

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CP5

Scaling States of an Aggregating, Ballistic Particle (ABP) Model

We study a class of continuous in time, aggregating 1D particle models, namely aggregating, ballistic particle (ABP) models, motivated by material science applications. We numerically validate the dynamic scaling hypothesis, and in particular identify the associated scaling functions that characterize the self-similar 1-point statistics of the coarsening ensemble. Interesting links to the scaling state of the 'Min-driven Clustering' model (Menon, Niethammer and Pego, 2008) are obtained in the 'infinite-speed' limit.

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CP5

Moments of the Grain Size Distribution Formed Via Nucleation and Growth in 3D

A common characteristic of a cellular structure is the cell-size distribution, which can be expressed as a series involving the moments. For the formation of domains via nucleation and growth, we show that the leading order moments are exactly solvable. We present a procedure to approximate the cell-size distribution using the first few moments. The procedure is validated by comparison with simulation results for selected nucleation and growth schedules in 3D.

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CP5

A Stochastic Approach to Coarsening of Cellular Networks

We prove existence for a system of master equations modeling grain growth proposed by K. Barmak, D. Kinderlehrer, I. Livshits and S. Ta'asan. The method used to prove existence for these nonlinear, integro-partial differential equations employs tools from both functional analysis and probability. The stochastic in- terpretation for the evolution of the mesoscopic properties of this large scale metastable system we provide here is general enough to apply to other cellular networks. This approach leads to an internally consistent theory, and opens a new discussion on asymptotics for the distribution of grains in a two dimensional network, which is the subject of future work.

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CP5

Stochastic Simulation for Self-Organization in Materials

Self-organization of components of two phase mixtures through diffusion is known as Ostwald ripening. This phenomenon can be described using mesoscopic models which are stochastic partial differential equations that were derived from the underlying microphysics of the system. In this talk, results from simulations using spectral schemes for stochastic partial differential equations are described and new results on improving the accuracy and efficiency of this method are given. Finally, simulation results for the mesoscopic model are compared with theoretical results such as the Lifshitz-Slyozov growth law.

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CP5

A Generalized Space-Time Poisson Voronoi Construction Applied to Crystal Nucleation and Growth

We present a generalization of the Poisson Voronoi construction in space-time that provides a mathematical framework for studying crystal nucleation and growth. We show that the construction naturally leads to a very efficient simulation technique that provides information about the crystallization history without a need for explicit time marching during the simulation. The excellent efficiency of the method enables us to perform large ensemble calculations to obtain reliable statistics of various microstructural characteristics.

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CP6

Building Effective Models from Scarce But Precise Data

Large-scale models in materials science are generally parameterized by least-squares fitting. To fit arbitrarily precise *ab initio* data, however, we argue that it is more appropriate to begin with a ensemble of models that overfit the data. Within a Bayesian framework, a most likely model can be defined that incorporates physical knowledge, provides error estimates for configurations not included in the fit, and reproduces the original data exactly. We apply this approach to the $Ca[Zr,Ti]O_3$ solid solution.

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CP6

Image-Based Analysis of Microstructures with OOF

Material scientists have access to a wealth of image data on microstructures from various sources, such as micro-CT, serial sectioning and various forms of microscopy, and often their interest is in inferring the relevant physics from these images. The software, Object-Oriented Finite Element Analysis for Microstructures (OOF), has been developed at NIST for this purpose; it enables users to segment microstructure images, create high-quality meshes for computation and simulate the physical behavior of the material. In this talk, we will describe the capabilities of OOF and demonstrate OOF's power with challenging examples.

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CP6

Methods for Obtaining True Grain Size Distributions from Cross Section Measurements

Sectioning methods are frequently used to measure grain sizes in materials. These methods do not provide accurate grain sizes, however, because random sections are always smaller than the true sizes of solid objects, as noted by Wicksell, [Biometrika, 17 (1925), pp. 84-99]. We present a method for deducing true grain size distributions from those determined from specimen cross sections, either by measurement of equivalent grain diameters or mean linear intercepts.

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CP6

A Study of Elastography Based on Image Mass Spectroscopy

Palpation is an important medical diagnostic tool which is based on the fact that tumors tend to be stiffer than the surrounding normal tissue. None of the non-invasive, imaging techniques used by clinicians to find and diagnose tumors provides the critical information about the stiffness of the imaged tissues. We propose a novel technique of differentiating between benign and malignant tumors based on their corresponding Youngs moduli obtained using information provided by image mass spectroscopy.

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CP7

Effective Properties of Random Elastic Media and Their Isotropy

We present sufficient conditions on a symmetry group of a random elastic medium that ensure isotropy of the homogenized limit. These conditions involve the irreducibility of certain representations of the group in question. Our results also lead to an alternative proof of the representation theorem for an isotropic elasticity tensor.

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CP7

Homogenization of a Weakly Randomly Perturbed Periodic Material

We present an approach aiming at computing the first-order homogenized behavior of a randomly perturbed periodic material. More precisely, we are interested in the homogenization limit as $\epsilon \to 0$ of the field

$$A_\eta\left(\frac{x}{\epsilon},\omega\right) = A_{per}\left(\frac{x}{\epsilon}\right) + b_\eta\left(\frac{x}{\epsilon},\omega\right) C_{per}\left(\frac{x}{\epsilon}\right)$$

where A_{per} and C_{per} are deterministic periodic matrices and b_η is a "small' stochastic perturbation. Our approach, which is rigorously founded in a certain class of settings, proves to be very efficient from a computational point of view for even more general settings.

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CP7

Numerical Simulation of Wave Propagation in Materials with Microstructure

Results of numerical simulations of one-dimensional wave propagation in microstructured solids are compared with corresponding results in given layered media. A linear microstructure model based on Mindlin theory is adopted in

the framework of the internal variable theory. Fully coupled systems of equations are rewritten in the form of conservation laws. A modification of wave propagation algorithm is used. It is shown how the initial microstructure model can be improved to match the better result.

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CP7

Two-Scale G-Convergence and Its Applications to Homogenisation of Non-Linear High-Contrast Problems.

It is a resent results of Bouchitte, Felbacq, Zhikov and others that passing to the limit in high-contrast elliptic PDEs may lead to non-classical effects, which are due to the two-scale nature of the limit problem. These have so far been studied in the linear setting, or under the assumption of convexity of the stored energy function. It seems of practical interest however to investigate the effect of high-contrast in the general non-linear case, such as of finite elasticity. With this aim in mind, we develop a new tool to study non-linear high-contrast problems, which may be thought of as a hybrid of the classical Γ-convergence (De Giorgi, Dal Maso, Braides) and two-scale convergence (Allaire, Briane, Zhikov). We demonstrate the need for such a tool by showing that in the high-contrast case the minimizing sequences may be non-compact in L^p space and the corresponding minima may not converge to the minimum of the usual Γ-limit. We prove a compactness principle for high-contrast functionals with respect to the two-scale Γ-convergence, which in particular implies convergence of their minima.

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CP7

Variance Reduction Methods for Stochastic Homogenization

The homogenized matrix of a random material is known from the solutions of the so-called corrector problems, which, in the stochastic framework, are stochastic equations posed on the *whole* space R^d. In practice, these equations are solved numerically on a truncated domain. Because of this truncation, the approximated homogenized matrix is *random*. In this work, we explain how to reduce its variance, using antithetic variables. Numerical simulations illustrate the efficiency of the approach.

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CP7

Correctors and Field Fluctuations for the $p_\epsilon(x)$-Laplacian with Rough Exponents

Properties of local fields inside mixtures of two nonlinear power law materials are studied. This simple constitutive model is frequently used to describe several phenomena ranging from plasticity to nonlinear dielectric media. This work addresses a prototypical problem in the scalar setting. We provide the corrector theory for the strong approximation of fields inside composites made from power law materials. These results are applied to deliver new multiscale tools for bounding the local singularity strength inside micro-structured media in terms of the macroscopic applied fields.

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CP8

Nanostructure Instability Induced by Anisotropic Epitaxial Stresses

The morphological evolution of an initially straight stripe lying on a semi-infinite substrate is studied in the linear regime when the mass transport mechanism is the diffusion of ad-atoms along stripe edges and when the heteroepitaxy between the line and the substrate is anisotropic. It is found that anti-phase fluctuations grows faster than in-phase ones for selected values of epitaxial stress components such that a pinched shape preferentially emerges.

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CP8

Micromechanics Model for Debonding of Elliptical Particles

A primary failure mode for particulate composites is the dewetting of particles from the surrounding matrix. This nonlinear process in an inherently multiscale system results in complex physical behaviour. A cohesive law is incorporated into a micromechanics formulation to investigate the debonding of elliptical particles, for which the macroscopic response depends strongly on the misalignment between the loading direction and the major axis of the ellipse.

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CP8

A Mathematical Tool for Investigating the Structural Response of Composites Subjected to Impact Loading

A tool for analyzing the propagation of a wave in composite material due to an impact load is described. It consists of a micromechanical model of wave propagation in composite material using a lattice structure of a two dimensional plate divided into subcells. The top of the plate is impacted by a wave (input) and a propagated wave is recorded at the bottom. The tool can allow the study of transmission loss due to impact of an acoustical wave or dissipation of a mechanical impact. Examples of specific materials and composites will be illustrated and mathematical problems associated with the current version will be discussed.

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CP8

Maximization of Fracture Energy by Variation of Shapes of Inclusions

Our goal is to design shapes of inclusions inside brittle composite materials yielding maximal fracture energy for a given load case. For each design the resulting crack pattern is computed as solution of an energy minimization problem. The uncracked domain is modeled by linear elasticity while the area close to the crack is described on a smaller scale taking into account non-linear cohesive effects. Numerically, this problem is solved by the FEM with cohesive elements.

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CP8

Refraction of Transverse Wave at a Plane Interface in Thermo-Elastic Materials with Voids

The problem of reflection and refraction of elastic waves due to incident plane transverse wave at a plane interface between two dissimilar thermo-elastic materials has been analyzed. The theory developed by Iesan (1986) for thermo-elastic materials with voids has been used. There exist three sets of reflected and refracted coupled longitudinal waves and transverse waves in the half-spaces of thermo-elastic materials with voids when a transverse wave is incident at the plane interface. The formulae for amplitudes and energy ratios of various reflected and refracted waves have been obtained. The amplitude and energy ratios of various reflected and refracted waves are computed numerically and the results are presented graphically for a specific model

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CP9

Multiscale Modeling of Flow-Induced Semicrystalline Morphologies in Polymer Fiber Spinning

A systematic multiscale approach is developed to model the flow-induced semicrystalline morphologies in polymer fiber spinning processes. It combines a non-equilibrium lattice-based microscopic Monte Carlo simulation of the polymer chains, implemented efficiently using a lattice subdivision technique, with a non-equilibrium thermodynamics continuum flow model of the polymer amorphous phase. We showed that as the extensional rate increases, the lamellar semicrystalline morphology becomes less favored than the fibrillar, in agreement with what has been observed experimentally.

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CP9

Adaptive Free Energy Computations for Crystalline Materials

Several processes in the thermo-mechanical behavior of crystalline materials arise from microscopic interactions between constituent atoms. As a result molecular dynamics simulations have become a valuable tool as they allow detailed resolution of such phenomena. Despite their accuracy, atomistic simulations at the engineering space/time scales are impossible with current or forseeable compuational capabilities. On the other hand, continuum theories are computationally efficient but their accuracy can be limited unless they are somehow informed from the atomistic properties. Important steps in this direction are a variety of sequential or hierarchical multiscale methods which combine atomistic models with coarse-graining schemes. The critical issue in coarse-graining equilibrium atomistic descriptions amounts to the computation of the free energy with respect to the collective variables of interest. Existing efforts along these lines frequently employ (local) (quasi)harmonic approximations to get a semi-analytic expression of the free energy. This approach however underestimates the temperature dependence, fails for tempera-

tures greater than half the melting point and is sensitive to unharmonicities of the interatomic potential which become prominent at transitions between microscopic equilibrium states. In order to connect atomistic and continuum descriptions we make use of the Cauchy-Born rule. At finite temperature, we consider a representative cell of the crystal and impose boundary displacements according to the macroscopic deformation gradient of the contiuum description. The problem therefore reduces to calculating the free energy landscape as a function of the nine (in three-dimensions) components of the deformation gradient (or six-components of the Cauchy-Green strain tensor due to frame indifference). The core contribution of this paper is a novel, adaptive technique for calculating such free-energy surfaces. The proposed procedure combines elements of adavanced Monte Carlo sampling and statistical learning. We utilize an extended-space formulation where sampling is performed with respect to the macroscopic variables (or reaction coordinates). The free energy is estimated from an evolving ensemble of non-equilibrium atomistic simulations. This estimate is used to bias the dynamics until the whole free energy landscpe is identified. In contrast to existing techniques that employ dynamical arguments, we are motivated from statistical learning theories and provide rigorous bounds for convergence. We investigate the use of Bayesian sparseness priors that favor the discovery of free energy surfaces in high-dimensional domains.

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CP9

In Silico Structure and Nanomechanics of Intermediate Filaments

Intermediate filaments (IFs) are a major component of the cytoskeleton in eukaryotic cells, playing a vital role in providing structural stability. Here we utilize an in silico materiomics approach to develop a structural model of IFs through the use of a multi-scale simulation. We report experimentally validated atomistic-level models of IF dimer and tetramer structures, and examine their response to mechanical stress. A comparison with experimental nanomechanics results shows good agreement.

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CP9

Reverse Monte Carlo Refinements of Local Atomic Structure in Crystalline Materials

Exploitable properties of many functional crystalline materials, such as ferroelectrics, high Tc superconductors, multiferroics, etc., are controlled by the local atomic ordering (i.e. chemical ordering in solid solutions or correlated atomic displacements from the average lattice sites). Reverse Monte Carlo refinements of local structure, which rely on the Metropolis algorithm to fit the experimental data, provide an opportunity for quantitative determination of the local atomic configurations. We developed computer algorithms and relevant software that enable simultaneous fitting of multiple types of experimental data under various bespoke restraints on atomic moves. Applications of this method to several practical material systems will be discussed to highlight the capabilities of this approach and the challenges that still need to be resolved.

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CP9

Coarse Variables As Adapted Projections

Given an autonomous ODE system we aim to define (non-trivial) scalar state functions that evolve autonomously. If possible, such functions can be useful as candidates for unambiguously initializable coarse dynamics in physical applications. The question motivates a mathematical restatement in terms of a first-order PDE. A computational approximation is developed and tested on the Lorenz system and the Hald Hamiltonian system with promising results and intriguing questions.

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CP9

Coupled Atomistic-Continuum Study of Inertial Effects for Brittle Cracks

A coupled method is proposed which employs the continuum elastodynamics model to introduce loading conditions and capture elastic waves, and uses molecular dynamics to resolve the local structures at the atomic scale. A consistent coupling condition with special treatment of the atomistic boundary condition is introduced at the interface. Application to the dynamics of a brittle crack under various loading conditions is presented, with a focus on the inertial effects of the crack tip.

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MS1

Bounds on the Rate of Coarsening for the LSW and Diffusive LSW Models

The Lifschitz-Slyozov-Wagner (LSW) model is one of the simplest models describing the phenomenon of domain coarsening. The talk is concerned with the problem of estimating in a mathematically rigorous way the rate of

coarsening for this model and its related diffusive (DLSW) version. Point-wise in time upper and lower bounds on the rate of coarsening are obtained for the classical LSW model with fairly general initial data. These bounds complement the time averaged upper bounds previously obtained by Dai and Pego, and the point-wise in time upper and lower bounds obtained by Niethammer and Velasquez for solutions with initial data close to a self-similar solution. Current work of the speaker and Mohar Guha to extend these results to the DLSW model will also be summarized.

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MS1

Coarsening Rates for the Degenerate Cahn-Hilliard Equations

Upper bounds on coarsening rates at long times are obtained for the degenerate Cahn-Hilliard equation, for all temperatures below the critical temperature and for all concentrations within the miscibility gap. These results generalize the results of Kohn & Otto (2001). Additionally, upper bounds on coarsening are obtained that are valid from early times, based on bounds from below on the free energy. Various time dependent transitions between various coarsening rates are shown to be possible.

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MS1

Crossover in the Coarsening Rates in Demixing Binary Viscous Liquids

We consider the demixing process of a binary mixture of two liquids after a temperature quench. In viscous liquids, the demixing is mediated by diffusion and convection. The typical particle size ℓ grows as a function of time t, a phenomenon called coarsening. Simple scaling arguments based on the assumption of statistical self-similarity of the domain morphology suggest the coarsening rate: from $\ell \sim t^{1/3}$ for diffusion-mediated to $\ell \sim t$ for flow-mediated. In joint works with Yann Brenier, Felix Otto, and Dejan Slepcev, we derive the crossover of both scaling regimes. The mathematical model is a Cahn-Hilliard equation with convection term, where the fluid velocity is determined by a Stokes equation. The analysis follows closely a method proposed by Kohn and Otto, which is based on the gradient flow structure of the evolution.

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MS1

Self Similarity During Coarsening of Morphologically Complex Mixtures

Coarsening of three-dimensional two-phase structures is examined using nonconserved and conserved dynamics. For systems with 50% volume fraction evolving via both dynamics and 36% and 40% mixtures evolving via conserved dynamics, we find that the domains are bicontinuous, and have time-invariant scaled morphologies and topologies. We will discuss the evolution equation for the principal curvatures of the interface, and the resulting flux of probability of finding a patch of interface with a given pair of principal curvatures.

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MS2

A Boundary Integral Approach and Its Applications to Crystal Growth

In this talk, we will develop a boundary integral method for solving the quasi-steady crystal growth and epitaxial thin film growth problem within the context of classical BCF model. We compare our numerical results with linear stability analysis and show that there exist critical conditions such that the evolving morphology can be controlled by the mass flux and related boundary conditions. This enables us to develop effective ways to control the evolving morphologies.

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MS2

A Phase Field Simulation of Step Flow Problem

Abstract not available at time of publication.

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MS2

A Level Set Simulation for Ordering of Quantum Dots

We present level set simulations for the ordering and self-organization of quantum dots. In particular, we will discuss how variations of the potential energy surface for adatom diffusion affects ordering. Our results are compared to recent experiments that use the cleaved edge overgrowth technique, which is a promising technique to obtain ordered arrays of quantum dots, where the size and position of the dots can be controlled very well. Our results then suggest what type of variations of the potential energy surface can potentially improve the uniformity of quantum dot arrays.

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MS2

Simulating Surface Energy Anisotropy Using Extended Cahn-Hilliard Model

We study the influence of surface and strain energies on heteroepitaxial thin-film growth. We propose an alternate way of simulating anisotropy for the surface energy by using the higher order terms in the free energy. To the second order, the system only have isotropic properties. We can produce different anisotropy by adding higher order terms to the energy. By choosing the right parameters, we can study the behavior SiGe/Si thin film. This type of extended Cahn-Hilliard model has been previously studied to the 4th order, but to our knowledge no one has ever implemented all the terms in this system. One advantage of this energy is that it has the intrinsic regularization. We present numerical results using an adaptive, nonlinear multigrid finite-difference method.

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MS2

Smoothed Boundary Method for Problems in Materials Science

In this presentation, we will describe an approach for solving partial differential equations with general boundary conditions imposed on arbitrarily shaped boundaries, along with the mathematical derivation. To demonstrate the general applicability of this approach, we provide four examples: the diffusion equation with both Neumann and Dirichlet boundary conditions, the diffusion equation with surface diffusion, the mechanical equilibrium equation and the equation for phase transformation with additional boundaries.

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MS3

Structured Elastic Media

This lecture treats a variety of properly invariant dissipative and regularizing mechanisms for the dynamics of nonlinearly elastic rods and of 3-dimensional nonlinearly elastic bodies. The constitutive equations for the resulting structured media play a central role in stability studies, the treatment of incompressibility, the theory of shocks in elasticity, and in computation.

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MS3

Nucleation of Austenite in Martensite

In recent experiments of H. Seiner, austenite was nucleated via localized heating in a single crystal of CuAlNi mechanically stabilized as a single martensitic variant. It was observed that the shape recovery process was always initiated at a corner irrespective of the point of contact of the localized heat source with the specimen. We present an analysis of this phenomenon in terms of quasiconvexity properties of the energy density.

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MS3

An Iterated Homogenization Method to Study Cavitation in Hyperelastic Solids

We propose a novel formulation to study cavitation in solids that: (i) is applicable to large classes of nonlinear elastic materials, (ii) allows for 3D general loading conditions with arbitrary triaxility, (iii) incorporates direct information on the initial shape, spatial distribution, and mechanical properties of the underlying defects at which cavitation can initiate, and (iv) is, at the same time, computationally tractable. The proposed framework is based on an iterated homogenization method that allows for the construction of exact solutions for the mechanical response of nonlinear elastic materials containing random distributions of initially infinitesimal cavities (or defects). The relevant analysis reduces to the study of Hamilton-Jacobi equations in which the initial size of the cavities plays the role of time and the applied load plays the role of space.

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MS3

On the Symmetry of Energy Minimising Deformations in Nonlinear Elasticity

We present a new symmetrisation procedure applicable to deformations of spherically symmetric, nonlinearly elastic, compressible shells. The procedure can be used to prove the symmetry of energy minimisers obtained using the direct method of the Calculus of Variations in the case when symmetric boundary conditions are imposed. Our meth-

ods apply to classes of polyconvex stored energy functions and involve use of the isoperimetric inequality to obtain lower bounds on the energy of deformed spheres in terms of their deformed area. These bounds turn out to be sharp in the case of the symmetrised deformation.

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MS4

Energy Minimizers for a Class of Incompressible Liquid Crystal Elastomers

We present results on existence of minimizers and qualitative behavior for the Warner-Terentjev energy in a certain material regime.

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MS4

The Effects of Strain on the Orientational Distribution of Particles on a Rubber Surface

We discuss the effect of strain on the orientational distribution of particles on a surface of a rubber sheet. Both experimental and modeling results will be presented for particles with various aspect ratios and strengths of attachement to the rubber.

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MS4

Motors Based on Shape Change: See How They Run

Motors are devices which produce motion due to the transfer of energy, but not of momentum, to the device. Recent advances in materials science have allowed the construction of motors where the motion is produced via changes in the shapes of solid objects. In this talk, we consider motors where the shape change is a bend, rather than an elongation or contraction. We analyze in detail the physical mechanisms which bring about the motion, and discuss the origins and path of the momentum current which is generated. We present the results of numerical simulations, and compare these with experimental observations. Some novel approaches to motor design will be discussed.

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MS4

The Mechanics of Nematic Glasses with Topological Defects - How to Develop a Non-developable Surface

Nematic solids suffer considerable elongations and contractions along or perpendicular to a uniform director on temperature change or illumination. Gradients of director instead lead to bend or curl. More subtle response occurs when topological defects in the director field cause flat sheets of nematic glass to thermally or optically develop localised Gaussian curvature. Reversibly inducing non-developable surfaces offers a new mechanics paradigm for actuation and for adaptive surfaces.

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MS4

A Nonlocal Model and Its Simulation of Liquid Crystal Elastomers

We consider a nonlocal model describing the dynamic behavior of nematic liquid crystal elastomers (LCEs) and solve the governing equations numerically. The model gives dynamics for the material displacement, the scalar order parameter and the nematic director, the latter two of which correspond to the order parameter tensor. The simulation shows that our model can successfully capture the shape changing phenomena of LCEs observed in experiments, and also track the dynamics of the order parameter tensor.

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MS5
Selected Features of Plasmonic Cloaking

One of the exciting topics in the field of metamaterials is the concept of cloaking and invisibility. There have been various different methods and techniques for cloaking suggested in the recent years. Among those, we have been developing the scattering-cancellation-based plasmonic cloaking. In this method, the induced dipole moment (and possibly any of the higher-order relevant multipoles) in a moderately-sized object when illuminated by electromagnetic waves can be canceled by the dipole moments generated in the metamaterial shells around the object. The material parameters, the geometry, and the size of such metamaterial invisibility cloaks can be judiciously selected in order to make the total induced dipole (or higher order) moments in the cloak and the object together vanish, resulting in significant reduction of total scattering cross sections. Such plasmonic cloaking does not require anisotropy, inhomogeneity nor a specific geometry in the metamaterial cloaks, since the integrative effects of dipolar cancellation is the main mechanism behind such invisibility. We have studied numerous features of this plasmonic cloaking in the past several years, and have obtained exciting results that exhibit the advantages and constraints of this cloaking method. In this talk, we will present an overview of our work in this area, and highlight key features of plasmonic cloaking.

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MS5
Cloaking vs. Shielding in Transformation Optics

It is generally believed that transformation optics based cloaking, besides rendering the cloaked region invisible to detection by scattering of incident waves, also shields the region from those same waves. We exhibit a coupling between the cloaked and uncloaked regions, and as one application, show how to hide sensors in the cloaked region and yet enable them to efficiently measure the waves incident on the exterior of the cloak, an effect similar to the plasmon-based approach of Alú and Engheta.

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MS5
Effective Constitutive Relations and Variational Principles for Waves in Composites and Metamaterials

This work considers materials whose microstructure is random. Effective constitutive relations and associated variational principles are derived via ensemble averaging. The form of the relations is preserved even if effective relations are expressed via "weighted averages' of the displacement (for elasticity) or the vector potential (for electromagnetics). Even for elasticity, this form is invariant under arbitrary coordinate transformations. The variational principles have stationary character; related minimum principles, applicable to dissipative media, will be mentioned briefly.

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MS5
Optical Cloaking and Transformation Optics

Metamaterials are artificially designed subwavelength composites that possess extraordinary properties not existing in naturally occurring materials. They can alter the propagation of electromagnetic waves resulting in negative refraction, subwavelength focusing and even in cloaking of macroscopic objects. Such unusual properties can be obtained by a careful design of dielectric or metal-dielectric composites on a deep sub-wavelength scale. Metamaterials can now be designed with spatially-varying properties using coordinate transformation for new range of applications. I will discuss a few recent experiments demonstrating intriguing phenomena associated with Metamaterials and transformation optics including 3D negative-index metamaterials, carpet cloak and other transformation optics applications.

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MS6
Physical Models for Describing the Forced Separation of a Molecular Bond

Over the past decade, direct measurements of the mechanical strengths of bio-protein bonds have been reported, and the data provide an glimpse into the realm of material structure and its evolution. The data also offer a challenge to develop a quantitative description of the molecular phenomena being interrogated. In particular, a unifying theme in the study of these phenomena has been to extract microscopic characteristics of the bonds from the macroscopic data obtained, with a view toward comparing bond structures based on behavior or controlling bond behavior through control of environmnent. The process of protein-protein debonding can be described functionally as a transition from one stable configuration of the system to another, with passage through an unstable intermediate configuration. Accessible configurations are defined by means of a landscape surface in a space spanned by both random coodinates and external coordinates representing loading. For the case of time dependent loading, the landscape itself is time-dependent, pushing the framework beyond the direct application of Kramers' theory and similar models for calculating bond reaction characteristics from physical properties of the landscape. In this contribution, we use the established picture of bond behavior for

time-indenpendent landsapes as the point of departure for considering resisting force probablity distribtions and interaction energy landscapes with multiple dimensions for transient bond separtion processes.

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MS6

The Non-equilibrium Thermodynamics and Kinetics of Focal Adhesion Dynamics

We present focal adhesion dynamics via a non-equilibrium thermodynamics treatment, which is derived from harmonic transition state theory. For this purpose we consider several competing thermodynamic driving forces that are both chemical and mechanical in origin. Crucially, we have found a work-based symmetry-breaking mechanism that enables the dominant treadmilling mode of focal adhesion dynamics. Our findings hold for a variety of models, suggesting that the underlying mechanisms are are widely applicable to the dynamics of a broad class of biological soft matter.

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MS6

Cytoskeletal Dynamics Simulations: A Minimalistic Approach

We discuss about coarse-grained approaches to modeling cytoskeletal dynamics in a living cell (Biophys. J. 88 (2005) 3707; PNAS 104 (2007) 4937), using the red blood cell as example. The fundamental distinction between living matter such as tissues and cells with traditional engineering materials is that living matter consumes high-quality energy non-stop. The effect of such metabolic energy consumption on cytoskeletal structural evolution and mechanical properties are investigated by computer simulations.

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MS6

Large Scale Simulations of Vesicles Suspended in 3D Viscous Flows

Vesicles are locally-inextensible closed membranes that possess tension and bending energies. Vesicle flows model numerous biophysical phenomena that involve deforming particles interacting with a Stokesian fluid. We will present new schemes for simulating the three-dimensional hydrodynamic interactions of large number of vesicles. They incorporate a stable time-stepping scheme, high-order spatio-temporal discretizations, spectral preconditioners, and a new reparameterization scheme capable of resolving extreme mesh distortions in dynamic simulations.

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MS7

Dynamic Homogenization of a Non-linear Lattice

The talk deals with a problem of dynamic homogenization which accounts for kinetic energy of phase transition in a bi-stable lattice. In the course of dynamic transition, a part of the energy is radiated and dissipated due to high frequency oscillations and waves. It is necessary to account for the dissipated high frequency part of energy in order to construct an adequate description of the behavior of the microstructured material or dynamically homogenized model. We derive a macrolevel description of a model problem, analyze the solution at the micro-level, and obtain consistent equations for the homogenized system. The computed on the micro-level quantities such as energy loss which accompanies the waves of transitions are used in the derivation.

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MS7

Hysteresis Due to Non-monotone Material Behaviour Inside Many Particle Systems

We study storage problems of the following kind. A many-particle system is used to reversibly store and release a foreign substance. Examples are the storage of hydrogen in small magnesium particles, the storage of lithium in small iron phosphate particles and the storage of air in elastic rubber balloons. The three storage systems have in common: 1. Non-monotone constitutive behavior of the individual particles and spherical rubber balloons. 2. Phase transition and hysteresis of the particle ensemble during loading and unloading.

We describe the evolution of the processes of loading and unloading by a kinetic equation of Fokker-Planck type. There are two small parameters that control whether those processes run in the vicinity of the Maxwell line or whether they exhibit strong hysteretic behavior.

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MS7

Wave Propagation and Thermalisation in Hamiltonian Lattices

Hamiltonian lattices provide simple models for crystals and solids but obey a quite complex dynamical behaviour, in particular when studied on a macroscopic scale. A key phenomenon in this context is the onset of dispersive shocks, in which a Hamiltonian lattice self-thermalises via modulated travelling waves. In this talk we present some new results about several types of travelling waves in FPU chains. In particular, we discuss the existence of action-minimising heteroclinic waves and show that their existence is closely related to a geometric area condition for the interaction potential. Afterwards we use these results and describe several macroscopic Riemann solvers for FPU chains which involve dispersive shocks, conservative shocks, and composite waves.

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MS7

Coherent Structures in Granular Crystals: from Traveling Waves to Discrete Breathers and Beyond

In this talk, we intend to give an overview of our recent theoretical, numerical and experimental activity in the theme of solitary nonlinear waves that arise in granular crystals made up of elastically interacting spherical beads subject to Hertz's law. We start by examining beads of a single type, reviewing the theory of highly localized (nearly compact) solitary traveling waves that exist therein and we consider the possibility of discrete breathers in the 1d granular chain. We then insert a single or multiple defect beads (e.g. of different mass) and examine how this insertion modifies the underlying linear spectrum and the nonlinear states emanating from it. We find interesting bifurcation phenomena especially when inserting multiple defects, such as next-nearest-neighboring ones. We illustrate how to generalize this paradigm of "defect insertion' to an infinite limit of the so-called dimer lattice. In that limit, we consider both solitary traveling waves and discrete breathers. Time permitting, generalizations to other heterogeneous or even disordered chains, as well as to higher dimensional examples will also be given.

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MS8

Self Assembly of Colloidal Spheres

We present an analytical method, using graph theory and geometry, that is capable of deriving all structures into which N colloidal particles can self-assemble in thermodynamic equilibrium. We derive such structures up to $N = 10$ and present conjectures for $N > 10$. We also present a method for directing the self-assembly of the particles such that any N particle equilibrium structure self-assembles with 100% yield.

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MS8

Growth of Objective Structures by Self-assembly

The ideas of Caspar and Klug (Physical principles in the construction of regular viruses, Cold Spring Harbor Symp. Quant. Biol. **27** (1962), 1–24) on equivalence and quasi-equivalence of viral capsids suggest a precise concept, termed "objective structures', that summarizes an essential feature about their construction. An objective structure is a collection of identical molecules for which corresponding atoms in each molecule see the same environment up to orthogonal transformation. Objective structures include many of the most widely studied structures in science today, including carbon nanotubes, the other parts of viruses like necks, tails and baseplates, the cilia of some bacteria, DNA octahedra, buckyballs, actin and collagen and many other common proteins, and typical nonrods, nanosprings and nanowires being synthesized by methods of self-assembly. We discuss quantitative mathematical theory for the self-assembly process, and present some experiments suggested by this theory.

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MS8

Minimal Energy Polymer Packings

We study the structural and mechanical properties of model collapsed polymers using tangent, 'sticky' hard-sphere chains. For small chains, using analytical techniques, we enumerate all low-energy packings. For larger chains, we employ molecular dynamics simulations to study how the quench rate affects the structure of packings and transitions from one low-energy packing to another. These studies will elucidate how chain connectivity affects the packing and dynamics of adhesive hard spheres.

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MS8

Particle Packing Problems: From Kepler and Be-

yond

Packing problems, such as how densely nonoverlapping particles fill d-dimensional Euclidean space R^d are ancient. We provide the putative exponential improvement on a 100-year-old lower bound on the maximal sphere-packing density due to Minkowski in R^d in the asymptotic limit $d \to \infty$. Our study suggests that disordered (rather than ordered) sphere packings may be the densest for sufficiently large d. We also conjecture that the densest packings of the Platonic and Archimedean solids with central symmetry are given by their corresponding densest lattice packings. This is the analogue of Kepler's sphere-packing conjecture for these solids.

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MS9

Phase-field Model of Stress Effect on Grain Growth

We report an efficient phase field formalism to compute the stress distribution in polycrystalline materials with arbitrary elastic inhomogeneity and anisotropy. The dependence of elastic stiffness tensor on grain orientation is taken into account, and the elastic equilibrium equation is solved using a spectral iterative perturbation method. We discuss its applications to computing residual stress distribution in systems containing arbitrarily shaped cavities and cracks (with zero elastic modulus) and to determining the effective elastic properties of polycrystals and multilayered composites. We implemented this approach in a grain growth model to study the stress-driven grain boundary migration and grain growth in two and three dimensions.

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MS9

Simulations of Anisotropic Grain Growth

We describe a new method for simulating anisotropic grain growth in which the interface between each pair of grains is permitted an arbitrary, constant surface tension. This algorithm is an extension of diffusion generated motion, with significant modifications made to ensure that the Herring angle conditions are satisfied at triple junctions. Preliminary results are shown for simulations of analytically-known three-phase evolutions and for large-scale simulations of anisotropic grain growth beginning from thousands of grains.

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MS9

Predictive Theory for the Grain Boundary Character Distribution

Most technologically useful materials are polycrystalline microstructures composed of a myriad of small grains separated by grain boundaries. The energetics and connectivity of the grain boundary network plays a crucial role in determining the properties of a material across a wide range of scales. Cellular structures coarsen according to a local evolution law, a gradient flow or curvature driven growth, for example, limited by space filling constraints, which give rise to changes in the configuration. There are two aspects of coarsening, geometric growth and texture development. The main objective of this presentation is to show that they may be decoupled and characterized by different types of evolution processes, leading to statistically different types of coarsening rates. We consider the grain boundary character distribution, the GBCD, a basic texture measure, and outline a possible entropy based theory for it which suggests that the GBCD statistic satisfies a Fokker-Planck equation. For this, we introduce and study a simplified critical event model which is driven by the boundary conditions and reflects the dissipation principle present in the real system. The proposed theory is consistent with the numerical simulations and experiments.

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MS9

Experimental Studies of Grain Boundary Migration

Grain boundary motion constitutes the microstructural mechanism of recrystallization and grain growth and is usually accompanied by a dramatic change of material properties. This contribution reports on experimental efforts and quantitative results of grain boundary migration mainly in aluminum. Various driving forces and different grain boundary geometries were chosen to study grain boundary mobility of flat and curved grain boundaries. Besides single boundaries also systems of grain boundaries were investigated to reveal the effect of grain boundary junctions on grain growth. The measurements were complemented by molecular dynamics simulations of grain boundary motion and vertex simulations of grain growth.

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MS10

Ferroelectric Phase Transitions, Domain Evolution and Switching in Thin Films

This presentation will discuss the applications of the phase field approach to predicting phase transitions, domain structures, and properties of ferroelectric thin films. In this approach, a nanoscale domain structure is described using a set of spatially inhomogeneous distributions of order parameters such as polarization and strains. Their temporal evolution toward equilibrium is obtained by solving the coupled time dependent Ginzburg-Landau equations as well as the electrostatic and mechanical equilibrium equations. In particular, it will be shown that one can use it to not only help interpreting experimental observations but also provide guidance to achieve desirable transition temperatures, specific domain states, domain wall orientations, and domain wall mobility. It will also be shown that mechanical boundary conditions and stress distributions may be manipulated to tune the coercive field and dramatically enhance piezoelectric responses of ferroelectric thin films. Examples to be discussed are drawn from recent collaborations between the authors group in continuum and mesoscale modeling and a number of experimental groups on oxide film growth and characterizations.

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MS10

Phase-Field Modeling of Grain-Boundary Premelting

Abstract not available at time of publication.

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MS10

Modeling and Simulation of Two Phase Flow on Rough Surface

In this talk, I will first describe a newly developed phase field model for two phase fluid flow based on Cahn Hilliard Navier Stokes equation with generalized Navier boundary condition. Efficient numerical method for the model will be discussed. We then present some numerical results on two phase flow on rough and patterned surfaces. Issues related to drop formation, dripping to jetting transition will also be discussed.

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MS10

Simulation of Dendritic Growth in Melt Flows

We simulate the evolution and free particle motion of an individual nucleus. The melt flow and the convective heat transfer around the dendrites are simulated using a phase-field model.

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MS11

Quasistatic Evolution for Cam-Clay Plasticity

Cam-Clay nonassociative plasticity exhibits both hardening and softening behavior, depending on the loading. For many initial data the classical formulation of the quasistatic evolution problem has no smooth solution. We propose here a notion of generalized solution, based on a viscoplastic approximation. To study the limit of the viscoplastic evolutions we rescale time, in such a way that the plastic strain is uniformly Lipschitz with respect to the rescaled time. The limit of these rescaled solutions, as the viscosity parameter tends to zero, is characterized through an energy-dissipation balance, that can be written in a natural way using the rescaled time. We can also give a differential characterization of the limit, based on a generalization of the flow rule in the rescaled time. It turns out that the proposed solution may be discontinuous with respect to the original time, and our formulation allows to compute the amouunt of viscous dissipation occurring instantaneously at each discontinuity time.

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MS11

Non Associative Plasticity

In this joint work with JFB and MGM we uncover a variational structure for a large class of materials that behave plastically, but with a flow rule which is unrelated to the yield surface. This is of special significance when studying various soil or rock-like materials.

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MS11

The Wigner-Fokker-Planck Equation and the Size Effect on Resistivity in Polycrystalline Materials

Recent experimental results attribute increased resistivity

in small conductors to grain boundary scattering. The Wigner-Fokker-Planck equation yields a temperature dependent open quantum kinetic model of electron flow in a polycrystalline wire. The equation models electron scattering from an electric potential representing the lattice and grain boundaries, and diffusive electron-phonon scattering with a Fokker-Planck operator. Resistivity is extracted from steady-state solutions computed with the discontinuous Galerkin method.

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MS12

Pressure Driven Flow of a Wormlike Micellar Mixture in a Straight Mircrochannel

The inhomogeneous (shear-banding) response of the VCM model (Vasquez, Cook, McKinley 2007) in steady rectilinear pressure-driven channel flow is examined. The VCM model is a microstructural network model developed to describe flows of concentrated solutions of wormlike micelles. The model comprises of a set of coupled, nonlinear partial differential equations, which incorporate breakage and reforming of two micellar species (a long species A and a shorter species B) in addition to reptative and Rousian stress-relaxation mechanisms. We report on results for pressure-driven flow in microfluidic devices with rectangular cross-sections. The velocity profile predicted in a straight channel deviates from the parabolic profile expected for a constant viscosity fluid and exhibits strong shear bands near channel walls. This (nonlocal) model involves diffusive terms both through Brownian motion and through the finite length of the worms. The relevant dimensionless (diffusive) parameter controlling the width of the transition region is a Peclet number; i.e. a microstructural diffusion length scaled by a typical device length scale. Recent experiments have shown that relative magnitude of such terms become increasingly important in microfludic devices. Simulations with the VCM model show that decreasing the characteristic size of the diffusive coupling between the stress and fluid microstructure results in pronounced non-local effects felt across the flow channel.

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MS12

Structure and Rheology of Fiber-Laden Membranes Via Integration of Nematodynamics and Membranodynamics

A study of the structure and dynamics of rigid fiber-laden deformable curved fluid membranes based on an viscoelastic model that integrates the statics of anisotropic membranes, the planar nematodynamics of fibers and the dynamics of isotropic membranes is presented. Based on the membrane's force and torque balance equations and the fiber's balance of molecular fields, the model provides the governing equations for the membrane's velocity and curvature and the fiber structure (fiber orientation and order).

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MS12

Kinetic Modeling of Biological Systems

I will present a kinetic theory for a biofilm system with active polymeric components. The networked biopolymers and bacteria interact with the surrounding nutrient and background fluid to produce the biofilm material system. I will give a detailed discussion on the structure of the governing system of equations, growth modes, and nonlinear interaction among the fluid components. Finally, rheological implication will be discussed as well.

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MS12

Maier-Saupe Theory in 4D

Maier-Saupe theory is the canonical mean field description of thermotropic nematic liquid crystals. In this talk, we examine the predictions of the theory in four spatial dimensions. Representations of the order parameter tensor and the existence of new phases will be discussed. The phase diagram, based on numerical solution of the self-consistent equations and Landau theory will be presented.

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MS13

The Continuum Mechanics of Liquid Crystal Elastic Fluids with Line Defects

We develop the continuum mechanics of nonlinear viscoleastic fluids with disclination and dislocation defects. Driving forces on the defects (under no dynamical restriction) are a natural outcome of our analysis. Both types of defect motion are dissipative, following rigorous kinematic conservation laws for line densities that allow the independent specification of defect kinetics. With appropriate restrictions on kinematic ingredients, the nematic, smectic (A and C), and cholesteric liquid crystal phases, the solid nematic and smectic elastomers and the nematic glass can all be modeled by our theory. A primary feature of this approach is the feasibility of numerical calculations of the interaction of multiple dynamic defects.

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MS13

Mathematical Analysis for the Peridynamic Nonlocal Continuum Theory

We develop a functional analytical framework for the nonlocal peridynamic models. Various properties of the nonlocal peridynamic operators are examined. The connections to the classical elastic models are also provided.

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MS13

Tight Bounds on Failure Surfaces for Random Elastic-Plastic Composites

The failure of load bearing structures made from composite materials is a multiscale phenomena. It involves quantifying force transfer from the structural length scale down to the microscale. In this talk we provide new tools for quantifying the effects associated with force transfer from structural length scales to the length scale of the heterogeneity of the reinforcement phase. We report on new tight bounds for the strength domains for elastic-plastic composite materials when only the volume fractions of the constituent materials are known. These calculations provide bench marks that can be used to validate phenomenological models and numerical computations.

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MS14

Convergence of Quasicontinuum Approximations

The quasicontinuum method reduces the computational cost of approximating the solution of atomistic equilibrium equations by directly coupling the atomistic model with a continuum approximation. We present numerical analysis for a one-dimensional model problem and evaluate the accuracy and efficiency of quasicontinuum approximations with a focus on the choice of coupling at the atomistic-to-continuum interface.

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MS14

A Field Theoretical Approach to the Quasi-Continuum Method

We present a field formulation for the quasi-continuum method based on the following ideas: (i) reformulation of the extended interatomic interactions into a local variational problem that describes the energy of a system via potential fields; (ii) quasi-continuum reduction of these potential fields using an adaptive finite-element discretization of the formulation. We demonstrate that the present formulation resolves inconsistencies present in previous formulations of the quasi-continuum method, and show using numerical examples the remarkable improvement in the accuracy of solutions.

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MS14

Analysis of Quasicontinuum Methods: Introduction and Overview

In the first half of the talk I will give a point-of-view- introduction and overview to the development of the quasicontinuum method, with particular emphasis on the analysis in the zero- temperature static case. I will conclude this part with some remarks on the most important open questions. In the second half of the talk, I will present a new force-based quasicontinuum formulation, developed in joint work with E. Süli and C. Makridakis. Our motivation and starting point are the unusual and potentially damaging stability properties of the "classical" force- based QC method (described in recent work with M. Luskin and M. Dobson). By formulating a variational form of the atomistic equilibrium equations and coupling stress tensors instead of pointwise forces we obtain an alternative force-based coupling scheme that has superior stability properties.

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MS14

Atomistic-to-Continuum Coupling Methods Based on Domain Decomposition

The atomistic-to-continuum coupling problem has similarities with the classical continuum-to-continuum domain decomposition problem. We will explore some of these similarities and address the extent to which both problems can be placed within the same mathematical and algorithmic framework. We will address domain decomposition methods that can be harnessed when solving the atomistic-to-continuum coupling problem, and provide some analysis giving guidance about when the scheme will produce a sat-

isfactory answer.

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MS15

Beating the Clock with Atomistic Simulation of Dislocations

Atomistic simulation is uniquely suited to study the interaction of dislocations with each other and with surfaces and interfaces. However, the accessible timescale is often a severe challenge. In this talk I will discuss about theoretical and numerical issues associated with predicting elementary dislocation behavior at anthropological timescales, namely seconds to hours. For strongly driven systems where the saddle-point is far from the ending equilibrium, a so-called free end modification to the Nudged Elastic Band method (PNAS 104 (2007) 3031; Phys. Rev. Lett. 100 (2008) 025502) has proven to be quite effective.

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MS15

Magnetism-induced Dislocation Mobility and Cross-slip in NiAl: A Multiscale Modeling

Can magnetism be responsible for dislocation mobility and cross-slip, thus the mechanical strength of materials? The answer is yes. With intermetallic NiAl alloy as an example, we perform multiscale simulations to study how magnetic impurities could affect dislocation mobility and cross-slip. More specifically, we examine the effect of 3d-transition metal impurities (Ni, Fe and Co) on the core structure, Peierls energy and stress of a screw dislocation in NiAl. The multiscale approach combines quantum mechanical description of the dislocation core with DFT and empirical atomistic simulations of long-range strain field with EAM. Both spin-polarized and non-spin-polarized DFT calculations are carried out and compared against each other. We find that Fe impurities can introduce local magnetic moments at the dislocation core and enhance dislocation mobility. Depending on concentrations, Ni and Co impurities can either dissociate the dislocation or render spontaneous dislocation cross-slip.

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MS15

Self-forces of Moving Dislocations and Inclusion Boundaries with Inertia Effects

On the basis of Noether's theorem and the dynamic J integral, the self-forces of Volterra dislocations moving in generally accelerating motions are calculated with regularization in the sense of distributions. A particular analysis involves the singularity at the forming Mach cone as the dislocation crosses the shear-wave-speed (with Surong Huang).The self-forces of dynamically expanding inclusion boundaries with eigenstrain, both spherical and plane (by a limiting procedure), are also obtained, and the analogy of the Peach-Koehler forces of dislocations and inclusions is shown.

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MS15

A Continuum Model for Dislocation Dynamics in a Slip Plane

We derive a continuum model for the PeachKoehler force on dislocations in a slip plane. To represent the dislocations, we use the disregistry across the slip plane, whose gradient gives the density and direction of the dislocations. The continuum model is derived rigorously from the PeachKoehler force on dislocations in a region that contains many dislocations. The resulting continuum model can be written as the variation of an elastic energy that consists of the contribution from the long-range elastic interaction of dislocations and a correction due to the line tension effect. We validate our model by performing linear stability analysis and numerical simulation and comparing the results with those of discrete dislocation dynamics model.

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MS16

Ab Initio Enumeration of 3-periodic Weavings and Catenated Nets from 2D Hyperbolic Tilings. Results, Applications and Open Questions

A variety of nets and weavings can be formed in 3D (euclidean) space by folding patterns created in 2D hyperbolic space onto triply-periodic minimal surfaces embedded in 3D space (see S. J. Ramsden, V. Robins and S. T. Hyde, ActaCryst. (2009). A65, 81–108; see also *epinet.anu.edu.au*). The "epinet" project offers a multitude of structures available for materials modelling. A number of fundamental questions arise from these patterns, some answerable, other not (yet).

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MS16

Three-periodic Tilings, Nets and Designed Synthe-

sis of Materials

Crystal structures can be abstracted as *nets* (periodic connected simple graphs). Such nets are carried by face-to-face tilings of space by generalized polyhedra (*cages*) and much of our knowledge of nets has come from systematic enumeration of tilings. Particularly interesting to chemistry are edge-transitive nets which are carried by the duals of face-transitive tilings. The taxonomy of such structures and their relevance to the designed synthesis of targeted materials will be described.

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MS16

The Mathematics and (Mathematical) Physics of Zeolites

I will discuss problems we face when designing algorithms to design zeolites. The problems range from purely combinatorial (how to explore the space of four-regular graphs?) to group theoretic and topological (how to represent such structures in a compact yet expressive way?) to physical (how to find a good model for the energy of such a structure).

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MS16

From Enumerated Graphs to Zeolites; The Mathematical Challenges of Identifying the Real Among the Fanciful

Zeolites are an important class of materials because of their microporosity. They contain sub-nanometer sized pores and channels that allow small molecules to enter. By modeling zeolites as periodic, corner-connected, regular tetrahedra (i.e. as periodic 4-valent graphs), we have been able to enumerate over 5 million hypothetical zeolite structures. However, in nature, there are fewer than 200 known structures. In this talk, I will discuss some of the subtle, and perhaps surprising, mathematical differences between a real zeolite and many of the relaxed 4-valent periodic graphs in our database.

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MS17

Kinetic Monte Carlo Simulation of Nanohut Assembly on Al(110)

Al(110) homoepitaxy exhibits nanoscale self-assembly into huts with well-defined (100) and (111) facets. We used density-functional theory (DFT) to identify the mechanisms needed to describe this three-dimensional assembly and incorporated these into a kinetic Monte Carlo (KMC) model. Our model predicts experimentally observed trends for this system. To achieve precise placement of Al nanohuts, we simulated thermal-field-directed assembly. Our results indicate that this technique can be used to create uniform arrays of nanostructures.

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MS17

Hierarchical Coarse-graining Methods for Complex Stochastic Lattice Systems

We will discuss a variety of coarse-graining methods for many-body microscopic lattice systems and in particular systems dominated by the competition of short and long range interactions. We focus on mathematical, numerical and statistical methods allowing us to assess the parameter regimes where such approximations are valid. Finally, motivated by related problems in the simulation of macromolecular systems, we discuss mathematical strategies for reversing the coarse-graining procedure. The principal purpose of such a task is recovering local microscopic information in a large system by first employing inexpensive coarse-grained solvers.

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MS17

An Energy Localization Principle and Its Application to Fast Kinetic Monte Carlo Simulation of Heteroepitaxial Growth

Simulation of heteroepitaxial growth using kinetic Monte Carlo (KMC) is often based on rates determined by differences in elastic energy between two configurations. This is computationally challenging due to the long range nature of elastic interactions. A new method is introduced in which the elastic field is updated using a local approximation technique. This involves an iterative method that is applied in a sequence of nested domains until a convergence criteria is satisfied. These localized calculations yield energy differences that are highly accurate despite the fact that the energies themselves are far less accurate: an effect referred to as the principle of energy localization. This is explained using the continuum analogue of the discrete model and error estimates are found. In addition, a rejection algorithm that relies on a computationally inexpensive estimate of hopping rates is used to avoid a substantial fraction of the elastic updates. These techniques are applied to $1+1$ and $2+1$ dimensional KMC simulations in physically interesting regimes. The simulations in $2+1$ dimensions introduce additional approximations in order to further improve the performance of the simulations.

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MS17

Extending the Computational and Phenomenolog-

ical Scope of Kinetic Monte Carlo Simulations

Two approaches are presented for extending the application horizon of kinetic Monte Carlo (KMC) simulations. First, a coarse-graining methodology is discussed in which lattice KMC simulations are mapped onto coarser grids. Using properly formulated rate averaging, the coarse-grained simulations are shown to retain essential ingredients of the full-resolution model that are required to capture dynamical and equilibrium properties. Secondly, approaches for incorporating convective flow into lattice KMC simulations of particle transport and clustering are discussed.

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MS18

Phase-Field Studies of Crystal Cohesion during Late-Stage Solidification

This talk will discuss recent progress made in using both conventional phase-field and phase-field-crystal simulations to characterize the complex interaction between solid-liquid interfaces that come into close contact during the late stages of solidification. When interfaces belong to different crystal grains, this interaction can be either attractive or repulsive depending on the br¿the two grains. For strong repulsion, crystal cohesion is retarded and interface bridging only occurs substantially below the liquidus temperature, thereby promoting hot cracking. Results will be presented that shed light on various factors that control interface bridging and the mechanical response of bicrystals in between the liquidus and bridging temperatures.

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MS18

Calculation of Interfacial Free Energies from Atomistic Simulation with Thermodynamic Integration

The solid-liquid interfacial free energy, γ_{sl}, plays a central role in understanding a number of technologically important phenomena in physics, chemistry and materials science, such as crystal nucleation and growth, dendritic solidification, liquid-metal embrittlement, and wetting. In this talk, I will review our work on the direct calculation of γ_{sl} for a number of model systems using molecular-dynamics simulation and thermodynamic integration. This discussion will highlight recent work where we use Cahn's reformulation of Gibbs' interfacial thermodynamics to determine γ_{sl} along a solid-liquid coexistence curve by integration of data for the excess interfacial energy and stress, with specific application to the Lennard-Jones system.

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MS18

Phase-field Modeling of Reactive Wetting

During reactive wetting the fluid and solid substrate can react together chemically, so that the solid undergoes further phase transitions. Such intermetallic formation introduces an additional free boundary into the problem description, which becomes even more challenging than the classical problem of droplet spreading on an inert substrate. A four-phase, diffuse interface model for a ternary alloy system has been formulated, and numerical solutions describing the dynamics of the interface motion are being computed.

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MS18

Phase Field Models of Grain Boundaries: The Good and the Bad

Over the years, there have been many different approaches to modeling the dynamics of grain boundaries. In particular, over the past two decades, a number of phase field models of grain boundary evolution have been developed, all with particular short-comings. In this talk I will review these approaches, discuss their advantages and disadvantages, and finally suggest a possible "way" out.

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MS19

Electroactive Polymers

This talk is motivated by soft dielectric elastomer actuators. In these materials, deformation is obtained by an applied electric field mediated by the Maxwell stress. The low electro-mechanical coupling efficiency has given rise to various attempts to improve the underlying materials. Of particular interest is heterogeneous media which can show an unexpectedly large increase in coupling. This talk will describe the basis of this increase, and potential instabilities which can give rise to even larger deformation.

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MS19

Material Instabilities in Nematic Elastomers

We discuss material instabilities in nematic elastomers, which are crucial for the interpretation of their mechanical response. These are mostly in the form of reversible,

elastic shear bands and they underlie the unusually soft response of these materials to imposed stretches.

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MS19

A Micromechanical Approach of Localization Phenomena in SMAs

Localization phenomena are frequently observed in polycrystalline SMAs, and are known to be partly related to material instabilities. Common micromechanical models of SMAs result in convex estimation of the free energy and therefore are not able to capture all the complexity of the localization phenomena. Using tools of quasiconvex analysis and homogenization, a non convex lower bound on the free energy of polycrystalline SMAs is proposed. That result is a step towards a better understanding of localization aspects in SMAs.

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MS20

Mathematical Differences and Similarities Between High-TC and Low-TC Superconductors

We present recent results on the behavior of the Lawrence-Doniach system for layered superconductors occupying a bounded domain in three dimensions. The Lawrence-Doniach system is the Euler-Lagrange system for a corresponding anisotropic Ginzburg-Landau energy used to describe anisotropic high-temperature superconductors. We prove that applied magnetic fields in a direction parallel to the layers do not produce vortices in energy minimizers, in contrast to the behavior of low-temperature three-dimensional superconductors or the anisotropic "effective mass" model in three dimensions. For nonparallel (tilted) applied fields, vortices do form at a sufficiently large field, and we characterize the critical modulus of this field in terms of the angle it makes with the layers. We also present results on the behavior of minimizers in parallel or slightly tilted magnetic fields.

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MS20

Patterns in Two-dimensional Nematics

I will present an extension of Onsager's variational theory of nematic liquid crystals to spatially inhomogeneous systems. Concentrating on the two-dimensional model I will provide a detailed description of vortex-like patterns and their evolution induced by the diffusive transport (Doi) dynamics.

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MS20

Dynamics of Colloidal Particles in Liquid Crystals

We employ 3D microscopy to study electrically-controlled dynamics of colloidal particles in a liquid crystal. Particles create defects of a dipolar type (hyperbolic hedgehogs) in the otherwise homogeneous director field. The particles levitate in the nematic bulk thanks to the elastic repulsion from the bounding plates. By applying electric field one causes three dynamic effects: (1) backflow of the nematic and bidirectional motion of particles; (2) electrophoresis of the particles; (3) electrorotation.

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MS20

Stable States in a Coupled Energetic Model for Incompressible Nematic Elastomers

We investigate an energetic model for incompressible nematic elastomers. A unit-length molecular director and an incompressible deformation are the unknown functions, minimizers of a proposed coupled energy in $\mathbf{R}^3$. Working in Sobolev spaces, we prove lower semi-continuity and existence of minimizers for the energy. Keeping incompressibility, we derive weak Euler Lagrange equations. Additionally, we consider 2-dimensional models with non-convex energy densities involving terms related to the volume constraint, and deduce existence and partial regularity results.

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MS21

Flux Norm in a Finite-demensiona Homogenization Approximation with Non-separated Scales

The homogenization of PDEs with periodic or ergodic coefficients and well separated scales is now well understood. In a joint work with H. Owhadi (Caltech) we consider the most general case of arbitrary bounded coefficients. Specifically, we study divergence-form scalar elliptic equations and vectorial equations with such coefficients. For these problems we establish two finite-dimensional approximations of solutions, which we refer to as finite-dimensional homogenization approximations. We introduce a flux norm and establish the error estimate in this norm with an explicit and *optimal* error constant independent of the contrast and regularity of the coefficients. A proper generalization of the notion of cell problem is the key technical issue in our consideration.

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MS21

Pade Approximations for Composites with Evolving Structure

The talk discusses a problem of approximation of effective transport properties of a two-phase composite with slowly changing structure. The Stieltjes integral represen-

tation is used to describe the effective properties of the composite. This representation relates the n-point correlation functions of the microgeometry to the moments of the spectral measure, which contain all information about the microstructure. Pade approximation of the spectral function can be used to construct a minimal lattice whose effective properties approximate the properties of the composite. The moments of the spectral measure characterizing the structure, are exactly calculated using poles and residues of Pade approximation; this allows us to monitor the changes in the microgeometry using a small number of parameters.

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MS21

Electromagnetic Circuits

Maxwell's equations bear a close resemblance with those of linear elastodynamics. So a natural question to ask is: what is the electromagnetic analog of a mass-spring network in elastodynamics? We assume the frequency is fixed and construct such an analog, which we call an electromagnetic circuit. By interchanging the roles of epsilon and mu we also obtain magnetoelectric circuits. Then one can join electromagnetic and magnetoelectric circuits to obtain hybrid circuits. Their response is measured in terms of the electric or magnetic field along or across the terminal edges of the circuit. This response is governed by a symmetric matrix with negative semidefinite imaginary part. Conversely given any such matrix a recipe is given for constructing a hybrid circuit which has that matrix as its response matrix.

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MS21

Controlled Self-assembly of Charged Particle Monolayers

Recently, self-assembly has emerged as an efficient method to create scale-independent regular structures. A problem commonly encountered in experiment is little or no control over the kinetics of structure formation. In this work, an optimal choice of macroscopic control parameters is identified. Using Molecular Dynamics, kinetics of self-assembly is evaluated in systems proposed by Whitesides *et. al.* An idealized model is put forward to rationalize the results observed in simulations.

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MS22

Bridging Fluctuating Hydrodynamics and Molecular Dynamics Simulations

We devise a scheme to map the atomic representation of a fluid to field variables and show that field fluctuations in FHD and all-atom MD simulations and their equation of state and transport coefficients can be matched quantitatively. We also show that the FHD equations can be generalized to use a viscoelastic rheological model with colored noise. Finally, we develop a coupling scheme based the Lum- Chandler-Week theory of hydrophobicity to enable combined particle/ field simulations.

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MS22

A Hybrid Particle-continuum Method for Hydrodynamics of Complex Fluids

We describe a hybrid method coupling a fluctuating compressible Navier-Stokes solver with the I-DSMC particle method. The continuum provides state boundary conditions to the particle subdomain, which in turn provides fluxes to the continuum subdomain. We study the Brownian motion of a large spherical bead, as well as the relaxation of an adiabatic piston, and we find that the hybrid correctly reproduces the particle simulations only if the continuum solver includes thermal fluctuations.

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MS22

Constrained Polymer Dynamics in a Mesoscale Solvent

While modeling polymer solutions, the presence of multiple time scales, such as the intermolecular bond potentials, makes quantitative analysis of results difficult, and simulations costly. Here, we show how these degrees of freedom can be replaced by rigid bond constraints—as commonly done in Brownian dynamics—for polymers embedded in a recently introduced hydrodynamic solvent known as Stochastic Rotation Dynamics (SRD) (or Multi-Particle Collision Dynamics - MPCD).

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MS23

Patterning and Intermittency in a PDE Model of Dislocation Plasticity

An exact 1-d reduction of a 3-d, time-dependent PDE model of dislocation mechanics will be discussed. The 1-d model takes the form of a level set equation whose velocity is the driving force of a Ginzburg-Landau equation. Computation of pattern formation and time-dependent behavior will be presented, including the formation of near-static dipolar dislocation wall and cell structures observed within persistent slip bands in bulk single crystals under fatigue loading.

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MS23

Variational Equivalence Between Ginzburg-Landau, XY Spin Systems and Screw Dislocation Energies

We introduce and discuss discrete two-dimensional models for XY spin systems and screw dislocations in crystals. We prove that, as the lattice spacing ε tends to zero, the relevant energies in these models behave like a free energy in the complex Ginzburg-Landau theory of superconductivity, justifying in a rigorous mathematical language the analogies between screw dislocations in crystals and vortices in superconductors. To this purpose, we introduce a notion of asymptotic variational equivalence between families of functionals in the framework of Γ-convergence. We then prove that, in several scaling regimes, the complex Ginzburg-Landau, the XY spin system and the screw dislocation energy functionals are variationally equivalent. Exploiting such an equivalence between dislocations and vortices, we can show new results concerning the asymptotic behavior of screw dislocations in the $|\log\varepsilon|^2$ energetic regime.

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MS23

Gradient Theory for Plasticity via Homogenization of Discrete Dislocations

We derive, in a mathematically rigorous way, a strain gradient theory for plasticity as a mesoscopic limit of systems of discrete dislocations, where only the elastic energy is taken into account and the presence of dislocations is determined by a topological constraint. This is joint work with A. Garroni and M. Ponsiglione.

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MS23

Coarse-graining in Atomistic Models of Dislocations

Dislocations and their dynamics play a major role in the response of materials to mechanical and thermal loading. Extensive work has been done on different scales of the problem from atomistic level, to dislocation level to macroscopic level. Yet the behavior of material under plastic deformation is still a source of many challenging mathematical problems. In this talk we focus on models at the atomistic level and deal with questions of coarse graining where higher level models are sought. We focus on distribution functions characterizing the atomic arrangement and discuss energy representation and dislocation motion in terms of these statistical properties. The evolution is formulated as a gradient flow.

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MS24

Coarsening of Surface Patterns in Growth and Ero-

sion

Surface patterns like ripples, mounds or pits are a ubiquitous feature of thin film deposition and erosion processes. In many cases such patterns are observed to coarsen, in the sense that the typical feature scale increases as a power law with growth or erosion time. Nonlinear continuum equations have played an important role in classifying possible coarsening laws as a function of the symmetries and conservation laws of the system. The typical scenario suggested by these studies is that coarsening is driven by the minimization of some energy-like quantity (more generally, a Lyapunov function of the process). After outlining this general framework, the talk will focus on recent experiments on the rapid coarsening of ripples by ion erosion under near-glancing incidence. In this system coarsening appears to be a purely kinematic phenomenon, which can be consistently described in terms of the ion-driven motion of pattern defects. The analogy to the evolution of wind-driven sand ripples is emphasized, and it is argued that a full quantitative theory of this type of coarsening dynamics poses an interesting challenge to the continuum modeling of surface structures. The talk is based on joint work with H. Hansen, A. Redinger, S. Messlinger, G. Stoian and T. Michely (Phys. Rev. Lett. 102, 146103, 2009).

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MS24

Effects of Additives on Restructuring of Two-dimensional Islands on Metal Surfaces

Addition of chalogen atoms (O, S, ...) generally enhance the rates of coarsening of nanostructures on coinage metals (Cu, Ag, Au, ...). While some metal-chalogen complex are found to be stable and can be observed through scanning tunneling microscope, surfactant assisted surface dynamics involves structures that could be highly transient and unstable. Using density functional theory, we calculate the formation energy of various Ag-S and Cu-S clusters on Ag(111) and Cu(111) surfaces. Some clusters has significantly lower energies than Ag and Cu adatoms, and can serve as more efficient carriers for mass transport on surfaces. A continuum model utilizing those calculated energies is developed to modeling the effect of additives on relaxation of surface nanostructures.

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MS24

Self-assembled Superlattice Patterns

On a solid surface a binary thin film may separate into two phases. The phases can self-assemble into nanoscale domains. We show that directed self-assembly via substrate elasticity, surface strain field and surface chemistry can produce a variety of patterns. Our study also reveals the important role of diffusion dynamics, and how a locally ordered seeding pattern propagates to the neighboring regions to form a large uniform supperlattice structures.

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MS24

Step Dynamics: Deterministic and Stochastic Effects in Mound Decay and Growth

This talk focuses on a class of models for the dynamics of line defects (steps) on crystal surfaces in homoepitaxy. Two topics to be discussed are: (i) The homogenization of microscale effects and resulting properties of effective deterministic partial differential equations for the surface height profile. (ii) Analytical aspects of adding noise to Burton-Cabrera-Frank-type models for steps under growth, with some emphasis on the variance of terrace widths and the comparison to 'mean-field' theories.

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MS25

Phase-Field Crystal Modeling of Morphology Evolution in 2D and 3D

Crystallization kinetics and morphological evolution are addressed using the phase-field crystal approach. We show that at low thermodynamic driving forces continuously decelerating diffusion-controlled growth is observed, while at large enough driving forces a steady-state diffusionless mode occurs. This is associated with dynamic broadening of the crystal-liquid interface that influences the anisotropy of interfacial properties. Consistently with experiments, this leads to a transition from faceted dendrites to curved dendrite tips in 2d and 3d.

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MS25

Multi-Scale Modeling of Phase Transformations: From Classical Density Functional Theory to Phase Field Methods

We review recent mathematical and numerical innovations in quantitative modeling microstructure formation using phase field methods. Their success in predicting steady state and transient spacing selection in solidification is reviewed. The new phase field crystal (PFC) methodology, and some of its variants, is then discussed as a simple yet fundamental method of addressing some of the shortcomings of traditional phase field theory. The PFC methodology is demonstrated by reviewing new research on the effects of elasto-plasticity, polycrystalline interactions and multiple phases on microstructure formation. Finally, new work on connecting phase field crystal models to density functional theory (DFT) is reviewed. Two applications that exploit this connection are discussed. The first deals with interfacing PFC models with molecular dynamics for more quantitative simulations than have been possible thus far. The second discusses new uses of course graining strategies, aimed at projecting out free energies, the forms of which are more fundamental than those used in traditional phase field modeling.

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MS25

Nucleation Barriers: Using a String Method for the Phase Field Crystal Model

Phase Field Crystal (PFC) is a well established model to study solid state phenomena in metals and colloids on an atomistic scale. It can be connected to time dependent classical density functional theory. We will use PFC to study nucleation. This requires to explore the transition path between two (meta)stable states. The nucleation barrier is then defined by the most probable transition path, which is equivalent to the minimum energy path (MEP) in configuration space. We use a simplified string method proposed by E, Ren and Vanden-Eijnden in order to calculate MEP based on PFC. Nucleation barriers as well as the morphology of minimal stable nuclei and the influence of walls on nucleation will be discussed.

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MS25

Energy Stable Schemes for the Phase Field Crystal Equation

The PFC and MPFC equations decribe crystals at the atomic scale in space but on diffusive scales in time. The models account for the periodic structure of a crystal lattice through a free energy functional of Swift-Hohenberg type that is minimized by periodic functions. The models naturally incorporate elastic and plastic deformations, multiple crystal orientations and defects and have been used to simulate a wide variety of microstructures. In this talk I describe energy stable and convergent finite difference schemes and their effcient solution using nonlinear multigrid methods. A key point in the numerical analysis is the convex splitting of the functional energy corresponding to the gradient systems. In more detail, the physical energy in both cases can be decomposed into purely convex and concave parts. The convex part is treated implicitly, and the concave part is updated explicitly in the numerical schemes. I will discuss both first- and second-order accurate convex splitting schemes. The proposed schemes are unconditionally stable in terms of the physical energy and unconditionally solvable, which allows for arbitrarily large time step sizes. This property is vital for coarsening studies that require very long time scales.

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MS26

Coexistent Phases and Critical Points in Thermoelasticity

Materials are known to behave in strange and novel ways in the neighborhood of critical points. The softening of various material moduli is commonly reported, and the smooth change of homogeneous states into complex multiphase microstructures is possible. For solids, the analysis of this behavior is complicated by the fact that the full notion of stress and deformation gradient (as tensors), including shearing, must be considered, rather than simply the classical effects associated with pressure, specific volume, and temperature. In this work, I consider sequences of equilibrium coexistent phases, induced by thermal and mechanical loading, and the asymptotic limits and relations between the thermodynamic fields of deformation gradient, temperature and the specific heat at constant deformation for elastic solids in the neighborhood of critical points. A generalized form of the famous Rushbrooke inequality from physical chemistry is obtained. Also, a generalized Clausius-Clapeyron equation is obtained.

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MS26

Metastable Elastic Equilibria with Surfaces of Discontinuity

We consider non-linearly elastic equilibrium configurations, that are smooth away from a a smooth phase boundary. We ask for conditions that would be necessary for such configurations to be strong local minimizers. We discuss classical necessary conditions and derive new ones from a unified point of view. We also discuss interrelations between all necessary conditions. Open questions remain, highlighting the fundamental difference between configurations with and without phase boundaries.

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MS26

Twisting Elastic Annuli, SO(n) and the Lifting of Stationary Loops to the Spinor Groups

In this talk I will consider the equilibrium equations of elasticity for an incompressible material having the geometry of an annulus (in any dimension) and examine a family of maps rooted in geometry and topology, i.e., generalised twists, as possible solutions. The analysis leads to a surprising multiplicity versus non-existence result depending on the dimension being even or odd. I will then move on to discussing some qualitative features of the solutions in particular introduce and evaluate an associated topological invariant namely their spin degree.

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MS27

Effective Properties of Polydomain Liquid Crystal

Elastomers

The talk concerns polydomain liquid-crystal elastomers, materials are not homogeneous with each mesoscale region having a distinct preferred director orientation. We present a theoretical analysis of the overall or collective behavior of this heterogeneous medium starting from the neo-classical soft and semi-soft free energies for LCEs. We show that there is a significant difference between polydomains cross-linked in homogeneous high symmetry states then cooled to low symmetry polydomain states and those cross-linked directly in the low symmetry polydomain state.

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MS27

Recent Results on the Mechanical Response of Nematic Elastomers

We present recent analytical and numerical results on the mechanical response of nematic elastomers. These are based on two fully nonlinear elastic energies and on their small strain expansions in the regime of small strains and large director rotations. We compare the behavior they predict with the currently available experimental evidence, and discuss their relation with other models recently proposed in the theoretical literature.

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MS27

A Phase Field Approach to Modeling Nonequilibrium Liquid Crystal Elastomer Behavior

Liquid crystal elastomers exhibit a number of fascinating and important material characteristics for a number of engineering applications including for aerospace applications, adaptive optics, and robotics. This class of materials is characterized by unusual nonlinear, anisotropic mechanics and field-coupled material behavior including light or pH induced deformation, flexoelectricity, shape memory behavior, and electrostriction. The constitutive behavior is strongly dependent on the interactions between liquid crystal domain structure evolution and deformation of the host elastomer during electrical or mechanical loading, application of heat, or exposure to light or chemical constituents. This has motivated an analysis of the interplay between microscopic liquid crystal domains and the host elastomer network to fully utilize these materials in various artificial muscle and sensor applications. A phase field description of liquid crystals is developed and coupled to photoisomerization behavior and nonlinear mechanics of the host elastomer. This provides a relatively simple computational modeling strategy that is implemented within a finite element phase field framework. The effects of nonequilibrium domain structure evolution under mechanical loading and light exposure are modeled. Computational results illustrating nonlinear microstructure evolution during finite deformation and photoisomerization are presented.

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MS27

Modeling Shape Change and Microstructural Evolution in Nematic Elastomers via Finite Element Elastodynamics

When a nematic elastomer is subject to external strain, the sample's shape and microstructure may both evolve over time. To model the resulting mechanical response of these fascinating materials, we have developed a three-dimensional finite element elastodynamics simulation technique. We apply this method to study the mechanical response and microstructural evolution of nematic elastomers as a function of the sample's initial state, geometry, and applied strain rate. For initially monodomain samples under external strain, simulations show the formation of striped textures accompanied by a pronounced plateau in the force-displacement curve. For polydomain nematic elastomers, simulation shows that applied strain drives a polydomain to monodomain transition, but the resulting mechanical response depends sensitively on the sample's thermomechanical history. In particular, we explore the role of the "crosslink memory" effect, in which the local preferred nematic director orientation is patterned in the polymer network upon crosslinking. Our results suggest that this memory effect is far more pronounced in polydomain samples crosslinked in the nematic phase (N-PNE) than in those crosslinked in the isotropic phase (I-PNE). Our simulation results are in good qualitative agreement with observed differences in the stress-strain behaviors of N-PNE and I-PNE materials, as seen in recent experiments (K. Urayama, Macromolecules 2009).

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MS27

Angular Momentum Transport in Complex Fluids

In dye doped nematics, the threshold intensity for the optical Freedericksz transition can be dramatically reduced due to an optical ratchet mechanism. Dye molecules absorb light and rotate; angular momentum is transported from the cell walls via shear flow generated by the rotation

[P. Palffy-Muhoray, T. Kosa and Weinan E, "Brownian Motors in the Photoalignment of Liquid Crystals', *Appl. Phys. A* **75**, 293-300 (2002)]. We describe the transport of angular momentum caused by singular vortices which generate flow, and which are transported by the flow which they generate. We provide analytic and numerical solutions for the vorticity distribution in simple and non-Newtonian fluids.

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MS28

Evolution of Brittle Damage with Multiple Damaged States

We present a variational formulation for the evolution of brutal brittle damage for isotropic materials which extends the earlier work of Garroni and Larsen by permitting multiple damaged states. If time permits we shall also present results for anisotropic and continuous (ie. non-brutal) damage.

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MS28

Exact Results for Effective Tensors of Fiber-reinforced Elastic Composites via General Theory

Exact relations, or cases when effective tensors of composites satisfy certain equalities regardless of the microstructure, are well-known in the literature. The general theory of exact relations developed by Graeme Milton, Daniel Sage and Yury Grabovsky permits a complete description of all such cases. In this talk I will report on my recent work on exact relations for fiber-reinforced elastic composites.

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MS28

The Attainability of the Hashin-Shtrikman's Bounds for Multiphase Composites

This paper addresses the attainability of the Hashin-Shtrikman (HS) bounds for multiphase composites, including those of conductive materials and elastic materials. It presents a novel derivation of these bounds and a necessary and sufficient condition for attainment. A key idea is to focus on the optimal gradient field and the associated gradient Young measures. In particular we find a series of sufficient conditions such that the HS bounds are attainable or not attainable.

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MS28

Complete Characterization and Synthesis of the Dynamic Response of Spring-mass Networks

The response function of a network of springs and masses, an elastodynamic network, is the matrix valued function $W(\omega)$, depending on the frequency ω, mapping the displacements of some accessible or terminal nodes to the net forces at the terminals. We give necessary and sufficient conditions for a given function $W(\omega)$ to be the response function of an elastodynamic network, assuming there is no damping. In particular we construct an elastodynamic network that can mimic a suitable response in the frequency or time domain. Our characterization is valid for networks in three dimensions and also for planar networks, which are networks where all the elements, displacements and forces are in a plane. Additionally, we prove stability of the network response to the addition of springs with small spring constants, which may serve to eliminate floppy modes.

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MS29

Dynamic Modeling of Lipid Bilayer Membranes: Simulation Studies Relating Molecular Level Interactions and Bulk Material Properties

A model is developed for lipid bilayer membranes which takes into account microscopic interactions and dynamics at the level of individual lipid molecules. The model also takes into account hydrodynamic coupling between the lipid molecules, bilayer embedded particles, and the surrounding solvent fluid. To carry out the studies, new stochastic computational methods are introduced which utilized a mixed Eulerian and Lagrangian description of the physical system. Stochastic forcing terms are introduced to account for thermal fluctuations in a manner consistent with statistical mechanics. Dynamic simulations studies are carried out for the bilayer which relate molecular level interactions and kinetics to bulk material properties. Specific results are presented which characterize how molecular

level interactions contribute to bilayer mechanics (stiffness, tension, compressibility), bilayer rheology (shear viscosity, normal stress differences), and the mobility of bilayer embedded particles (single and pair diffusivity tensors). Applications of the bilayer model and computational methods to problems in cell biology are also discussed.

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MS29

Studying the Thermodynamic Folding Characteristics of Peptides Using Coarse-grained Simulations

One of the central problems of computational biology is to predict the three-dimensional shape of proteins starting from their primary sequence of amino acids. I will show how one can use coarse-grained simulations to address certain aspects of this problem which are amenable to a simplified biophysical analysis, and how well-known (but not widely used) thermodynamic principles can be employed to shed further light on it. I will also point out the problems and suggest ways to overcome them.

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MS29

An Implicit Interface Formulation of the Stochastic Immersed Boundary Method

We present the derivation and some mathematical analysis of the recently proposed stochastic implicit interface models for an elastic interface immersed in a background fluid subject to fluctuation forces. This provides an implicit interface formulation of the stochastic immersed boundary methods. We discuss the implication of the fluctuation-dissipation theorem and present suitable a priori estimates and the well-posedness of pathwise solutions for a couple of different elastic energy functionals and an incompressible Stokes fluid.

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MS29

Fluid-structure Interactions in Flagella and Cilia

Flagella and cilia are used by microorganisms to swim. A complete understanding of the mechanics of flagella requires integrating the physics from the molecular scale of the driving motors with the fluid mechanics of flagella. In this talk I will describe several problems from flagellar mechanics, such as the determination of the shape of a model rotating flagellum, and how hydrodynamic interactions lead to synchronization of nearby beating cilia.

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MS30

Domain Decomposition for Nonlocal Problems

We generalize iterative substructuring methods to nonlocal settings and characterize the impact of nonlocality upon the scalability of these methods. We present a nonlocal variational formulation and establish spectral equivalences to characterize conditioning of the underlying stiffness matrix and the Schur complement by proving a nonlocal Poincare inequality. Furthermore, we introduce a nonlocal two-domain variational formulation utilizing nonlocal transmission conditions, and prove equivalence with the single-domain formulation, a first step in establishing rigorous theory for nonlocal domain decomposition methods.

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MS30

A Nonlocal Vector Calculus with Application to Nonlocal Boundary Value Problems

We develop a calculus for nonlocal operators that mimics Gauss' theorem and the Green's identities of the classical vector calculus for scalar functions. The operators we treat do not involve the gradient of the scalar function. We then apply the nonlocal calculus to define variational formulations of nonlocal "boundary' value problems that mimic the Dirichlet and Neumann problems for second-order scalar elliptic partial differential equations. For the nonlocal variational problems, we derive fundamental solutions, show how one can derive existence and uniqueness results, and state conditions under which the solution is a member of a fractional Sobolev space.

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MS30

Length Scales and Time Scales in Peridynamics

The peridynamic theory of continuum mechanics is based on integro-differential equations that model interactions within groups of particles over finite distances. These distances provide a length scale within the theory. The boundedness of the dispersion curves for peridynamic materials results in a time scale that emerges naturally from a given length scale. This talk will explore the origins and significance of peridynamic length and time scales in numerical discretization and predictions of physical phenomena.

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MS30

Green's Functions in Non-local Three-dimensional Linear Elasticity

In this talk small deformations due to the presence of point loads in a linear locally elastic body are compared to the corresponding deformations in the peridynamic, non-local formulation. Owing to the linearity of the problem, the response to a point load can then be used to obtain the response to general body force loading functions by superposition. Using Laplace and Fourier transforms, an integral representation for the dynamic three-dimensional peridynamic solution is obtained with the help of Greens functions. This new theoretical result is illustrated by dynamic and static examples in one and three dimensions. It is demonstrated that the non-local peridynamic formulation regularizes the singular response encoutered in local elasticity.

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MS31

Modeling Thermal Based Damage Detection in Porous Materials

We use the heat equation to simuate a thermal interrogation method for detecting damage in porous materials, which is being developed in collaboration with scientists at NASA Langley Research Center. We first use probability schemes to randomly generate pores in a sample material; then we simulate flash-heating of the compartment along one of the boundaries with and without damage due to oxidation which is represented with a large ellipse. We will discuss the computational complexity from the complicated geometry of the porosity. We then investigate techniques from homogenization theory to alleviate this problem by approximating the thermal effect of the porosity with a matrix A^{Ω} in the conductivity term of the heat equation. We compare this approximation with the results of the simulations.

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MS31

Model Development and Analysis of Granular Avalanches

A model developed by Gray and Thornton (2005) is used to describe the phenomen of particle-size segregation in granular avalanches. In my presentation, we study the formation of shocks, which are jumps in the concentration of dissimilar particles, as well as the mixing zone that results from a shock breaking. Finally, I will talk about the lab experiment that has been run to show how well the model performs in reality.

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MS31

Analysis of Preisach and Homogenized Energy Models for Ferroic Compounds

There presently exist a number of modeling frameworks to quantify hysteresis in ferromagnetic, ferroelectric and ferroelastic (ferroic) compounds including Preisach, Prandtl-Ishlinskii and homogenized energy models. Whereas the formulations differ, all are comprised of kernels integrated against density functions quantifying the distributions of various parameters. In this talk, we will discuss the similarities and differences between these models and indicate the degreee to which unifying frameworks can be constructed. Attributes of the models will be illustrated through comparison with experimental data.

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MS31

A Fast Quadrature Method for the Continuous Spectrum Biphasic Poroviscoelastic Model of Cartilage

The talk presents a new fast numerical method for the continuous poroviscoelastic model of soft tissue. The reduced continuous stress-relaxation function is approximated with high accuracy by a Gauss-Legendre integration formula. This leads to an update rule for the stress-strain integral with similar accuracy compared to the full method but a reduction of the computational cost from $O(N^2)$ to $O(N)$. Numerical results and comparison to other methods are presented.

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MS32

Is Step-flow Epitaxial Growth Ever Stable Against

Bunching and Meandering?

Recent experiments have established that bunching and meandering instabilities coexist during step flow, in contrast to the predictions of existing Burton–Cabrera–Frank models. Indeed, in the BCF framework, meandering is predicated on an Ehrlich–Schwoebel barrier whereas bunching requires an inverse ES effect. The two appear therefore to be mutually exclusive. Herein, an alternative theory is presented that resolves this apparent paradox. Its main ingredient is a generalized Gibbs–Thomson relation, derived via an energy-rate calculation and resulting in jump conditions that couple adjacent terraces. Specialization to a periodic step train reveals a competition between the stabilizing ES kinetics and a destabilizing energetic correction that leads to step collisions. This can be understood in terms of the tendency of the thin film to minimize its total grand canonical potential.

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MS32

Anti-coarsening of Step Bunches with Non-conserved Dynamics

Step bunching is a ubiquitous morphological instability of vicinal crystal surfaces that occurs during nonequilibrium processes such as growth, sublimation or surface electromigation. In the standard scenario, bunching is initiated at a small length scale determined by the linear instability and proceeds by the unlimited coarsening of bunches, often characterized by a power law growth of the mean bunch size. Here we point out that the reverse process, the breakup of a large bunch into several smaller bunches, occurs generically in situations (such as sublimation with or without electromigration) where the step dynamics is coupled to the change of the total volume of the film. Extensive simulations of a discrete step model are presented in combination with a phenomenological continuum theory. The talk is based on joint work with Marian Ivanov and Vladislav Popkov.

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MS32

Dewetting of Ultra-Thin Solid Films

The dewetting dynamics of ultra-thin solid films is discussed. The dynamics is found to be controlled by atomic step formation and motion. Two regimes are found: layer-by-layer dewetting, and a regime with a facetted rim. A analytical model is obtained, which is in quantitative agreement with Kinetic Monte Carlo Simulations. The stability of the dewetting fronts is also discussed. Finally we discuss the relevance of these results for experiments.

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MS32

Linear Stability Analysis and Phase-Field Simulations of Step Flow Dynamics

We examine the dynamics of step flow growth using a linear stability analysis and a phase-field model that include the effects of the Ehrlich-Schwoebel Barrier and elastic stress. We summarize the instabilities observed from the linear stability analysis, including the transition between patterned and random morphologies. The full simulations using the phase-field model provide the evolution of the step morphologies beyond the linear regime.

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MS33

Localized and Propagating Oscillation Modes for Spin-torque Induced Magnetic Excitations in Structures with Different Dimensionalities

In this talk we present an overview of localized and propagating magnetization oscillation modes, excited in magnetic elements of various dimensionality (nanodots, nanowires, extended films) due to the torque induced by spin injection. The mode nature qualitatively depends on the system dimensionality, current strength, current-flooded area size, stray field from other layers, Oersted field. Qualitatively different localized modes (relatively homogenous 'bullet mode', highly inhomogeneous vortex and vortex-antivortex pair modes) can be excited when these parameters are varied.

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MS33

Nonlinear Magnetization Dynamics and Spin-wave Instabilities in Magnetic Nanostructures

The discovery that large-amplitude magnetization motions can be induced by spin-polarized electron currents through spin-transfer torques has generated renewed attention on Landau-Lifshitz equation for magnetization dynamics. The analysis of the stability of magnetization motions induced by time-dependent magnetic fields or by spin-transfer torques leads to the introduction of a generalized notion of spin-wave, applicable to far-from-equilibrium conditions. On this basis, analytical predictions are obtained for the onset of spin-wave instabilities in large magnetization motions. These instabilities can be viewed as the far-from-equilibrium generalization of Suhl's instabilities occurring in ferromagnetic resonance. These results are compared with numerical simulations of Landau-Lifshitz dynamics in sub-micron magnetic elements.

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MS33

Modelling Spin Transfer Induced Dynamics in Point Contact Devices

Micromagnetic modelling of point contact devices is not straightforward because the computational region one can realistically consider is typically one order of magnitude smaller than the lateral dimensions of the real device. Therefore, depending on the features of the dynamics under study, some ad-hoc techniques are to be developed in order to avoid unphysical effects due the computational boundary. For instance, if a propagating linear mode is excited, spin wave reflections at the boundaries need to be minimized. On the other hand, if a localized vortex is oscillating around the point contact in a well defined orbit, the charges in the boundaries need to be removed. I will discuss how with these ad-hoc techniques one can satisfactorily simulate point-contact devices. The results are compared to some recent experimental data.

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MS33

The Effect of Disorder on Domain Wall Propagation in Magnetic Wires

The dynamics of magnetic domain wall structures driven by fields or currents is a subject of practical importance related to possible schemes for nanoscale magnetic memory devices. Experimental results are typically interpreted in comparison to ideal models that ignore the effects of extrinsic disorder and internal dynamics of domain wall structures. To understand the effect of disorder and internal dynamics, we study the dynamics of vortex wall propagation driven by fields or currents, and vortex wall gyration driven by an external magnetic field pulse in the presence of extrinsic random potential. We analyze micromagnetic simulations using ideal models and observe that effective damping increases due to the disorder.

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MS34

Some Problems in Heterogeneous Griffith Fracture

We describe some examples of Griffith fracture in a microstructured material, and how the effective macroscopic behavior can be very different from what might be expected. In particular, considering Griffith fracture in a material with elastic properties obtained by homogenizing the elastic properties of the microstructured material, and fracture toughness obtained as a function of only the toughnesses of the microstructured material, will not in general produce the correct behavior.

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MS34

Strong Deformations of and at Soft Interfaces

I will discuss some simple examples of how soft interfaces behave when strongly deformed. I will start by considering how a thin film peels off from a substrate to which it is adhered in the presence and absence of a fluid. I will then move to the question of how creases form on soft interfaces, and then close with the question of how cracks and cuts appear at such an interface. In each example, geometry and physics meld with each other interestingly and lead to a rich variety of mathematical problems.

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MS34

The Time-dependent von Kármán Plate Equation as a Limit of 3d Nonlinear Elasticity

In this talk we discuss the asymptotic behaviour of solutions of three-dimensional nonlinear elastodynamics in a thin plate, as the thickness of the plate tends to zero. Under appropriate scalings of the applied force and of the initial values, we prove existence of strong solutions for large times and sufficiently small thickness and we show their convergence to solutions of the time-dependent von Kármán plate equation.

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MS34

Universal Interfacial Morphologies near Topological Singularities in Materials

It is well known that interfacial energy will induce a rod of one phase embedded in another to develop undulations by the well-known Rayleigh instability. We show that sufficiently close to the pinching event the interfacial morphology for systems evolving by interface-energy-driven bulk diffusion becomes universal, independent of the initial morphology and material system. We find an excellent agreement between theory and experiment in both the morphology and the kinetics of the pinching process

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MS35

Linear Stability and the Role of Rotational Diffusion for Active Suspensions

The dynamics of active suspensions has been modeled through a modification of Doi rod theory. We investigate the structure of this system linearized near a state of isotropy and uniformity. We show that while long-wave instability depends upon the swimming mechanism, short-wave stability does not. Further, we find a critical volume concentration or system size for the onset of instabilities in the presence of both rotational and translational diffusion.

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MS35

Hydrodynamics of Active Suspensions: Instabilities and Rheology

Bacterial suspensions and extracts of cytoskeletal filaments and motor proteins are examples of assemblies of interacting self-driven units that form active fluids. These systems exhibit fascinating collective behavior, including nonequilibrium phase transitions and pattern formation. In this talk I will review our work on using nonequilibrium statistical physics to derive a continuum description of active suspensions from specific models of single particle dynamics, highlighting the role of physical interactions in controlling the large-scale behavior.

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MS35

Hydrodynamics of Active Fluids: Pattern Formation and Phase Transitions in Bacterial Suspensions

I will present simulations of the hydrodynamics of active bacterial fluids. Firstly, I will discuss concentrated active gels, which undergo a transition between a passive and a spontaneously flowing phase at high enough density. Secondly, I will consider a run-and-tumble bacterial colony with logistic growth, where the swimming speed decreases with density. If the velocity decrease is strong enough, the system forms patterns usually attributed to chemotaxis,

but in the absence of any diffusing chemical.

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MS35
Active Films, Drops and Filaments

The study of self-driven particles, such as cytoskeletal filaments with motors, pumps in biomembranes, or swimming organisms, is a new frontier in the hydrodynamics of suspensions. In my talk I will focus on the unique phenomena engendered by the presence of active contractile or tensile force dipoles in Stokesian fluids, in thin-film, strand and droplet geometries. The results I will present include waves, surface-undulation instabilities, and anomalous spreading laws.

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MS35
Modeling and Simulation of Biologically Active Suspensions

Active suspensions, of which a bath of swimming bacteria is a paradigmatic example, are fluid systems whose microstructure is motile, and constitute a fundamental example of nonequilibrium pattern-forming systems. In this work, we apply a kinetic theory previously developed by Saintillan and Shelley (Phys. Fluids **20**, 123304, 2008) to study the nonlinear dynamics and pattern formation in active suspensions in a variety of situations. We first consider the case of a uniform isotropic suspension, where we show using a linear stability analysis that long-wavelength fluctuations are unstable as a result of hydrodynamic interactions. The long-time dynamics and pattern formation are studied using large-scale three-dimensional numerical simulations, where we report results on the coherent structures that are seen to appear and their relation to the disturbance flows driven by the particles. Second, we extend this study to investigate the effects of an external shear flow: in this case, it is found using a stability analysis that the external flow is stabilizing at high shear rates, and nonlinear simulations demonstrate the existence of several regimes of instability at low and moderate shear rates.

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MS36
Ideal Cloaking and Local Density of States

We discuss cloaking or hiding the objects from detection by electromagnetic probes, and means of detecting cloaked objects. Among these are passive schemes, whereby radiation absorbed and then reradiated at different wavelengths is detected. To study these, we calculate the Local Density of States (LDOS) of the cloaking system as a function of position and frequency, which quantifies the radiative ability of sources. We derive LDOS from Green's functions and illustrate its properties.

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MS36
Limits to Cloaking and Optical Devices

For cloaking, we show that causal cloaking is generally impossible, regardless of the material used. It is easily discoverable by pulsed probing. We also show how perfect cloaking can be approached. For optical devices, we prove a fundamental bound that depends only on the maximum variation of dielectric constant and the physical volumes involved, independent of the design details, and show applications to slow light, dispersion and volume holography.

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MS36
Cloaking Via Change of Variables for the Helmholtz Equation in the Whole Spaces

In this talk, I will discuss a cloaking device which is composed of a standard near cloak based on a regularization of the transformation optics, and a fixed lossy-layer, for the Helmholtz equation in the whole space of dimension 2 or 3. Two important features of this problem will be presented: i) degree of near invisibility, ii) necessity of the lossy-layer. A similar problem for a bounded domain was previously studied by Kohn-Onofrei-Vogelius-Weinstein.

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MS36
Approximate Cloaking for the Helmholtz Equation

I shall give a brief review of the estimates that may obtained for the effect of a very natural approximate cloaking scheme. The particular cloaking scheme is of the "cloaking-by-mapping" type, and efficacy estimates have been obtained at all frequencies. This represents joint work with Kohn, Onofrei, Weinstein and Nguyen.

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MS37
Some Recent Progress on Quantum Simulations

Abstract not available at time of publication.

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MS37

Continuue Limit for the Electronic Structure Models

We analyze the electronic structure of smoothly or elastically deformed crystals by studying various quantum mechanics models at different levels of complexity, including the Kohn-Sham density functional theory, Thomas-Fermi type of models and tight-binding models. Our overall objective is to establish the microscopic foundation of the continuum theories of solids, such as the nonlinear elasticity theory and the theory of piezoelectric or magnetic materials, in terms of quantum mechanics and to examine the boundary where the continuum theories break down. This is joint work with Jianfeng Lu of NYU.

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MS37

Heuristics for Accelerating Electronic Structure Calculation

Under the Kohn-Sham density functional theory framework, the electron density ρ associated with a ground state atomistic system can be obtained by solving the nonlinear equation $\rho = f(H(\rho))$ where f is the Fermi-Dirac distribution function and H is the Kohn-Sham Hamiltonian. One way to solve this nonlinear equation is to apply a Broyden type of method. I will discuss a number of heuristics for constructing an effective Jacobian approximation and efficient ways to evaluate $f(H(\rho))$.

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MS37

Some Recent Progress in Fast Algorithms for DFT Calculation

Abstract not available at time of publication.

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MS38

Dislocation Mobility and Stiffness in Dislocation Dynamics

Crystal's ability to withstand applied loads is ultimately defined by the behavior of lattice dislocations. The method of Dislocation Dynamics (DD) seeks to compute plastic response of a crystalline material directly from the motion of interacting dislocations lines. This is achieved by forward integration of coupled equations of motion (ODE) for dislocation segments and/or nodes. The resulting set of equations can be more or less stiff depending on the type of material and dislocation motion mechanisms. This presentation will describe several physical sources of ODE stiffness in Dislocations Dynamics, including anisotropy of dislocation mobility as a function of line and slip plane orientations, elastic anisotropy and dislocation collisions.

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MS38

Dislocation Dynamics in Micro-Pillars and Thin Films

Understanding plasticity and strength of crystalline materials in terms of the dynamics of microscopic defects has been a goal of materials research in the last seventy years. The size-dependent yield stress observed in recent experiments of sub-micrometer metallic pillars provides a unique opportunity to test our theoretical models, allowing the predictions from defect dynamics simulations to be directly compared with mechanical strength measurements. The balance between the dislocation multiplication rate and exhaustion rate (at the surface) may be the key to understand the observed size effect in flow stress. Here we report two counterintuitive observations from Molecular Dynamics and Dislocation Dynamics simulations. In body-centered-cubic (BCC) metals, the surface itself is sufficient to induce dislocation multiplication as a single dislocation moves across the pillar. In face-centered-cubic (FCC) metal pillars and thin films, however, even jogs of the Lomer-Cottrell type are not strong enough pinning points to cause dislocation multiplication. These results highlight the need for better calibration of Dislocation Dynamics models against the more fundamental atomistic models.

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MS38

Ginzburg-Landau-type Energy of a Crystalline Lattice with Defects

We propose a Ginzburg-Landau-type energy functional that describes a crystalline lattice with defects. The motion of dislocations can be described as a gradient flow for this energy; we show that the predicted dynamics corresponds to the known results for the standard models.

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MS38

Atomic Diffusion in Dislocation Cores Studied by Molecular Dynamics

We report on molecular dynamics simulations of self-diffusion along screw and edge dislocations, both isolated and assembled in low-angle grain boundaries. While vacancy migration is confirmed to be the most important diffusion mechanism, the unexpected finding is that diffusion can occur without pre-existing point defects. This intrinsic diffusion mechanism is mediated by dynamic vacancy-

interstitial pairs whose activation can be assisted by thermal jogs. The dislocation interactions in low-angle boundaries result in acceleration of dislocation diffusion.

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MS39

On a Mean Field Model for 1D Thin Film Droplet Coarsening

A thin liquid film coating a solid substrate is unstable and the late stage morphology is essentially quasiequilibrium droplets connected by an ultra thin film. Droplets exchange mass and coarsening occurs – the total number of droplets $N(t)$ decreases while the average size of droplets increases. It is predicted that $N(t)$ obeys a power law $N(t) \sim t^{-2/5}$ in the 1D case. We study a mean field model proposed by Gratton and Witelski for the one-dimensional thin film coarsening and prove a universal one-sided bound on $N(t)$ that partially justifies the power law. A corresponding bound on the average drop size is also obtained. Then we study the relation of this model and the mean field model for Ostwald ripening and show that they are equivalent after a nonlinear rescaling of time. Finally we present some further estimates on the coarsening rates for the Ostwald ripening.

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MS39

Novel Coarsening Kinetics for Islands on Surfaces: Effects of Anisotropy, Quantum Size Effects, and Additives

Metal islands on surfaces in homoepitaxial fcc(111) systems often provide ideal examples of 2D Ostwald ripening limited by isotropic terrace diffusion. LSW theory describes such details as the decay of individual small islands [Thiel et al., J. Phys. Chem. C 113 (2009) 5047]. We describe the refinement of LSW theory to treat more complex situations: (i) Introducing trace amounts of chemical additives can dramatically accelerate coarsening due to facile mass transport via metal-additive complexes. (ii) For homoepitaxial fcc(110) systems, diffusional and energetic anisotropies exist, and deviations from expected equilibrated island shapes occur. (iii) In heteroepitaxial systems, quantum size effects (QSE) can impact island structure and coarsening kinetics.

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MS39

The Theory of Herring Crystals: Morphology, Morphometrics, and Emergent Symmetries

Herring's model of crystal interface energy combines the (non-convex) orientation-dependant Wulff energy with a curvature penalisation. Herring crystals evolve when in contact with their melt through a fourth order hyperbolic-parabolic geometric evolution equation (GE). We demonstrate, contrary to expectation, that such Herring interfaces generally violate the classical Wulff construction. Further, we characterise the singular limit of GE, identify the associated scaling laws and scaling functions (morphometrics), and close with a curious emergent symmetry.

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MS39

Transient and Self-similar Dynamics in Thin Film Coarsening

The dynamics of arrays of droplets formed by the dewetting of viscous thin films on hydrophobic substrates can be reduced to a coarsening dynamical system (CDS) consisting of a set of coupled ODEs and deletion rules for when droplets vanish. We write a Lifshitz-Slyozov-Wagner-type (LSW) continuous mean-field model for the drop size distribution and compare it with simulations of discrete models derived from the CDS. Large transient deviations from self-similar LSW dynamics are shown to conform to bounds given by Kohn and Otto.

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MS40

Dynamics of Faceted Solid-liquid Interfaces Probed by Atomistic Simulations

This talk will discuss recent work involving the application of molecular dynamics simulations in the study of the dynamics of faceted solid-liquid interfaces in both bulk and nanometer-scale confined geometries. We discuss examples highlighting the ways in which the structural, thermodynamic and kinetic information derived from such simulations can be used both to parametrize and refine continuum theories for growth of faceted bulk and nanoscale crystals from the liquid state.

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MS40

Utilizing MD-based Information on Interfacial Dynamics to Understand Microstructure Evolution

Molecular dynamics can determine interfacial properties for specific boundaries. We discuss two modes of using mobility results. Interpolation in the 5-dimensional space of grain boundaries allows their incorporation into mesoscale models, but requires an appropriate metric and a sufficient density of data. The results can also be used to infer the presence of classes of values, in this case fast and slow boundaries. The presence of these classes provides insight into grain growth stagnation.

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MS40

The Composition Dependence of the Anisotropy in the Crystal-melt Interfacial Free Energy: A Progress Report

Recent phase field simulations have shown that the variation in the crystallographic growth direction of dendrites as a function of increasing solute concentration arises from an interplay between the four-fold and six-fold anisotropy parameters, which characterize the orientation dependence of the solid-liquid interfacial free energy. In this talk we will summarize several molecular dynamics simulation studies of the dependence of interfacial energy anisotropy on solute additions. Systems discussed include: Lennard-Jones, hard sphere, Al-Mg and Cu-Ag-Au.

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MS40

Surface Mechanics and its Coupling to Electronic Structure and Chemical Reactivity

Surface stress quantifies the elastic interaction of the matter at solid surfaces and interfaces with the adjacent regions of bulk solid. From a materials point of view, surface stress is relevant since balance equations for stress and chemical potential couple the simultaneous mechanical and chemical equilibrium in the material to its capillary parameters and to microstructural quantities such as surface net area, curvature, roughness, and orientation distribution as well as the net line length of step edges or triple lines. Furthermore, thermodynamics also suggests an important link between surface mechanics and reactivity.

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MS41

Step Evolution for Crystals of Finite Size

We study the step evolution of crystal structures relaxing toward flat surface when the number of steps is finite. The model is 1-dimensional and the rate limiting transport process is attachment-detachment limited (ADL). Starting with the step equations, we write down ODE's for the discrete slope of the profile. These are the l^2-steepest descent of an energy functional. Using this structure, we prove existence, uniqueness, and stability of the self-similar solution for profiles with "monotone' initial data.
We then propose a fourth order PDE whose natural discretization is the slope ODE's. We prove existence and uniqueness of a positive self-similar solution this continuum setting. Moreover, we give some qualitative features of the self-similar solution and the corresponding height profile.

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MS41

Understanding the Shape Evolution of Nanoscale Objects: Continuum Models from the Atomistics of Jets, Menisci, Catalyst Particles and Protective Coatings

Abstract not available at time of publication.

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MS41

Multi-scale Modeling of Ion-beam Irradiation: Linking Atomistic Simulation to Continuum PDEs

Energetic particle irradiation of solids – long used in industry for surface ultra-smoothening – can lead to nanoscale pattern formation under the right environmental conditions. The widespread use of this technology in current industrial settings for smoothening suggests the promise of

harnessing spontaneous pattern formation to create novel devices. However, existing theoretical models of ion irradiation fail to agree broadly with experiment even in the linear regime. To investigate this dilemma, we conduct molecular dynamics simulations of the average crater shape caused by ion bombardment of an initially flat silicon surface, and develop a multi-scale framework that directly predicts a parameter-free continuum PDE for the surface topography. Analysis of the PDE yields a parameter-free phase diagram for pattern formation and the characteristic wavelength as the incidence angle is varied. The results agree remarkably well with the pattern wavelength and transition angle between patterns and smoothening observed in experiments on silicon. In addition, they overturn the long-held assumption that pattern formation is due to the removal of target atoms by sputter erosion; instead, these phenomena are dominated by the impact-induced redistribution of target atoms that are not sputtered away.

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MS41

Continuum Model for the Long-range Elastic Interaction on Stepped Epitaxial Surfaces

In heteroepitaxy, the mismatch of lattice constants between the crystal film and the substrate causes misfit strain and stress in the bulk of the film, driving the surface of the film to self-organize into various nanostructures. Below the roughening transition temperature, an epitaxial surface consists of facets and steps and changes its morphology by lateral motion of steps. We present a 2+1-dimensional continuum model for the long range elastic interaction on stepped surface of a strained film. The continuum model is derived rigorously from the discrete model for the interaction of steps; thus it incorporates the discrete features of the stepped surfaces. We validate our model by performing linear stability analysis and numerical simulation in the nonlinear regime.

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MS42

Near Boundary Vortices in a Magnetic Ginzburg-Landau Model: Their Locations via Tight Energy Bounds

Given a bounded doubly connected domain $G \subset R^2$, we consider a minimization problem for the Ginzburg-Landau energy functional when the order parameter is constrained to take $\S^1$-values on ∂G and have degrees zero and one on the inner and outer connected components of ∂G, correspondingly. We identify intervals of the GL parameter where the minimizers always exist and never exist. For the critical values of the GL parameter we show limited locations of vortices (that correspond to the singularities of the limiting currents) by deriving tight upper and lower energy bounds. These locations are described via a scalar linear PDE problem in the entire domain G and therefore they are not determined by local characteristics of the boundary such as maximal curvature of of ∂G (as conjectured previously).

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MS42

Gauge Uniqueness of Solutions to the Ginzburg-Landau Equations of Superconductivity in Small Samples

In this talk, we present some results on the solutions of the Ginzburg-Landau system for small two-dimensional superconducting samples. We show that up to a gauge, the system has only two solutions: the normal and the vortex-less superconduting states. Additionally, we identify a critical field below which the vortex-less solution is the global minimizer and above which the normal solution is the only possible state.

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MS42

Some Remarks Regarding a Ginzburg-Landau Type Model for Liquid Crystals

We will discuss some results regarding the Landau De Gennes energy, often used to model liquid crystals, in the framework developed by Bethuel, Brezis and Helein for the Ginzburg-Landau energy of superconductivity. Our eventual aim is to describe the types of singularities allowed by this model.

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MS42

Order Parameter Models for Problems from Liquid Crystals

In this talk I will describe our work on order parameter models for liquid crystals where we investigate the structure of solutions and their defects.

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MS42

Variational Characterization of the Abrikosov Lattice

The Abrikosov Lattice is the name of the hexagonal lattice in the context of superconductivity, where superconducting vortices arrange themselves in this way. In a joint work with S.Serfaty we derive from the Ginzburg-Landau model an energy for configurations of points in the plane for which the optimal lattice is the Abrikosov lattice. The question of minimization among all possible configurations remains open.

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MS43

Discrete Inhomogeneous Materials

We study lattice models of inhomogeneous materials, deriving compatibility conditions, phase equilibrium and eigendeformation, effective properties of discrete composites and their lower bound, and discrete polyconvexity. We discuss similarity and difference of discrete and continuum models, homogenization, and lower limit of the size of a material grain.

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MS43

Patterns in Ferromagnetic Anti-ferromagnetic Spin Systems

We consider a simple variational model for a ferromagnetic anti-ferromagnetic spin system with nearest-neighbors and next-to-nearest-neighbors interactions. By tuning the interaction parameters the system develop, in the continuum limit, interfacial energies parameterized on the set of the ground states. We introduce a new set of phases and a phase transition energy to describe such a phenomenon. Finally, we briefly compare this model with its continuous counterpart.

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MS43

Sub-Wavelength Plasmonic Crystals: Dispersion Relations and Effective Properties

Plasmonic crystals are representative of a class of microstructured dielectrics known as meta-materials. The period of the meta-material crystal lies below the wavelength of illumination and the propagation of light is influenced by local electromagnetic field resonances on the length scale of the period. In this talk we report on recent work that develops a new type of power series expansion for the first branch of the dispersion relation for plasmonic crystals. The expansion parameter is given by the product kd where k is the wave number and d is the period of the crystal. Explicit error estimates show that a good approximation to the true dispersion relation is obtained using only a few terms of the expansion.

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MS43

A Geometric Approach to Bounds of Discrete Composites

Cherkaev and Rogora proposed a discrete approach to composites based on the concept of monad, A discrete composite is an arrangement of monads, glued together at their boundary points. The associated simplicial complex of a discrete composite covers the composite and each of its 2-dim simplexes contains one and only one monad. On the associated simplicial complex, discrete forms and the basic operators of exterior calculus can be define. The discrete wedge product allows one to define translators . We shall discuss for which kind of monads these translators can be used to get translation bounds as in continuum theory.

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MS44

Multiscale Science of Protein Materials in Extreme Conditions and Disease

Protein materials feature hierarchical structures, ranging from the atomistic, molecular to macroscopic scales to form functional biological tissues as diverse as silk, bone, skin, hair or cells. I will present integrated theoretical, computational and experimental multiscale materiomics studies,

focused on how protein materials deform and fail due to extreme mechanical conditions, disease and injuries. Specific focus is on collagenous tissues including tendon and bone, where we investigate the mechanisms of brittle bone disease *osteogenesis imperfecta*.

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MS44

Mechanics of Adhesion Between Elastic Mediua Via Molecular Bond Clusters: Implications on Cell Adhesion

Cell adhesion depends on the collective behavior of a large number of molecular bonds. While the behavior of a single molecular bond is governed by statistical mechanics, continuum mechanics should be valid at a large scale. How to model this transition and can this tell us something about mechanics of cell adhesion? With a long-term objective towards quantitative understanding of cell adhesion, we consider an idealized theoretical model of a cluster of molecular bonds between two dissimilar elastic media subjected to an applied tensile load. In this model, the distribution of interfacial traction is assumed to obey classical elastic equations while the rupture and rebinding of individual molecular bonds are governed by stochastic equations. Monte Carlo simulations that combine the elastic and stochastic equations are conducted to investigate the lifetime of the bond cluster as a function of the applied load. We show that the interfacial traction is generally non-uniform and for a given adhesion size, the average cluster lifetime asymptotically approaches infinity as the applied load is reduced to below a critical value, defined as the strength of the cluster. The effects of elastic moduli, adhesion size and rebinding rate on the cluster lifetime and strength are studied under strongly non-uniform distributions of interfacial traction. While overly simplified in a number of aspects, our model seems to give predictions that are consistent with relevant experimental observations on focal adhesion dynamics.

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MS44

Elasticity of Random Networks

We study the role of connectivity on the linear and nonlinear elastic behavior of amorphous systems using a two-dimensional random network of springs as a model system. A natural characterization of these systems arises in terms of the network coordination relative to that of an isostatic network δz; a floppy network has $\delta z < 0$, while a stiff network has $\delta z > 0$. We use numerical simulations to compute the exponents which characterize the onset of elasticity in these networks and also determine the scaling exponents for the shear modulus, the heterogeneity of the response, and the network stiffening as a function of δz. We also derive these theoretically and consider the effect of the probability distribution of the random network on the properties of these networks.

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MS44

Mesoscale Modeling of Cell Membrane-Mediated Trafficking

Trafficking of receptors and nanocarriers on cell membranes regulate important intracellular processes governing cell growth and hold promise in targeted drug delivery, but their optimization require accurate descriptions of hydrodynamics as well as dynamics of cell membranes. We will describe our computational approach for modeling protein-mediated membrane deformation as well as energy landscapes and hydrodynamic interactions in nanocarrier binding to cell membranes. The method consists of employing the time-dependent Ginzburg Landau approach for conformational sampling, flat histogram methods for defining the free energy landscape, and fluctuating hydrodynamics for quantifying the hydrodynamic interactions. From a biological standpoint, we describe the importance of cooperativity and spatial order in curvature inducing proteins and the effect of flexure, bond-stiffness in receptor-ligand interactions as well as the effect of shear force and resistance due to glycocalyx in binding and trafficking mechanisms.

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MS45

Defect Dynamics in Graphene

We have proposed a nonlinear lattice model for defects in graphene (single sheet of carbon atoms arranged in a hexagonal lattice) with overdamped or conservative dynamics. Solving numerically our model with initial and boundary conditions corresponding to edge dislocations and dislocation dipoles, we study the associated defect cores. Stable cores include pentagon-heptagon pairs and shuffle dislocations (octagons with a dangling bond). Stone-Wales defects are dynamically unstable, collapse and disappear. Recent experiments agree with our predictions.

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MS45

Nucleation of Defects and Incipient Plasticity in Crystals

By performing a bifurcation analysis in a lattice model of two dimensional nanoindentation we show that discontinuities in the load versus penetration depth curve correspond to the nucleation of dislocation loops. Another prediction of the model is the possibility of reversible homogeneous nucleation and annihilation of dislocation loops as the stress is released. Recent experiments confirm these predictions.

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MS45
Lattice Models in Fracture

Mass-spring and bending beam lattices are considered, and lattice fracture phenomena and the analytical technique are discussed. Crack resistance and continuum limit. Discrete and continuum fields coupling. Discrete versus continuum stress distributions. Lattice trapping and the local-to-global energy release ratio. Dynamic factor and crack speeds. Green's functions, causality principle, remote load and homogeneous equations. Dynamic-to-static crack growth transition and the related continuous-to-discrete transition of the Fourier transform.

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MS45
Continuum Linear Elasticity Theory with a Set of Internal Length Scales

We propose a method of constructing a series of nested continuum models, which describe linear elastic behavior of crystal lattices at successively smaller scales. The relevant scales are dictated by the interatomic interactions and are not arbitrary. The essence of the model is a decomposition of the displacement field into the coarse part and the micro-level corrections. The coarse contribution is the conventional homogenized displacement field used in classical continuum elasticity. The micro-level corrections are sub-continuum fields representing the fine structure of the boundary layers exhibited by the discrete equilibrium configuration. The model is based on a multi-point Pad approximation in the Fourier space of the Greens function for discrete problem. Joint work with M. Charlotte

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MS46
Far-from-equilibrium Growth of Multicomponent Films: Ni+Al/NiAl(110)

Homoepitaxial growth of single-element films (A on A) has provided an ideal testing ground for assessing the fundamentals of crystal growth. Equilibrated films have simple structure, but deposited films display complex morphologies reflecting kinetic limitations [Evans et al. Surf. Sci. Rep. 61 (2006) 1]. For homoepitaxial growth of binary alloys (A+B on AB), an additional issue is the interplay between growth morphology and alloy ordering. Several studies explored these issues using generic models with an idealized treatment of diffusion. However, morphology and ordering in systems driven out of equilibrium depends sensitively on the details of the diffusion kinetics. This motivated our development of a realistic atomistic model for deposition of Ni+Al on NiAl(110).

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MS46
Patterns in Strained Epitaxial Layers: Beyond the Frenkel-Kontrova Model

Although the structures of strained layers have been understood in terms of the classical Frenkel-Kontorova model, our work shows that these structures can have a quantum mechanical origin. We consider the striped phases of Ag on Pt(111). Using Monte Carlo simulations based on substrate-mediated Ag-Ag pair interactions obtained up to the 53^{rd} neighbor with DFT, we find striped phases with all the experimental characteristics. Angular variations in the potential are important in producing these phases.

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MS46
Nucleation, Growth, and Self-assembly of Strained Islands on Patterned Surfaces

Abstract not available at time of publication.

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MS46
Compositional Patterning in Alloy Nanostructures

Knowledge of composition profiles within alloy nanostructures such as heteroepitaxial nanowires, alloy nanocrystals/quantum dots and self-assembled surface patterns is critical for applications in electronic, photonic and memory devices as variations in composition at the nanoscale can substantially influence electronic and optical properties. Obtaining a quantitative description of composition profiles in these small-scale structures is a challenging task due to the complex coupling between composition variations, shape and long-range elastic interactions. In addition, differences in the bulk and surface transport properties of the alloy components can lead to rich pattering phenomena that cannot be observed in single-component systems. In this talk I will present efficient numerical schemes to study both equilibrium and far-from equilibrium composition profiles in alloy nanostructures. I will illustrate application of our methods for 1) determination of compositional patterning in strained alloy quantum dots, 2) analysis of the morphology and instabilities of heteroepitaxial nanowires and 3) the formation of compositionally modulated ripples during sputtering of alloy surfaces.

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MS47

Ultrafast Micromagnetics at Elevated Temperatures

It has recently been shown experimentally that magnetization reversal can occur following the application of circularly polarised laser light. The reversal mechanism (K. Vahaplar et al, Phys. Rev. Lett., 103, 117201 (2009)) involves a strongly non-uniform magnetization state achieved by heating close to T_c. We will describe a micromagnetic model based on the Landau-Lifshitz-Bloch equation. The model will be applied to the prediction of laser assisted reversal processes including opto-magnetic reversal.

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MS47

Strategies for the Efficient and Accurate Micromagnetic Modeling of Static Hysteresis Loops

The attention is focused on the computation of equilibrium states for the determination of static hysteresis loops of submicron samples. Starting from the space-time integration of the Landau-Lifshitz-Gilbert equation, the magnetization is time-updated by means of a norm-conserving algorithm based on Cayley transform. The analysis gives hints for the definition of a correct criterion of convergence towards equilibrium states and for the improvement of the numerical efficiency, exploring the possibility of reducing the simulation duration.

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MS47

The Magnetic Effect of Dislocations in Small Ferromagnetic Minerals

Dislocations have a major effect on magnetic hysteresis in large ferromagnetic crystals, but very little is known about their effect in nanocrystals. Any effect arises from the coupling between the magnetization and the strain field around the dislocation. Strain fields in finite crystals are difficult to calculate because of the boundary conditions. A new method is presented that solves the boundary value problem. Magnetic hysteresis curves are calculated for nanocrystals with screw and edge dislocations.

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MS47

Mathematical Treatment of Nanoscale Multilayer Materials: Is a Continuum Limit Useful?

Micromagnetic methods are well established for the treatment of homogeneous materials described by a bulk exchange constant A, and for discrete grains or layers coupled at their boundaries by a surface energy σ. In the latter case, magnetization variation within a grain is ignored. We have developed a consistent scheme involving both A and σ, in which $A \to \infty$ gives the usual discrete theory, and $\sigma \to \infty$ gives the continuum theory.

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MS48

Energy-minimizing Weak Solutions in Second-gradient Nonlinear Elasticity

We consider a class of second-gradient nonlinear elasticity models in which the stored energy density is assumed to grow unboundedly as the local volume ratio approaches zero. We provide a general setting in which the determinant of any admissible deformation with bounded energy is strictly positive on the closure of the domain. We obtain energy-minimizing weak solutions for a wide variety of mixed boundary conditions on bounded Lipshitz domains.

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MS48

A Quantitative Rigidity Result for the Cubic to Tetragonal Phase Transition in the Geometrically Linear Theory with Interfacial Energy

We are interested in the cubic to tetragonal phase transition in a shape memory alloy. We consider geometrically linear elasticity. In this framework, Dolzmann and Müller have shown the following rigidity result: The only stress-free configurations are (locally) twins (i.e. laminates of just two of the three Martensitic variants). However, configurations with arbitrarily small elastic energy are not necessarily close to these twins: The formation of microstructure allows to mix all three Martensitic variants at arbitrary volume fractions. In this paper, we take an interfacial energy into account and establish a (local) lower bound on elastic + interfacial energy in terms of the Martensitic volume fractions. The introduction of an interfacial energy introduces a length scale and thus, together with the linear dimensions of the sample, a non-dimensional parameter. Our lower Ansatz-free bound has optimal scaling in this parameter. It is the scaling predicted by a reduced model introduced and analyzed by Kohn and Müller with the purpose to describe the microstructure near an interface between Austenite and twinned Martensite. The optimal construction features branching of the Martensitic twins when approaching this interface.

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MS48

Everting Elastic Spherical Caps

It is common experience that a half tennis ball or a contact lense can be made to snap from a load-free and stress-free configuration into another loqd-free but not stress-free equilibrium configuration, characterized by a macroscopic change in sign of the mid-surface's curvature and a further curvature flipping localized about the rim. Such a snap instability is called eversion. A mathematical model that accounts for eversion is discussed.

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MS48

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MS49

Hydrogels and Microfluidic Devices

Hydrogels consist of crosslinked polymeric networks, holding fluid able to sustain ions. We propose a model based on mixture theory that the couples equations of elasticity and Navier Stokes that account for the mechanical properties of gels with the Nearst-Planck equations for ion transport. We apply the model to the design of a microfluidic valve activated by an alternating current.

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MS49

Undulation Instability in Smectic Liquid Crystals

We study layer undulations of smectic A liquid crystals when a magnetic field is applied in the direction parallel to smectic layers. Using the Landau-de Gennes model of smectic A liquid crystals, we characterize the critical field and obtain the asymptotic expression of unstable modes using the Γ-convergence theory. Under the assumption that the layers are fixed at the boundaries, the maximum undulation occurs in the middle of the cell and the displacement amplitude decreases as approaching the boundaries. We also obtain the estimate of the critical field, which is consistent with Helfrich-Hurault theory. With the natural boundary condition, however, the displacement amplitude weakly depends on the vertical z-coordinate and the critical field is reduced compared to the one calculated in the classic theory. This is consistent with the experiment done by Laverentovich. Numerical simulations will be presented to confirm the predictions of the analysis.

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MS49

Transient Rheological Responses in Sheared Biaxial Liquid Crystals

We study the rheological response of monodomain ellipsoidal biaxial liquid crystal polymers as well as bent-core or V-shaped liquid crystal polymers subject to steady and time-dependent small amplitude oscillatory shear. Transient shear stresses and normal stress differences corresponding to steady and small amplitude oscillatory shear are investigated.

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MS49

Physical-Chemical Based Modeling of Biofilm Induced Mineralization

We consider the following biomineralization problem. Urea hydrolysis catalyzed by biofilm increases the pH value and produces carbonate ions. In the presence of calcium ions, calcite ($CaCO_3$) will precipitate and form crystal once its saturation index exceeds certain critical value. We present a mathematical model including the important chemical, physican and biological processes (Ureolysis and pH value change, advection, diffusion and crystal precipitation, biofilm growth and deformation) involved in the problem. Some computation results and discussion will also be given.

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MS49

Kinetic Structure Simuations of Nematic Polymers in Shear

We numerically simulate the structure formation of nematic rigid-rod liquid crystalline polymers confined in a Couette cell using the kinetic model equations coupled with the Navier-Stokes equation. The transient defect cores associated with the flow for large Erickson number will be examined in detail.

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MS50

Phase-Field Modelling of Bi-Crystal Grain Boundaries via an Orientation Parameter

Grain Boundaries are of paramount importance in Materials Science; they influence the macroscopic properties of materials in very profound ways such as tensile strength and creep. Thus, the ability to accurately describe their behavior and extract material properties from their behavior is important. In this talk, we present a phase-field model that incorporates the effect of temperature of the structure and free energy of grain boundaries in order to describe the behavior of grain boundaries. The model was obtained

numerically using a copper bicrystal with symmetrical tilt grain boundaries of different misorientaion angles. To evaluate the accuracy of this phase-field model, its solutions will be compared with molecular dynamics simulations of the same set of grain boundaries.

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MS50

A Level Set Simulation of Theta Phase Dissolution in Al-Cu Alloys

A common approach to particle dissolution is the phase-field approach which is based on the minimization of a free energy function over a diffuse interface. Although recent studies have shown agreement between a phase-field approach and sharp interface approach, the diffuse interface is unrealistic and the free energy function parameters are difficult to obtain. The level set method is one of the several numerical methods available for solving Stefan problems with a sharp interface. It is also capable of handling complex topological changes that allow particle break-up in a natural way. The goal is this study is to replicate the sharp interface diffusion obtained from the software package DICTRA for theta phase particle dissolution in Al-Cu alloys. The results from two-dimensional and three-dimensional models using the level set method are then compared with experimental data.

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MS50

Modeling Phase Separation in Ternary Alloys

Alloys have many desirable properties and numerous applications, however sometimes nature combats their use with phenomena known as phase separation. Specifically, we examine a type of phase separation called nucleation which occurs after an alloy is quenched. Nucleation is characterized by the formation of discrete droplets of an individual material speckled throughout the otherwise homogeneous domain; this process weakens the composition and diminishes the value of the material. We model this phenomenon using the Cahn-Morral system by employing numerical continuation via AUTO. We discuss the model, associated numerical techniques, and comparison of nonlinearities.

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MS50

Toward Accurate Computation of Ternary Phase Diagrams Using Low-discrepancy Sequences

The effective and accurate computation of phase diagrams plays a critical role in allowing materials scientists to fully exploit the potential of cutting-edge manufacturing technology. It is currently possible to compute satisfactory phase diagrams for simple materials, however multi- component materials are proving to be less tractable. Our work focuses on these complicated systems, and in scenarios where existing techniques fail. We explore methods that do not require difficult-to-obtain a priori knowledge of the system, and employ sampling techniques that do not require a uniform domain discretization. Specifically, we employ adaptive search methods, and sample the domain using low-discrepancy sequences. Various combinations of these methods will be compared with each other and with conventional techniques.

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MS51

Multiscale Modeling and Simulation of Multi-walled Carbon Nanotubes (MWCNTs)

We will review recently developed models for multiwalled carbon nanotubes, hierarchically built from the atomistic interactions up to mesoscopic scales. These include surface models, foliation models, and non-linear phase-transforming elastica models. These models serve as the basis for efficient simulations, which are able to make a direct connection with the experimental observations.

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MS51

Finite-Temperature Extension of the Quasicontinuum Method based on Langevin Dynamics

The concurrent bridging of molecular dynamics and continuum thermodynamics remains one of the most challenging problems in multi-scale material modeling. The challenge lays in being able to derive an accurate description of the energy transfer across all length-scales involved. We propose a framework for simulating coarse-grained dynamic systems in the canonical ensemble using the Quasicontinuum method (QC). The equations of motion are expressed in reduced QC coordinates and are derived from dissipative Lagrangian mechanics. The derivation naturally leads to a classical Langevin implementation where the time-scale is governed by vibrations emanating from the finest length scale occurring in the computational cell. The equations of motion are integrated by recourse to Newmark's method, which is parametrized to ensure over-damped dynamics. Thus, spurious heating due to reflected vibrations is suppressed, leading to stable canonical trajectories. To estimate the errors introduced by the QC reduction in the resulting dynamics, we quantify the vibrational entropy losses in Al uniform meshes by calculating the thermal expansion coefficient for a number of conditions. The limitations of the method and alternatives to mitigate the errors introduced by coarsening will also be discussed.

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MS51

Finite Temperature Coarse-graining of Atomistic Models: Some Simple Cases

Molecular dynamics is a classical method to simulate materials at constant temperature. For instance, the evolution of an atomistic system according to the Langevin equation is simulated, while some relevant observables are averaged along the trajectory. On the basis of such a microscopic

model, macroscopic quantities can be computed. It is often the case that interesting observables actually do not depend on all the particles, but only on the position of some of them. In this case, it is natural to try and design a strategy to compute more efficiently the quantities under study. We will review some recent progress on that question. Efficient methods will be described, that are supported by rigorous error analysis. Numerical simulations will illustrate the obtained theoretical results.

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MS51

Multiscale Modeling of Surface-Induced Instabilities in Nanomaterials

The objective of the present work is to investigate the recently-developed Wallace instability criterion with a particular emphasis on studying defect nucleation and instabilities arising from the failure of nanomaterial surfaces. We study this within the context of FCC metals using both a mode Lennard-Jones potential, as well as a realistic embedded atom (EAM) potential.

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MS52

Simulating Fracture Interfaces with Curvature Dependent Surface Tension

The classical theory of linear elastic fracture mechanics for static cracks in an infinite linear elastic body has two significant defects: it predicts unbounded crack-tip stresses and elliptical crack opening profiles. A new model of fracture based on extending continuum mechanics to the nanoscale corrects these anomalous effects, predicting finite crack-tip stresses and cusp-like opening profiles. We describe how this new fracture modeling paradigm can be implemented in a finite element analysis.

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MS52

Sublinear Scaling Algorithms for Electronic Structure Calculations

The electronic structure calculations based on Kohn-Sham density functional theory is limited to small systems due to its expensive computational cost. By coupling with continuum theory derived from the Kohn-Sham density functional theory, we develop a sublinear scaling algorithm for electronic structure calculations. This extends the solution of density functional theory to macroscopic systems with local defects. Joint work with Weinan E (Princeton) and Carlos Garcia-Cervera (UCSB).

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MS52

Fem for Geometric Problems: Application to Bio-Membranes and Shape Optimization in Continuous Mechanics

A parametric FEM for free boundary problems is discussed. Some applications include geometric and fluid-membrane interaction in bio-membranes. With slight modification the method can be successfully applied in shape optimization problems such the design of an obstacle with minimal drag or a cantilever with minimal compliance. The last in the context of inexact sequential quadratic programming. Inexactness is a consequence of using adaptive finite element methods (AFEM) to approximate the state equation, update the boundary, and compute the geometric functional.

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MS52

The Effect of Surface Tension in Modeling Fracture

The talk will focus on the analysis of a class of fracture models based on a new approach to modeling brittle fracture which incorporate molecular scale effects. Ascribing curvature-dependent surface tension to the fracture surfaces and using the appropriate crack surface boundary condition, given by the jump momentum balance, leads to bounded stresses. This allows for a fracture criterion based on Critical Crack Tip Stress, in addition to an energy based criterion.

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MS52

Debonding of a Material Interface

We discuss mixed mode de-bonding of a material interface within the context of a new theory of fracture incorporating curvature dependent crack surface tension and a mutual force correction to the balance of linear momentum within a thin region enveloping the interface. It is shown that once chemical bonds are broken, neither pure mode III (anti-plane shear) nor mode II (in-plane shear) deformations are possible even under pure anti-plane or in-plane shear loading leading to new crack growth criteria.

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MS53

Resonant
Properties of Complementary Filled Nanospheres and Nanocylinders: Optical Nanoswitch, Focusing and Extreme Anisotropy

We discuss here the closed-form analytical solution for inhomogeneous spheres and cylinders partially filled by plasmonic materials. We show that under proper conditions these nanoparticles may constitute optical nanoswitches, characterized by extremely anisotropic scattering behavior, or focusing devices. In our talk, we will provide mathematical details and physical insights into the anomalous optical response of these 2-D and 3-D nanostructures, and its interpretation in terms of optical nanocircuit theory.

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MS53

One-dimensional High-contrast Models and the Associated Defect Modes

Several recent works made an advance on the rigorous analysis of localised, or "defect', modes in mathematical models of photonic crystal fibres. One of the key geometric assumptions for the validity of the related results is that the "matrix' component of the high-contrast fibre cladding be a connected set. In the present talk we focus on the analogous 1D setting, where the above assumptions can not be fulfilled. We study the limit S of the spectra of the associated differential operators. One of the marked differences of our results from those in 2D is that, in the case of a fibre whose cross-section is bounded, the limiting set S contains a union of disjoint intervals. We also discuss the conditions under which defect modes emerge in this kind of 1D model.

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MS53

Focussing Bending Waves via Negative Refraction in Perforated Thin Plates

We propose a design of a periodically perforated thin plate leading to a lensing effect of bending waves via negative refraction. To achieve this goal, we first analyse the band spectrum of the bi-harmonic operator for an array of freely vibrating square voids using both numerical (finite elements) and asymptotic methods. We then find some point in the reciprocal space where the acoustic dispersion surface displays a convex isofrequency contour shrinking with frequency.

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MS53

More Defective Knowledge About Photonic Crystals

This talk describes recent progress in deriving semi-analytic models for defects created in photonic crystals, such a resonant cavities and waveguides. The presence of the defect modifies Bloch states of the perfect crystal, giving them an envelope function which gets broader and broader as the defect weakens. We derive analytic expressions for the envelope function, using perturbation ideas and the Luttinger-Kohn model from solid state physics. The semi-analytic results are verified using accurate electromagnetic theory numerical methods.

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MS54

Towards a Unified Statistical Theory of Texture Evolution in Polycrystals

We present an account of recent developments in mesoscale theory of texture evolution in polycrystalline materials. The talk will demonstrate how a carefully chosen combination of simulation, theory and modeling techniques can bring a deeper understanding to coarsening processes governed by the motion of triple junctions. By means of modulated stochastic process characterization and kinetic evolution equations, we will quantify the rates of grain boundary disappearance events and predict the influence of these events on macro-level materials properties. Comparison with large-scale 2D and 3D simulations will provide the necessary validation and reveal similarities and differences between these approaches.

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MS54

Grain Boundary Pore Interaction

The talk will focus on large-scale simulations of grain boundary pore interaction in three dimensions to capture the drag on grain boundaries when the pores move due to the presence of a temperature gradient. The simulations will be extended to three-dimensional grain structures to identify the path of a moving pore as a function of pore size, grain boundary character distribution and grain morphology. The application of the simulations to fission gas bubble evolution in nuclear fuels will be discussed.

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MS54

Challenges in Interpretation of Statistical Properties of Grain Growth Models

Polycrystalline materials are composed of small grains interconnected through a network of grain boundaries. Macroscopic properties of such materials including their response to mechanical and thermal loading are affected by the structure of the network of grains. It is expected that predictive macroscopic theories of such materials must include some features of the mesoscopic structure, yet the precise details are still unknown. Extensive work has been done on some statistical properties characterizing these networks. These include the well studied grain size distribution function, the grain orientation distribution function (texture), and more recently the grain boundary character distribution function. These functions are known to have important effect on macroscopic behavior, yet they are not stationary and may evolve as a result of loading. Therefore, it is important to understand their evolution on the proper time scales under relevant thermal and mechanical conditions. In this talk we will review some aspects of well studied distribution functions and discuss challenges in constructing theories for their evolution and their place in a macroscopic theory of material behavior. We will use simulation combined with analysis in our discussions of challenges and possible solutions.

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MS54

Are Grain Boundaries Like Glass?

It has long been hypothesized that GBs have features in common with glass-forming liquids based on the processing characteristics of polycrystalline materials. We ?nd remarkable support for this suggestion, as evidenced by string-like collective atomic motion and transient caging of atomic motion, and a non-Arrhenius GB mobility describing the average rate of large-scale GB displacement. Time permitting, I will also discuss a new model of creep in grain boundaries.

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MS55

A Grid Based Particle Method for Moving Interface Problems

We propose a novel algorithm for modeling interface motions. The interface is represented and is tracked using quasi-uniform meshless particles. These particles are sampled according to an underlying grid such that each particle is associated to a grid point which is in the neighborhood of the interface. The underlying grid provides an Eulerian reference and local sampling rate for particles on the interface. It also renders neighborhood information among the meshless particles for local reconstruction of the interface. The resulting algorithm, which is based on Lagrangian tracking using meshless particles with Eulerian reference grid, can naturally handle/control topological changes. Moreover, adaptive sampling of the interface can be achieved easily through local grid refinement with simple quad/oct-tree data structure.

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MS55

Phase Field Models of Fluids with Evaporation and Condensation

I will present phase field models of fluids undergoing evaporation and condensation with inhomogeneous temperature, where latent heat transport is crucial. I will also discuss Marangoni effect arising from the surface tension inhomogeneity in binary fluid mixtures. Evaporation, spreading, and boiling are examples of simulation.

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MS55

Phase Field Modeling and Simulation for Contact-Line Motion in One-Component Liquid-Gas Systems

The dynamic van der Waals theory has recently been presented for the study of hydrodynamics in liquid-gas systems. We derive the boundary conditions at the fluid-solid interface by introducing two dissipative processes on the solid surface and requiring the surface entropy production rate to be positive definite. We then carry out numerical simulations to investigate the quantitative effects of the boundary conditions on contact-line motion, with an emphasis on the fluid slip at solid surface.

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MS55

A New Phase-field Model for Incompressible Two-phase Flows with Large Density Ratios

We present a new phase-field model for the incompressible two-phase flows with variable density which admits an energy law. We also construct weakly coupled time discretization schemes that are energy stable. Efficient numerical implementations of these schemes are also presented. The model and the corresponding numerical schemes are particularly suited for incompressible flows with large density ratios. Ample numerical experiments are carried out to validate the correctness of these schemes and their accuracy.

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MS56

Branch-following and Bifurcation Methods for Crystals: A Study of Stability and Meta-stability in a One-dimensional Crystal Model

Branch-following and bifurcation (BFB) techniques are used to explore a one-dimensional crystal model of a phase transforming material. At bifurcation points group-theory methods are combined with an asymptotic analysis to determine all bifurcating branches. Multiple observable (stable) phases of the crystal are identified and this information is used to predict the strain-rate dependent material behavior. Molecular dynamics simulations at various deformation rates are performed and the results are compared and contrasted with the BFB predictions.

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MS56

Entropic Stabilization of Austenite in Shape Memory Alloys

Recent calculations have revealed that the observable high temperature austenite structure in shape memory alloys (SMAs) is *entropically stabilized* by nonlinear dynamic effects. The phenomenon of entropic stabilization in SMAs will be explicitly demonstrated with a *realistic three-dimensional all-atom model* using Molecular Dynamics (MD). Additionally, some observations about the transition pathways for the martensite to austenite and austenite to martensite transformations are discussed.

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MS56

Cavitation in Nonlinear Elastic Solids Under 3D Loading Conditions with Various Triaxilities

In this work, we study the problem of a single vacuous cavity of initially spherical shape embedded in a nonlinear elastic solid of infinite extent that is subjected to affine displacement loading conditions on its boundary, i.e., at infinity. By means of the Finite Element Method (FEM), we generate solutions for a variety of materials (including incompressible Neo-Hookean solids) and loading conditions (with various triaxilities) and analyze in detail the onset of cavitation corresponding to the event at which the size of the cavity grows unbounded.

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MS56

Shear Localization Instabilities in Porous Metals

Making use of a recently developed homogenization model for porous metals with evolving microstructure, we investigate the possible development of shear localization and cavitation instabilities. In particular, we explore the dependence of these different types of instabilities on the applied loading conditions, as characterized by the triaxiality (i.e., the ratio of the hydrostatic and deviatoric stresses) and the Lode angle (i.e., the third invariant), as well as on the elastic and plastic properties of the material.

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MS57

Transition Layers from the Normal to the Superconducting State in the Preence of Electric Currents

Abstract not available at time of publication.

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MS57

Meissner States of 3-Dimensional Superconductors and a Quasilinear System Involving Curl

Meissner state of bulk superconductors of type II loses its stability as the applied magnetic field increases to a critical field H_S. The Meissner states are described by the solutions of a partial differential system in 3-dimensional space, which are called Meissner solutions. In this talk we shall show the existence of the Meissner solutions, and examine the convergence of the Meissner solutions to a solution of the limiting system as the Ginzburg-Landau parameter increases to infinity. Our results suggest that in order to determine the critical field H_S one needs to measure the maximum value of the tangential component of the induced magnetic field on the surface of the superconductor.

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MS57

Ginzburg-Landau Vortex Dynamics Driven by an Applied Boundary Current

This talk concerns recent results on the time-dependent Ginzburg-Landau equations on a smooth, bounded 2-D domain, subject to both an applied magnetic field and an applied electrical current on the boundary. The energy of such solutions does not dissipate, but it is possible to estimate the growth of the energy in time. This estimate then allows for the derivation of the dynamics of the vortices in the limit as the Ginzburg-Landau parameter vanishes. In an appropriate time scale, we show that the vortex motion is driven by a novel Lorentz drift term induced by the presence of the applied boundary current.

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MS57

Quantized Vortices in Ginzburg-Landau Models with an Applied Current

We study the single-vortex solutions of a two-dimensional high-κ high-field Ginzburg-Landau model of superconductivity with a constant applied current. Under a nondegeneracy condition and for appropriate ranges of the applied magnetic field and applied current, we construct some special solutions which, up to a constant shift of phase in time, are the stationary solutions of the model equation. Our result provides partial justification to the existence of a critical applied current.

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MS58

Nonequilibrium Molecular Dynamics of Complex Structures using Objective Structures

The method of Objective Structures generalizes the notion of crystallinity to important non-crystalline nanostructures such as carbon nanotubes. This allows the calculation of properties of these nanostructures through efficient techniques developed for crystals. We apply the method to the non-equilibrium deformation and failure of carbon nanotubes at an imposed strain rate, using the Tersoff potential for carbon. Simulations with different strain rates ($10^4/s - 10^8/s$), temperatures and unit cells show that Stone-Wales defects play no role in the failure (though partials are sometimes seen just prior to failure), a variety of failure mechanisms is observed, and most simulations give a strain at failure of 15–20%, except those done with initial temperature above about 1200 K and at the lower strain rates. The latter have a strain at failure of 1–2%.

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MS58

A Quasicontinuum for Multilattice Crystals Exhibiting Martensitic Phase Transformations: Cascading Cauchy-Born Kinematics

The quasicontinuum (QC) method is a multiscale method coupling atomistic regions with a surrounding continuum modeled within a nonlinear finite element formulation. Application of QC to multilattice crystals is straightforward in principle, however a question arises as to which description of the crystal structure should be used with Cauchy-Born kinematics. Here a methodology referred to as *Cascading Cauchy-Born kinematics* is developed to detect deformations that require an increase in the periodic size of the unit cell. Applications to one- and $2\frac{1}{2}$-dimensional test problems that highlight the salient features will be presented.

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MS58

A Relation Between Compatibility and Hysteresis and its Role in the Search for New Active Materials

We present some recent measurements of hysteresis, in materials undergoing big first order phase transformations, that resulted from a systematic program of tuning of the lattice parameters by changing composition. The lattice parameters were tuned so that a certain non generic condition of compatibility between phases was satisfied. An exceptionally sharp drop of size of the hysteresis of the transformation was observed at the special lattice parameters. The data has some fascinating features, including an apparent singularity. We re-examine the origins of hysteresis in light of these measurements, commenting also on the role of defects and pinning, and the use of this kind of tuning to discover "unlikely" new materials. These thoughts lead us to consider hysteresis as arising from an elastic energy barrier associated with the failure of certain conditions of compatibility. We calculate this barrier based on methods of Gamma-convergence, where the small parameter is related to the near satisfaction of this non-generic condition of compatibility. A recent study suggest suggests a tantalizing relation between the emerging alloys with minimum hysteresis and stability of the transformation under cycling. Joint work with Stefan Mueller, Nick Schryvers and Jerry Zhang.

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MS58

Moving Interfaces in Rod-like Molecules as Agents of Conformational Change

We model coiled-coil molecules in viscous fluids as one-dimensional continua with a multi-well free energy. These molecules suffer a conformational change in response to large forces. We assume that the conformational change proceeds via a folded/unfolded interface that represents a jump in strain and is governed by the Abeyaratne-Knowles theory. The model agrees with experimental data on the melting transition in DNA and is able to predict the speed at which the interface moves.

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MS58

Waves in Lattice Models for Moving Interfaces and Macroscopic Implications

We study the motion of interfaces on the atomic (lattice) scale and seek to obtain related macroscopic information, for example kinetic relations. As the microscopic model, we consider a one-dimensional chain of atoms with nearest neighbour interaction, with the dynamics governed by Newton's law. To describe phase transitions, the elastic potential is chosen to be nonconvex in the discrete elastic strain. Travelling waves are particularly simple instances of moving interfaces. The topic of the talk is the existence and non-existence of travelling waves for 'heteroclinic' solutions, that is, solutions which explore both wells of the energy and thus have an interface moving with the speed of the wave. We will discuss the existence of waves and sketch a mathematical setting for the proof.

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MS59

Friction in F-actin Knots

We use existing data of force-extension experiments on F-actin molecules tied into knots to compute a value of 0.15 for the static friction coefficient for contact between different parts of the same molecule with itself. This estimate for protein-protein friction is relevant for the stabilization of the 273 known proteins with knots, one percent of the structures deposited in the Protein Data Bank.

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MS59

Mechanics of Myosin VI Molecular Motor and its Reverse Directionality

Myosin VI moves toward the (-) end of actin filaments, despite sharing extensive sequence and structural homology with (+) end directed myosins. We designed a range of myosin VI constructs with artificial lever arms to identify key structural elements dictating its reverse directionality. Using molecular dynamics simulation, we examined the mechanics in the converter domain of myosin VI. The results demonstrate that an alpha helix of 18 amino acids are enough to change the directionality.

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MS59

Heterorgeneous Fluctuating Rod Models for Unfolded Proteins and Application to Fibrin Networks

We present a theory to efficiently calculate the thermomechanical properties of fluctuating heterogeneous rods and chains and their networks. The central problem is to evaluate the partition function and free energy of a general heterogeneous chain/network under the assumption that its energy can be expressed as a quadratic function in the kinematic variables that characterize the configurations of the chain. The results from the model are verified through Monte Carlo simulations.

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MS59

Mechanics of the Power Stroke in Myosin II

Power stroke in skeletal muscles is a result of a conformational change in the globular portion of the molecular motor Myosin II. We show that the fast tension recovery data reflecting the inner working of the power stroke mechanism can be quantitatively reproduced by a Langevin dynamics of a simple mechanical system with only two structural states. The proposed model is a generalization of the two state model of Huxley and Simmons. The main idea which dates back to Eisenberg and Hill is to replace the rigid bi-stable device of Huxley and Simmons with an elastic bi-stable snap-spring. In this new setting the attached configuration of a cross-bridge is represented not only by the discrete energy minima but also by a continuum of intermediate states where the fluctuation induced dynamics of the system takes place. Joint work with L. Marcucci

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MS60

Mechanical and Transport Properties of Polymer Electrolytes for PEM Fuel Cells

Water and temperature alter the mechanical and transport properties of the Nafion, and in turn the operation of Polymer Electrolyte Membrane (PEM) fuel cells. Sorption and permeation involve interfacial mass transport, diffusion and polymer swelling. Water is transported through the hydrophilic phase of Nafion. The volume fraction of the hydrophilic phase increases with water activity, which increases permeation. At high water activity, interfacial mass transport at the membrane/vapor interface is the limiting resistance to permeation. Water absorption into Nafion is initially limited by interfacial mass transport; above critical water content water sorption is limited by polymer relaxation dynamics associated with swelling. The dynamics of water absorption show that at room temperature it takes more than 10^5 s for Nafion to equilibrate to changes in water activity. The mechanical properties of Nafion (elastic modulus and creep rate) show complex behavior as functions of water activity and temperature. The elastic modulus goes through a maximum and creep rate goes through a minimum at intermediate water activity that depends on temperature. Below 50C Nafion is plasticized by water, its modulus decreases and creep strain increase with increasing water activity. Above 80C water stiffens Nafion, its modulus increases and creep strain decreases with increasing water activity. The mechanical properties show the existence of structural transitions in Nafion. In this talk we shall examine the recent experimental results for the mechanical and transport properties of Nafion, relate them to structure and structural transitions and discuss the implications for PEM fuel cell operation.

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MS60

Fan the Flame with Water: Operation of PEM Fuel Cells with Dry Feeds

Water management is a major technological problem with Polymer Electrolyte Membrane (PEM) Fuel Cells. Bad performance is seen with membranes operating at low relative humidity or with liquid water flooding the fuel cell. Employing model fuel cell reactors that elucidate the basic physics of Polymer Electrolyte Membrane (PEM) fuel cell reactors we have been able to demonstrate that the water produced at the cathode can auto-humidify the fuel cell and operate with dry feeds to 130C. PEM fuel cells reactors are shown to be conceptually identical to exothermic reactions, e.g. flames! Current ignition in PEM fuel cells is analogous to thermal ignition in flames. Current density fronts propagate in fuel cells resulting from a balance between convection and diffusion, this is analogous to flame fronts that propagate resulting from a balance between convection and heat conduction. Our model fuel cells have been employed to elucidate the mechanism of liquid water motion through the PEM fuel cell. These experiments have illustrated the importance of gravity of PEM fuel cell operation. We have also exploited gravity to facilitate liquid water removal in the channel-less self-draining PEM fuel cell, which operates with operates with current densities $>$ 1 A/cm2 with dry feeds and T $>$120C and high current densities. This design has facilitated control and fuel utilization; we have been able to directly control power output to fixed load impedance with 100% fuel utilization with a system that requires no temperature control. In this talk we shall review the use of reaction engineering principles to arrive at improved PEM fuel cell design.

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MS60

Electrodes for Energy Applications Including Effects of Diffuse Space Charge: Microscopic vs. Phenomenological Modeling

To describe charge transfer at porous and planar electrodes in energy systems, the structure of the nanoscopic space charge region which forms at the electrode/electrolyte interface is generally not considered, even though details of this layer are of utmost importance for correct and self-consistent microscopic modeling of electrochemical processes. We show how these effects can be included in an

insightful, comprehensive and transparent framework and present numerical examples both for planar and porous electrodes.

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MS60

Ion Conduction in Polymer Electrolytes

Polymer electrolyte membranes play a central role in energy conversion. By spontaneously forming pore networks then preferentially conduct ions of prescribed charge. For applications to PEM fuel cells, dye-sensitized solar cells, and lithium ion batteries, it is desirable to have membranes with high conductivity, as well as robust structural characteristics. One method to achieve this is by dissolving a functionalized and a crystallizable polymer in solvent, and evaporating off the solvent. We present a class of models for the phase separation which occurs within the casting process of these blended membranes, as well as for the pore network created when the membranes are exposed to water.

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MS61

The Theory of Stranski Krastanov Transition: What We Truly Understand

The self assembly of quantum dots in the Hetero-epitaxial growth occurs though the Stranski Krastanov transition. This refers to the process where the flat surface of a strained thin film of a certain thickness (critical thickness) becomes unstable. This unstable film forms islands (quantum dots) that sit on top of a strained film known as the wetting layer. This transition is understood theoretically as a strain driven instability known as the Grinfeld instability. The Grinfeld instability however fails to predict a non-zero critical thickness or a wetting layer. Thus the relation between the Critical thickness and Wetting layer is also not understood. In this talk using a Kinetic Monte Carlo approach the Stranski Krastanov Transition in the epitaxial growth of strained alloy films is explored. It will be shown that the intermixing of the film and substrate material is entropy driven at the cost of increasing the energy of the system. The importance of entropy and intermixing and its role in stabilizing the initial layers will be discussed. The Stranski Krastanov transition and the existence of a wetting layer, is then understood in the context of the competition between entropy and energy.

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MS61

Accurate Acceleration of the Kinetic Monte Carlo Method

While kinetic Monte Carlo (KMC) is a powerful materials modeling tool, it is computationally expensive when rare-events are present. We present a novel method called the accelerated superbasin KMC (AS-KMC) method, that enables a more efficient study of rare-event dynamics than KMC, while maintaining control over the error. In AS-KMC, the rate constants of frequent processes are lowered. We show that AS-KMC can provide large CPU savings over KMC without significant loss in accuracy.

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MS61

Numerical Methods for Stochastic Bio-chemical Reacting Networks with Multiple Time Scales

Multiscale and stochastic approaches play a crucial role in faithfully capturing the dynamical features and making insightful predictions of cellular reacting systems involving gene expression. Despite their accuracy, the standard stochastic simulation algorithms are necessarily inefficient for most of the realistic problems with a multiscale nature characterized by multiple time scales induced by widely disparate reactions rates. In this talk, I will discuss some recent progress on using asymptotic techniques for probability theory to simplify the complex networks and help to design efficient numerical schemes.

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MS61

Connections Between Kinetic Monte Carlo and Continuum Models

In this talk the connections between traditional continuum models and kinetic Monte Carlo, as applied to heteroepitaxy will be explored. The advantage and disadvantages of both approaches will be outlined. One crucial aspect of kinetic Monte Carlo is that it naturally captures the discrete and stochastic nature of heteroepitaxial growth at the atomistic scale. Some examples will be shown where this

has consequences on bigger scales.

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MS62

Generalized Thermodynamics of Solid Surfaces with Application to Nucleation

When considering the thermodynamics of solid-fluid surfaces, Gibbs restricted attention to single-component solids. Attempts to generalize Gibbs approach for multicomponent solids are problematic because the chemical potentials for substitutional components are not well defined at the surface. It is proposed that this difficulty can be overcome by using the concept of thermodynamic availability (exergy). It will be discussed how this method can be used in the thermodynamics of nucleation and other applications.

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MS62

Cleaving Method for Determining Solid-liquid Interfacial Free Energy in Molecular Systems: Results for Simple Models of Water

The cleaving method for computing solid-liquid interfacial free energy has been very successful in atomic systems (hard and soft spheres, Lennard-Jones). The challenge for molecular systems is to take into account the rotational degrees of freedom of a molecule. I will present an extension of the cleaving method to molecular systems and results for several simple models of water, TIP4P, TIP4P-Ew, TIP5P-Ew, also elucidating the effect of including full electrostatic interactions.

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MS62

Interface Thermodynamics for Strongly Non-hydrostatic Solids

We derive thermodynamic relations for the free energy, interfaces stress tensor, segregation and other excess properties of interfaces between fluids and strongly non-hydrostatically stressed solid phases in multi-component systems. These relations lead to various thermodynamic integration schemes and are presented in forms convenient for atomistic simulations. The new relations are illustrated by several examples of calculation of interface thermodynamic properties in solid-liquid coexistence systems using Monte Carlo and molecular dynamics methods with embedded-atom potentials.

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MS62

Thermodynamics and Atomistic Modeling of Solid-solid Interfaces: An Overview

We discuss interfacial thermodynamics of coherent and incoherent solid-solid interfaces, deriving an adsorption equation with additional terms representing the effect of applied mechanical stresses on excess quantities. This equation predicts a number of stress-strain, stress-segregation and other cross effects that do not exist in fluids. New thermodynamic integration schemes are proposed, which are useful in atomistic simulations of interfaces. We demonstrate applications to atomistic simulations of grain boundaries and other interfaces subject to applied stresses.

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MS63

Bifurcations, Instabilities and Localizations of Deformations in Gradient Damage Models with Softening

This work is devoted to the mathematical study of softening damage models which are regularized by gradient damage terms. We first give the variational formulation of the damage evolution problem. Then we analyze the stability of homogeneous responses and we propose a construction of localized solutions when the homogeneous states are no more stable.

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MS63

A Variational Model for Cavitation and Fracture in Nonlinear Elasticity

We propose a variational model for cavitation and fracture in the context of nonlinear elasticity. The energy to minimize is the sum of the elastic energy plus a surface energy

accounting for the creation of surface. We prove the existence of minimizers that are one-to-one and orientation-preserving. We explain the connections with the theory of Cartesian currents and with the regularity of inverses of weakly differentiable functions. This is a joint work with Duvan Henao.

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MS63

Structured Flow and Fracture of Solids: A General Regularized Variational Model

The regularized formulation *à la* Ambrosio-Tortorelli of the variational approach to fracture mechanics by Francfort-Marigo (1998) is here generalized through Structured-Deformation theory, to consider that the inelastic (structured) deformations associated with flow and fracture may be different according to the characteristic loosening of the underlying material microstructure. Changing the class of functions for admissible structured deformations, we show also through numerical experiments that different responses, such as cleavage-, shear- and masonry-like-fractures, can be obtained.

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MS63

On the Global Stability of Two-dimensional, Incompressible, Elastic Bars in Uniaxial Extension

A bar, when stretched, often deforms uniformly until a neck or shear bands develop. This experiment is sometimes modeled as the in-plane deformation of a two-dimensional, elastic material. We show that, for many commonly used constitutive relations, the uniformly deformed state always minimizes the energy. Such stored-energy functions cannot therefore predict these phenomena. Thus, either these stored energies are inappropriate, this phenomena is three dimensional, or else necks and shear bands are beyond the scope of nonlinear elasticity.

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MS64

Stabilizing Fluid-fluid Interfaces by Nanoparticles - A Navier-Stokes-Cahn-Hilliard-Phase-Field-Crystal Approach

Bicontinuous interfacially jammed emulsion gels ('bijels') were proposed in 2005 as a hypothetical new class of soft materials in which interpenetrating, continuous domains of two immiscible fluids are maintained in a rigid state, by a jammed layer of colloidal particles at their interface. We derive a model for such a system which combines a Cahn-Hilliard-Navier-Stokes model for the macroscopic two-phase system with a surface Phase-Field-Crystal model for the microscopic colloidal system along the interface. First numerical results will be presented.

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MS64

Compositional Patterning on Surfaces via the Phase-Field Crystal Approach

In this work, we study compositional domain formation in binary alloys when deposited on a substrate, using the phase-field crystal (PFC) method. These alloys normally do not mix in the bulk, whereas they do mix when deposited on a substrate due to the reduction of elastic energy. We derive a set of amplitude equations, starting from a PFC based energy functional that models the presence of compositional variables. Using this approach, we model the formation of misfit dislocations to study the case of compositional domain formation for asymmetric mixtures.

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MS64

Phase Field Crystal Modeling with an Improved Correlation Function

We present an alternative fitting method for describing the direct correlation function used in the free energy functional of the Phase Field Crystal model. This method can easily be expanded to capture details beyond the first peak of the correlation function without increasing the stiffness of the equations. The applicability of this new fitting method is demonstrated by simulating the liquid-solid transition of copper and iron.

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MS64

Phase Field Crystal Models for Cubic Crystals and

Grain Growth

We study grain growth at the nanoscale using the phase field crystal model. Our results show that grains can both translate and rotate during grain growth. Consistent with recent theory, we find that low angle grain boundaries have a misorientation-dependent mobility. For intermediate misorientations, we observe a pronounced tangential motion of grain boundary dislocations that changes the morphology of the grains. We will also discuss phase field crystal models for cubic crystals.

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MS65
Cloaking Bending Waves in Structured Thin Plates

We introduce a cylindrical cloak to control the bending waves propagating in thin-plates. This is achieved through radially dependent isotropic mass density and radially dependent and orthotropic flexural rigidity deduced from a coordinate transformation for the biharmonic propagation equation. A homogenization approach allows to obtain such parameters. We note that the studied bending waves are of different physical and mathematical nature than their electromagnetic and acoustic counterparts.

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MS65
An Analysis and Performance Evaluation of the Optical Black Hole

The almost ideal absorption of the optical black hole (OBH) makes this conceptual device the very promising choice for designing broadband and omnidirectional light absorbers for solar energy harvesting and infrared sensing. Our study investigates the design of a realistic OBH utilizing both the exact frequency domain solutions for TM and TE waves, and time-domain results obtained from a finite-volume time-domain numerical solver. The dynamic behavior of the light pulse propagation in OBH is presented.

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MS65
Non-Euclidean Cloaking and Perfect Imaging

Optical materials act on light as if they change the geometry of space. In this lecture I show how implementations of certain curved geometries are useful for making broadband invisibility devices and for perfect imaging without negative refraction.

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MS65
Mathematical Analysis of the Active Exterior Cloak

The mathematical ideas behind the active exterior cloak will be presented. We will discuss in detail the quasistatic case and briefly highlight the ideas behind the fixed frequency active exterior cloaking for Helmholtz equation. To support our analysis numerical result will be presented.

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MS66
Gaussian Approximation Potentials: Quantum Mechanical Accuracy Without the Electrons

In this talk, we address the problem of approximating the Born- Oppenheimer potential energy surface (PES), without recourse to representing the electronic problem explicitly.This is essentially an interpolation problem, with the added requirements of maintaining the exact physical symmetries of the PES. We introduce a transformation of the atomic coordinates to describe the neighbourhood of atoms and use a Gaussian Process, which is a non-linear regression method, to solve the interpolation task. The accuracy of the interpolated PES (which we call a Gaussian Approximation Potential, GAP) is remarkable for the bulk phases of a wide variety of systems, including semiconductors, metals and polarizable crystals. The speedup obtained for a force evaluation using the approximate PES in comparison with plane wave density functional theory can reach a factor of a million for metallic systems. In addition

to being a practical calculation method, this success sheds new light on the nonlocal nature of the solutions to the Kohn-Sham equations.

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MS66

Orbital Minimization with Localization

Orbital minimization is among the most promising linear scaling algorithms for electronic structure calculation. However, to achieve linear scaling, one has to truncate the support of the orbitals and this introduces many problems, the most important of which is the occurrence of numerous local minima. In this talk, we introduce a simple modification of the orbital minimization method, by adding a localization step into the algorithm. This localization step selects the most localized representation of the subspace spanned by the orbitals obtained during the intermediate stages of the iteration process. We show that the addition of the localization step substantially reduces the chances that the iterations get trapped at local minima. Numerical experiments for alkane molecules are also presented. This is a joint work with Weinan E, Carlos J. Garcia-Cervera and Jianfeng Lu.

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MS66

Electronic Structure Calculations at Macroscopic Scales Using Orbital-free DFT

Recently proposed Quasi-Continuum Orbital Free Density Functional Theory (QC-OFDFT) is a seamless multi-scale scheme that has enabled the computation of electronic structure at macroscopic scales, and has paved the way for an accurate electronic structure study of defects in materials [V. Gavini, K. Bhattacharya, and M. Ortiz., 2007, Quasi-Continuum orbital-free density-functional theory: A route to multi-million atom non-periodic DFT calculation, J. Mech. Phys. Solids 55, 669]. It combines a real-space formulation of OFDFT with a finite-element discretization that is amenable to coarse-graining. The initial development of QC-OFDFT, for the purpose of demonstration, used Thomas-Fermi-Weizsacker family of kinetic energy functionals. However, more accurate kinetic energy functionals have been proposed in the form of kernel energies that are non-local in real-space [Y.A. Wang, N. Govind, and E.A. Carter., 1999, Orbital-free kinetic-energy density functionals with a density-dependent kernel, Phys. Rev. B 60, 16 350]. In the present study, we develop a local variational formulation for these kernel energies through a system of coupled Helmholtz equations. We incorporate these kernel energies into the quasi-continuum framework and investigate the convergence of the method with respect to coarse-graining and cell-size through studies on mono-vacancy and di-vacancies in aluminum. Our results show remarkable cell-size effects in the energetics of vacancies, and suggest much larger computational domains than those considered previously are necessary in electronic structure studies on defects. We further discuss the behavior of vacancies, in their dilute limit, from electronic structure calculations.

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MS66

Non-periodic Real-space Formulation of Kohn-Sham Density Functional Theory

The Kohn-Sham Density Functional Theory (KSDFT) is widely used for "ab initio" studies of materials. We describe a real-space formulation and finite-element implementation of KSDFT, and demonstrate it with selected examples. We then discuss approaches to coarse-grain KS-DFT for application in crystalline solids with isolated defects.

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MS67

A Discrete Model for Reversible Unzipping

The extraordinary material properties of several biological and bio-inspired materials derive from a judicious design, at the microscale, of chain networks constituted by elastic and breakable links. The energetic competition of these two components regulates the resulting macroscopic constitutive properties. We present two new type of discrete models, both characterized by elastic and breakable links, for the description of reversible unzipping in biological adhesion (with application to geckos adhesion) and of damage in amorphous solids (with application to spider silks and nanopolymers). [De Tommasi, G. Puglisi, G. Saccomandi, *Localized versus Diffuse Damage in Amorphous Materials*, Phys. Rev. Lett. **100** (2008), article]

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MS67

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MS67

Shocks Versus Kinks in a Discrete Model of Displacive Phase Transitions

We consider dynamics of phase boundaries in a bistable one-dimensional lattice with harmonic long-range interactions. Using Fourier transform and Wiener-Hopf technique, we construct traveling wave solutions that represent both subsonic phase boundaries (kinks) and intersonic ones (shocks). We derive the kinetic relation for kinks that provides a needed closure for the continuum theory. We show that the different structure of the roots of the dispersion relation in the case of shocks introduces an additional free parameter in these solutions, which thus do not require a kinetic relation on the macroscopic level. The case of ferromagnetic second-neighbor interactions is analyzed in detail. We show that the model parameters have a significant effect on the existence, structure and stability of the traveling waves, as well as their behavior near the sonic limit.

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MS67

Effect of Nonlinearity on the Kinetics of Twinning Dislocations

We consider the steady motion of a twinning dislocation in a Frenkel-Kontorova lattice with double-well substrate potential that has a non-degenerate spinodal region. Semi-analytical traveling wave solutions are constructed for the piecewise quadratic potential, and their stability and further effects of nonlinearity are investigated numerically. We show that the width of the spinodal region and the nonlinearity of the potential have a significant effect on the dislocation kinetics, resulting in stable steady motion in some low-velocity intervals and lower propagation stress. We also conjecture that a stable steady propagation must correspond to an increasing portion of the kinetic relation between the applied stress and dislocation velocity.

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MS68

Strain Dependence of Microscopic Parameters and its Effect on Ordering during Epitaxial Growth

In this talk, we will present density-functional theory calculations that examine the effect of strain on a number of microscopic growth parameters, such as diffusion, dissociation of small islands, detachment of adatoms from islands, and diffusion of adatoms along island edges. We will use growth of Ag on Ag(100) as our model system. We will then illustrate in growth simulations that employ the level-set technique how such strain dependence of microscopic parameters affects the ordering during growth. In particular, we will discuss the effect of strain on the scaled island size distribution in the submonolayer growth regime.

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MS68

Simulation of Heteroepitaxy in 3 Dimensions Using Kinetic Monte Carlo

In this talk, the efficient simulation of strained heteroepitaxial growth in three dimensions growth using kinetic Monte Carlo is discussed. The presentation will outline several different methods of varying fidelity and speed, the fastest of which is based on updating the elastic displacement field on a mesoscopic time scale. Examples of self assembled stacked quantum dots and growth of quantum dots on patterned substrates will be presented.

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MS68

Phase Field Crystal Simulations of Stress-Driven Surface Evolution

The stress-induced morphological instability of an interface is examined with the recently developed phase field crystal approach. We find that the critical wavenumber of the instability deviates from the prediction of the continuum theory when the length scale of the instability is on the order of the interface width. In addition, we find that large stresses induce nonlinear elastic effects that alter both the wavelength of the instability and the interfacial morphology.

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MS68

Heteroepitaxy - Interplay of Dislocations and Surface Instabilities

By using the phase-field-crystal (PFC) model, we investigate heteroepitaxial growth of thin films on vicinal substrates with step and terrace structure reproduced by a sharp film-liquid interface and substrate rigidity adjusted using an external pining potential. A phase diagram of the stress-induced morphology of the strained film near equilibrium is constructed, which identifies diverse growth

regimes, such as equally-spaced step flow, step bunching, and hill-and-valley facet growth with or without dislocation appearing, according to the increasing mismatch strain and the vicinal angle of the substrate. The morphology of the growing strained thin film follows the equilibrium morphological phase diagram, but indicating less critical mismatch strain for the dislocation formation. The mismatch strain dependence of the dislocation formation indicates the morphological instability properties of the strained thin film grown on the vicinal substrate, such as the step instability and the hill-and-valley growth. Our simulations demonstrate the potential of the PFC model for understanding the thin film growth morphology with steps, islands and dislocations interconnected.

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MS69

Phase Field Modeling as a Numerical Tool to Solve Coupled Bulk/surface Problems

Simulations for almost all applications of interest require to solve partial differential equations in complex geometries. We have introduced a diffuse domain method which can handle such problems for general equations with general boundary conditions. In the approach the complex geometry Ω_1 is embedded into a larger regular domain Ω and represented using a phase-field function, which is a smooth approximation of the characteristic function of the domain Ω_1 such that the sharp boundary of the domain $\Gamma_1 = \partial\Omega_1$ is replaced by a narrow diffuse interface layer. The equation to solve is reformulated on the larger, regular domain Ω with additional source terms that approximate the boundary conditions. The resulting partial differential equation in Ω converges to the original partial differential equation with the original boundary conditions if the width of the diffuse interface layer turns to zero. The diffuse domain approach does not require any modification of standard finite element or finite difference software and thus offers a simple way to implement general problems which have to be solved on complex geometries. We demonstrate the applicability of the approach by solving two-phase flow problems in complex geometries, e.g. sliding droplets over nanostructured surface and chaotic mixing in droplets flowing through a winding channel.

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MS69

Phase Field Method for Feature-Sensitive Curve/Surface Smoothing

A novel weighted phase field model for feature-sensitive variational curve and surface smoothing is proposed. Various numerical examples demonstrate the efficiency, effectiveness and robustness of the proposed numerical algorithms. Furthermore, adpation based on 3D FEM superconvergence and CVT has been realized for efficient surface smoothing.

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MS69

Phase Field Modeling of Dissolutive Wetting

Accurately modeling a spreading drop on a reactive substrate is enormously complicated. A minimal model requires the inclusion of three phases (and associated phase changes), two alloy components (and associated advection-diffusion), and hydrodynamics. We solve several such a models, obtaining crucial insights into the nature of the spreading process, and are able to compare our results with recent state-of-the-art experiments.

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MS69

Phase Field Modeling of Nucleation in Solid State Phase Transformations

We investigate the critical nucleus and equilibrium morphologies during precipitation of a second-phase particle in a solid. We show that a combination of diffuse-interface description and a constrained string method is able to predict both the critical nucleus and equilibrium precipitate morphologies simultaneously without *a priori* assumptions. Using the cubic to cubic transformation as an example, it is demonstrated that the maximum composition within a critical nucleus can be either higher or lower than that of equilibrium precipitate while the morphology of an equilibrium precipitate may exhibit lower symmetry than the critical nucleus resulted from elastic interactions.

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MS70

Macroscopic Instabilities in Fiber-reinforced Elastomers at Finite Strain

We investigate "macroscopic" (i.e., long wavelength) instabilities in fiber-reinforced elastomers at finite strain. We make use of recently developed homogenization estimates, together with a result of Geymonat, Muller and Triantafyllidis linking the development of these instabilities to the loss of strong ellipticity of the homogenized estimates. For composites with very stiff fibers and random microstructures, we derive a closed-form formula for the critical macroscopic deformation, and compare the result with classical (2-D) estimates for laminates.

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MS70

Non-uniqueness in Energy Minimization of Atomistic Problems: A Branch-following and Bifurcation Investigation

Static atomistic simulations aim to obtain local energy minimum (stable equilibrium) configurations of a body composed of discrete atoms subject to applied boundary conditions. In general, many such minimum energy configurations are expected. This work performs a *Branch-Following and Bifurcation* (BFB) investigation to map out a large number of stable equilibrium configurations. From this picture of the system's *potential behaviors* it is possible to draw conclusions about the most likely behavior of the system.

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MS70

Failure Surfaces for Fiber-Reinforced Elastomers Under General 3D Loading Conditions

We present a thorough investigation of local instabilities — including matrix cavitation, fiber debonding, and fiber failure — and global instabilities — defined as the loss of strict rank-one convexity of the effective properties — in fiber-reinforced nonlinearly elastic solids. The results are generated by means of an innovative iterated homogenization method, which incorporates direct microstructural information up to the two-point correlation functions and requires the solution to a Hamilton-Jacobi equation with the fiber concentration and the macroscopic deformation gradient playing the role of time and spatial variables, respectively.

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MS70

Microscopic and Macroscopic Onset-of-Failure Curves in Finitely Strained, Porous Elastomers Under Plane Strain Loading

The present work investigates the connections between microstructural instabilities and their macroscopic manifestations defined as the loss of rank-one convexity of the effective properties in finitely strained porous elastomers with a) random iso-disperse and b) periodic microstructures. The powerful second order homogenization (SOH) approximation technique, initially developed by P. Ponte Castaneda for random media, is also used here to study the onset of failure for periodic microstructures and the results are compared to more accurate finite element method (FEM) calculations. The influence of microgeometry (random and periodic with square and hexagonally arranged pores), initial porosity, matrix constitutive law (neo-Hookean and Gent) and macroscopic load orientation on the microscopic instability (loss of uniqueness of the principal solution for the case of periodic microstructures) and the macroscopic instability (loss of rank-one convexity of the homogenized energy density for all microstructures) is investigated in detail. In addition to the above-described stability-based onset of failure mechanisms, limitations to the elastomers response at finite strains (such as void surface instability, percolation, pore closure and strain locking) are also addressed, thus giving a complete picture of the different possible failure mechanisms present in finitely strained porous elastomers.

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MS71

High-order Modeling of the Smectic-A Mesophase: Defect Structure, Kinetics, and Dynamics

A modeling and simulation study of material transformations from the disordered state to the lamellar-ordered/smectic-A liquid crystalline state is presented. Two-dimensional smectic defect structure, kinetics, and dynamics are presented and compared with an experimen-

tal system sharing phase-transition symmetries. The formation, structure, and complex interactions of giant split-core edge dislocations, composite structures are presented and validated by experimental observations of this phenomena.

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MS71

Hydrodynamics and Rheology of Active Suspensions of Rigid Ellipsoids

Active soft materials are a challenging class of systems driven out of equilibrium by an internal or an external energy source. Examples are self-propelled particles in bacterial colonies, or the membrane and the cytoskeleton of eukaryotic cells, etc. In this talk, I will present a hydrodynamic theory of flowing active ellipsoidal suspensions and discuss the flow and rheological behaviors of these materials.

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MS71

Anomalous Diffusion of Tracer Particles in Viscoelastic Fluids

Due to compelling experimental observations using passive microrheology there is theoretical interest in anomalous sub-diffusion – stochastic processes whose long-term mean-squared displacement satisfies $E[x^2(t)] \sim t^\nu$ where $\nu < 1$. Such behavior can be observed for the Generalized Langevin Equation with a Prony series memory kernel for the friction. We introduce a single parameter for the structure of the Prony series which can be tuned to produce any sub-diffusive exponent ν and discuss issues of simulation, inference and first passage times from an interval.

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MS71

Numerical Study of Chemical Reaction in Blood Flow

Activated platelets play very important role in blood clotting since they are at the central stage of the process of aggregation and coagulation in blood flow. To study the effect of chemical reactions on platelet surface for clotting, we use embedded boundary technique to numerically simulate the reaction. Our numerical methods in 2D and some results will be presented in detail.

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MS72

The Inertial Manifold and Dimension Reduction for Systems of ODEs

In our continuing investigation of methods to reduce the dimensionality of systems of ordinary differential equations we are exploring an approach inspired by the center-manifold technique of dynamical systems. In this talk we will discuss the generl ideas, give some examples, and present results. (Joint work with Shouhong Wang, Indiana University.)

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MS72

AsymptoticAnalysis for the Generalized Langevin Equation

I'llbe presenting various properties of the Generalized Langevin equation and its approximation in higer dimensions,such as ergodicproperties, homogenization theorems, short timeasymptotics and hypoelliptic-type estimates.

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MS72

Mescoscopic Dynamics of Large ODE Systems

The main question addressed in the talk is how to obtain continuum equations for mesoscale averages from the ODE of classical particle dynamics. Balance equations for continuum mechanical averages (density, linear momentum, energy) were derived by Noll, Hardy, Murdoch and others. The missing ingredient in these works was closure: the equations were exact but calculation of fluxes required solving the underlying ODE system. We present a new closure method based on the use of regularized deconvolutions. The applications discussed in the talk include one-dimensional chains of non-linear oscillators, granular acoustics and discretizations of solid-fluid flows. Some error estimates for closure approximations will be presented as well.

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MS72

On the Continuum Limit for a Discrete Model of An Elastic Body

Waves, internal energy and fracture energy in the discrete and continuum models. Wave localization. Lattice spacing and crack resistance: a zero resistance in the limit. Crack-speed-dependent crack resistance and the cell-size-independent energy release ratio. Quasi-static limit. Discrete and continuous stress distribution in a hyper-singular mode of fracture. Generalized continuum limits and prelimiting states. Discrete-continuous structures. A sound-

less crack.

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MS72

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS73

Numerical Analysis of a Basic Electronic Density Functional

We study a mixed finite element discretization of a basic density functional, in which the electrostatic potential is introduced as an additional variable (Gavini et al.). We will outline the convergence analysis including effects of numerical integration. The analysis is based on a local notion of stability and techniques from nonlinear analysis to deal with the nonconvexity of the problem. We will also comment on optimal convergence orders. Time permitting we will present a few recent developments regarding the coarse graining of the density functional.

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MS73

Exact Embedding of Local Defects in Quantum Crystals

In this talk I will present a new model for quantum crystals with local defects. The main idea is to describe at the same time the electrons bound by the defect and the (nonlinear) behavior of the infinite crystal. This leads to a (rather peculiar) bounded-below nonlinear functional whose variable is an operator of infinite-rank. I will provide the correct

functional setting for this functional and discuss the properties of bound states. I will in particular relate them to the dielectric properties of the crystal. Finally, I will discuss discretization issues and show preliminary numerical results in 1D. This is a review of joint works with Eric

Cancs and Amlie Deleurence (Ecole des Ponts, Paris).

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MS73

A Priori Error Estimates for Nonlinear Eigenvalue Problems and Applications in DFT

Abstract not available at time of publication.

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MS73

Theory of Tunneling Transport in Periodic Molecular Chains

There exists now a large body of high quality experimental data for charge transport through single molecules. In particular, the data on insulating molecular chains reveals the expected tunneling behavior displayed in the exponential decay of the conductance with the length of the chains, but also intricate and sometime unexpected effects related to the contacts between the electrodes and the chains. In this talk I will discuss an analytic expression of the asymptotic tunneling conductance, which pinpoints, with atomistic precision, the effects of the contacts on the tunneling conductance and gives a fresh insight into the tunneling properties of the molecular chains. The theoretical exposition will be complemented by first-principle calculations for alkyl and benzene chains connected to gold electrodes via amine linkers and for alkyl chains covalently bonded to (semiconducting) silicon nano-wires. A comparison with the experiments will also be given.

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MS74

Modeling the Microstructural Effects in Electrochemical Systems

Electrochemical systems often undergo phase transformation and morphological evolution. We perform simulations of electrochemical systems, including fuel cell and battery electrodes, using a phase-field model and a smoothed boundary method. We demonstrate the linkage between microstructures and their predicted performance, as well as the means to understand the electrochemical impedance spectra, which is often difficult to interpret due to the microstructural effect.

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MS74

Nanoscale Phenomena in Catalyst Layers of PEM Fuel Cells

Structures at the nanoscale determine properties and operation of cathode catalyst layers of polymer electrolyte fuel cells. We consider a cylindrical water-filled nanochannel, decorated with Pt nanoparticles. The model couples electrostatic effects in the pore, incorporated via Poisson-Nernst-Planck theory, with kinetic effects at pore walls in order to rationalize the current conversion efficiency. Implications of this coupling for materials selection and for structural design of catalyst layers with reduced Pt loading will be discussed.

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MS74

Pore Network Formation in Polymer Electrolyte Membranes

Energy conversion, and in particular conversion of chemical and photonic energy to useful voltage, requires the selective conduction of charged ions through membranes. Polymer electrolytes membranes are a common class of sensitized membranes for selective ion conduction. They are created by emerging polymer electrolytes in a solvent in which the polymers spontaneously form nanoscale pore networks which serve as primitive ion channels. We present a novel model for the formation of the nanoscale pore network as the gradient flow of novel classes of competing interfacial and bending energies. We compare numerical solutions of the model equations to experimental data and derive sharp-interface evolution laws for pores. We show that they are given by a high-order nonlinear curvature-driven flow. This curvature-driven flow gives rise to various configurations of pore networks, including meandering pore channels, circular channels and straight channels.

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MS74

Stack Level Models of Fuel Cells

A model of steady state operation of Polymer Electrolyte Membrane Fuel Cell (PEMFC) stacks with straight gas channels is presented. The model is based on a decoupling of transport in the down-channel direction from transport in the cross-channel plane. Further, cross-channel transport is approximated heuristically using one-dimensional processes. The model takes into account all mass, heat and charge transport phenomena of interest and is a nonstandard system of non-smooth boundary value Differential Algebraic Equations (DAEs) with strong, nonlocal coupling. A discretization of the system and a successful iterative strategy are described. Representative computational results, validation against existing experimental data and a numerical convergence study are shown.

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MS75

Control of Crystallographic Texture and Grain Microstructure in Non-ferromagnetic Metals Through Application of a Magnetic Field

The current research on texture and grain structure evolution during recrystallization and grain growth in non-magnetic metals in high magnetic fields will be reviewed. The magnetically induced changes can be caused by the generation of an additional magnetic driving force which arises from a difference in magnetic free energy density between differently oriented grains. Furthermore, the mobility of grain boundaries can be enhanced in the presence of a magnetic field.

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MS75

Level Set Modeling of Grain Growth

Substantial progress has been made with the development of a level set method and code. We are now able to simulate the following phenomena using a single code: grain boundary motion in a polycrystalline network with grain boundary energy depending on interface normal as well as misorientation; interaction between moving boundaries and particles; interaction between moving boundaries and solute fields (i.e. solute drag); dissolution/growth of particles with diffusion of solute away from/to the particle.

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MS75

Grain Boundary Migration, Grain Growth and Grain Growth Microstructures: Cause and Effect

The mechanism of grain boundary migration and grain boundary structure are intimately linked. Similarly, polycrystalline microstructure and the dynamics of grain boundary migration are intimately linked. Both of these linkages are extremely complicated in the general case. We therefore propose a series of limiting assumptions and track their implications from structure, to boundary migration, to grain growth to the final grain growth microstructures. Our approach is based upon dislocation dynamics methods to study the migration of low angle grain boundaries and use these results as input to grain growth simulations, ending with an analysis of the corresponding steady state grain growth microstructure. These studies are performed in both two and three dimensions. The final results show the causal link between boundary structure and steady state grain growth microstructure.

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MS75

Recent Progress on Quantifying Intrinsic and Extrinsic Grain Boundary Mobility

This talk addresses two main issues related to computational efforts aimed at quantifying interfacial mobilities in polycrystalline materials: i) the largely atomistic efforts employ driving forces that are orders of magnitudes higher than those in experiments, and ii), the role of solutes in determining the mobilities remains unclear, in spite of the existence of several theoretical frameworks. The first part of this talk will focus on the use of the fluctuation dissipation theorem to extract the mobility of grain boundaries

in the zero-driving force limit. Molecular dynamics studies on fluctuating high angle grain boundaries in Al will be used as a benchmark to compare the results with past studies, both computational and experimental. The second part of this talk will focus on the application of a Monte-Carlo approach based on classical interatomic potentials for an Al-Mg alloy to extract the solute-boundary interaction energies, a key chemical parameter that allows for the first time to directly quantify the effect of solute concentration on grain boundary mobilities in alloy systems. I will conclude by discussing the implications of the generated atomistic datasets on annealing phenomena in crystalline materials.

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MS76

Computational Steering of Parallel Micromagnetic Calculations

We describe the design of the micromagnetic Nmag simulation framework (http://nmag.soton.ac.uk) and its choice of extending an existing general purpose programming language (Python) through a library module that provides the micromagnetic simulation capabilities. This approach allows great flexibility in how the micromagnetic simulation can be steered as the simulation user can combine the use of the Nmag Python module with the use of other (existing) scientific, numerical, data processing and visualization modules. We show how the interactive control of the simulation session at the Python prompt can be combined with parallel execution of the computationally demanding operations. The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under Grant Agreement nr 233552 (DYNAMAG), and from EPSRC (EP/E040063/1).

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MS76

Convergence of a Geometric Integrator for LLG

In our talk, we consider a finite element scheme for the Landau-Lifshitz-Gilbert equation (LLG) which describes the dynamics of ferromagnetism. In contrast to previous works, cf. [S. Bartels, A. Prohl, Convergence of an implicit finite element method for the Landau-Lifshitz-Gilbert equation, SIAM J. Numer. Anal., vol. 44, no. 4, 1405–1419 (electronic), 2006], [F. Alouges, A new finite element scheme for Landau-Lifchitz equations, Discrete Contin. Dyn. Syst. Ser. S, vol.1, no. 2, 187–196, 2008], we examine the LLG including the total magnetic field induced by several physical phenomena described in terms of exchange energy, anisotropy, stray-field, and exterior field. Besides a strong non-linearity, a non-convex side-constraint represents a challenging task for the numerical integrator. Nevertheless, we aim at proving unconditional convergence for the approximation of a weak solution.

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MS76

Large-scale Finite Element Micromagnetic Simulations with Hierarchical Matrices

In micromagnetic FEM simulations, solving Poisson's equation is an established approach to calculate the magnetostatic interaction. The memory requirements can however be large, since the computation involves a densely populated matrix. By implementing the H-matrix method in our hybrid FEM-BEM code, we have achieved significant improvement concerning the memory requirements. In this talk, a brief outline of the method will be presented and a few applications on the magnetization dynamics in microstructures will be discussed.

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MS76

Finite Element Numerical Micromagnetics: Old Problems and New Solutions

This talk will discuss some of the problems and limitations in numerical micromagnetic models and review recent advances. We developed and implemented new methods and algorithms for the calculation of the magnetostatic field in a finite element model, which are enabling micromagnetic simulations of significantly larger systems while reducing the memory requirements. Simulations of magnetic recording systems, which demonstrate the new capabilities, will be presented.

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MS77

Energy and Structures of Optimal Multimaterial Anisotropic Elastic Composites

We consider an elastic composite from three isotropic elastic materials, assembled with fixed volume fractions and placed into an arbitrary homogeneous plane stress field. We are seeking a structure that minimizes the energy of this composite, or maximizes its stiffness. We find a lower bound for the energy using Localized Polyconvexity technique, a modification of the Translation method by accounting of inequalities on the range of field in the materials in an optimal structure. When one of the three mixed materials is void, the lower bound of he energy is found explicitly. Depending of volume fractions and the loading type, the bound assumes one of six analytic expressions. For one of these regimes, it coincides with the Translation bound; the other bounds are new. The obtained bounds are exact in all but one regime. We show that special finite-rank laminates realize the bound in the five regimes. In the regime where the lower bound is nonexact, we suggest a laminate structure that provides an upper bound for the optimal energy, and compute the gap between them. All multimaterial optimal structures are found by the same regular procedure, that also demonstrates nonuniqueness

of optimal geometries.

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MS77

The Energy Density of Martensitic Thin-structures via Dimension Reduction

Variational limits defined on the space of one- or two-dimensional Young measures are obtained from three-dimensional elasticity via dimension reduction. The rate at which the energy becomes infinite when the volume locally vanishes characterizes the domain of the limit energy. The obtained limit problems uniquely determine the energy density of the thin-structures.

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MS77

Macroscopic Instabilities in Nematic Elastomers

We consider elastomers that are reinforced by aligned stiff inclusions and investigate the possible development of 'macroscopic' instabilities in these systems by computing the loss of strong ellipticity (or strict rank-one convexity) of the homogenized constitutive relation. We show that these instabilities can lead to 'soft' deformation modes that are similar to those observed in nematic liquid crystal elastomers, and make comparisons with these systems.

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MS77

Microscopic and Macroscopic Instabilities in Finitely Strained, Fiber-Reiforced Elastomers Under Plane Strain Loading

The present work is a detailed study of the connections between microstructural instabilities and their macroscopic manifestations as captured through the effective properties in finitely strained fiberreinforced elastomers, subjected to finite, planestrain deformations normal to the fiber direction. The work, which is a complement to a previous and analogous investigation by the same authors ("Microscopic and Macroscopic Instabilities in Finitely Strained Porous Elastomers," by: J. C. Michel, O. Lopez-Pamies, P. Ponte Castaneda, and N. Triantafyllidis, J. Mech. Phys. Solids, 55, 2007, pp. 900-938) on porous elastomers, uses the powerful secondorder homogenization (S.O.H.) technique, initially developed for random media, to study the onset of failure in periodic fiberreinforced elastomers and to compare the results to more accurate finite element method (F.E.M.) calculations. The influence of different fiber distributions (random and periodic), initial fiber volume fraction, matrix constitutive law and fiber crosssection on the microscopic buckling (for periodic microgeometries) and macroscopic loss of ellipticity (for all microgeometries) is investigated in detail. In addition, constraints to the principal solution due to fiber/matrix interface decohesion, matrix cavitation and fiber contact are also addressed, thus giving a complete picture of the different possible failure mechanisms present in this class of elastomeric composites.

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MS79

Simulation of the Dielectric Response of Compositionally Graded Ferroelectric Films with Wedge Domains

Functional materials with non-linear dielectric response are suited for frequency tuning devices. Developing the theory of wedge domains in graded ferroelectrics, we present a quantitative model of domain evolution and dielectric response of compositionally graded ferroelectric multilayers. We show that the domain structure adapts itself to the applied electric field. The domains are swept away layer-by-layer upon the application of the electric field; resulting in a non-linear field dependence of the dielectric constant and tunability. We demonstrate that by controlling relative thicknesses of the layers that make up the graded heterostructure, one could further enhance the dielectric response and tunability.

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MS79

Phase-Field Model of Phase Transformations and Microstructure Evolution in Polycrystals

Most materials in applications are polycrystalline, containing grains of different crystallographic orientations separated by grain boundaries. To predict the kinetics of phase transformations such as precipitation reactions and the accompanying microstructure evolution in the presence of grain boundaries is significantly more challenging than those in a uniform single crystal. Precipitation reactions in a polycrystalline material involve the complicated coupling among a number of different processes: solute segregation or depletion near grain boundaries, grain boundary migration, precipitate nucleation, growth and coarsening. Furthermore, the elastic moduli for a polycrystal are always spatially inhomogeneous: each grain has different elastic modulus and the elastic constants in the grain boundary regions are generally different from those inside the grains. In this presentation, a phase-field model will be presented

for modeling solute segregation and precipitation of second-phase particles in a polycrystal in the presence of the elastic strain with inhomogeneous modulus. Examples to be discussed include segregation behavior at grain boundaries in the presence of coherent precipitates inside grains, the morphological evolution during isostructural phase separation in the presence of grain boundaries, and precipitation of tetragonal particles in polycrystalline cubic materials.

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MS79

Austenite-Martensite Interfaces in Shape Memory Alloys

A two-scale phase field simulation is developed for austenite-martensite interface to understand the effects of crystalline symmetry and geometric compatibilities on the reversibility of structural phase transformations in shape memory alloys. It is observed that when the middle eigenvalue of martensite transformation strain is equal to 0, an exact austenite-martensite interface is formed with negligible elastic energy. On the other hand, when the middle eigenvalue is different from 0, an inexact interface between austenite and martensitic twin is formed, and the corresponding elastic energy increases with the increased magnitude of the middle eigenvalue, resulting in substantially higher energy barrier for austenite-martensite transformation, and thus higher thermal hysteresis in shape memory alloys.

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MS79

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MS80

Modeling and Analysis of Two-Phase Lipid Bi-layer Vesicles

We present and analyze a new model for two-phase lipid bilayer vesicles. We study symmetry-breaking patterns, as observed in experiment, in the presence of two fluid phases: an ordered phase and a disordered phase. We propose a rational continuum model that engenders no intrinsic curvature in either phase. We study the problem from the point of view of both global bifurcation and energy minimization.

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MS80

Equilibrium and Non-equilibrium Mechanics of Semiflexible Cytoskeletal Networks

Elasticity of cytoskeletal networks in cells appears to rely on a combination of passive equilibrium properties of filaments and active internal stresses generated by molecular motors, with changes in crosslink density and motor activity each capable of producing hundred-fold differences in network elastic moduli. We present theoretical and computational studies examining the effects of anisotropy and polydispersity in filament distributions, and activity of molecular motors on the nonlinear mechanics of semiflexible cytoskeletal networks.

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MS80

Micromechanical Modeling of Affine-Nonaffine Deformation in Cytoskeleton Mechanics

Semiflexible polymer network, such as cell-cytoskeleton, differ significantly from their flexible counter-part in the deformation energy storage mechanism. As a result, the network elasticity is governed by both enthalpic and entropic variations. In addition, the enthalpic effect shows two predominantly distinct regimes of energy storage mechanism, affine regime and non-affine regime. Recently some computational models, based on finite element analysis of the actual network, such as Mikado Model, were used to demonstrate the basic physics involved in the mechanical deformation of semiflexible network. These models are computationally expensive and it is very difficult, if not impossible to develop a macroscopic constitutive relation based on them. In the present paper, we are proposing a constitutive model (stress-strain relation) for a 2D semiflexible random network. We idealize a semiflexible network through a unit-cell representation, consisting of four semiflexible main chains and four equivalent springs. The

unit cell representation captures the actual networks distinct elastic energy storage mechanisms under the externally applied deformation field. The transition from non-affine (bending dominant) to affine (axial stretching dominant) is captured through the change of the relative positions of joints of the four chain, which also correspond to the crosslinking density. The current model provides a model frame to develop efficient continuum constitutive models of cytoskeleton in the future. The possibility of applying current model to large deformation is explored at the end.

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MS80

Mechanics of Bacterial Shape Regulation and Division

Bacterial cells utilize a ring-like organelle (the Z-ring) to accomplish cell division. The Z-ring actively generates a contractile force and influences cell wall growth. We will discuss a general model of bacterial morphogenesis where mechanical forces are coupled to the growth dynamics of the cell wall. The model suggests a physical mechanism that determines the shape of bacterial cells. The role of several bacterial cytoskeletal proteins and the Z-ring are discussed. We will explore molecular mechanisms of force generation by the Z-ring and how cells can generate mechanical forces without molecular motors.

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MS81

Peridynamics of Heterogeneous Media

Multiscale analysis of peridynamics inside two-phase heterogeneous media is discussed. A two-scale asymptotic method that captures the fluctuations of the local deformation field is introduced. The asymptotic method provides a multiscale numerical method with a cost that is far less than solving the full microscale peridynamic equation over the entire macroscopic domain.

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MS81

Peridynamic Theory Based on Variational Principle

Classical continuum mechanics presents obstacles for predicting crack initiation and growth in materials. Recently introduced non-local peridynamic theory removes these obstacles, and it is applicable at different length scales. This study presents an approach based on variational principle to rederive the peridynamics equations of motion. It also shows peridynamics can utilize any material model of the classical continuum mechanics provided that the Piola-Kirchhoff stress can be obtained directly or by using incremental procedures.

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MS81

Exact Mappings from Newtonian Particle Mechanics to Continuum Mechanics

Newtonian particle mechanics of the kind used in molecular dynamics (MD) simulations is a well known technique for modeling a wide class of material behaviors in fluids and solids. In this presentation we discuss the relationship between these discrete simulations and continuum mechanics where the basic variables are fields (density, mass velocity or momentum, stress, etc.) and we are able to show that there exists exact mappings from the discrete system to a continuum system that obeys the usual set of equations. This procedure allows us to define the continuum quantities as averages of microscopic observables. We have some new results for general force-fields for construction of microscopic stress as well as a construction of nonlocal force density (e.g. peridynamic force density). We will discuss how this mapping can be implemented as a post-processing step for MD simulations. We also point out that the averaging process is not unique and so the continuum system is not unique either except in the limit of large length and time scales. This does lead to an interesting theorem about correct averaging procedures for continuum theories, and the discussion of the exact relationship between microscopic models such as MD and continuum models lends new insight into informed construction of the latter.

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MS81

A Domain Decomposition Method for Local/nonlocal Coupling

We investigate the coupling of local and nonlocal models through the nonlocal continuum peridynamic theory. We extend the nonlocal domain decomposition results in [Burak Aksoylu and Michael L. Parks, "Towards domain decomposition for nonlocal problems', submitted, 2009] to the case of nonlocal models with variable interaction ranges, of which local/nonlocal coupling is a special case. We derive transmission conditions for local/nonlocal coupling, and show their connection to the classical theory. We explore, analytically and numerically, the suitability of these transmission conditions.

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MS82

Uses and Shortcomings of One-Dimensional Models of Step-Flow Growth: Some Examples

Kinetic Monte Carlo on a 2D model shows that terrace-width distributions (TWD) of steps on vicinal surfaces narrow progressively with increasing flux until the model breaks down. The narrowing corresponds to kinetic repulsion between moving steps, due to the intrinsic asymmetry of the adatom diffusion current on growing surfaces. To make analytic progress, we consider a 1D model, from a Burton-Cabrera-Frank approach. This model leads to attachment asymmetry in essentially the same way as does electromigration or Ehrlich-Schwoebel barriers. Work supported by U. of Maryland NSF-MRSEC under Grant DMR 05-20471, with ancillary support from CNAM.

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MS82

Instability and Growth on a Silicon Surface: From Homeoepitaxy to Heteroepitaxy

Abstract not available at time of publication.

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MS82

Phase-field Modeling of Epitaxial Growth: Applications to Step Trains and Island Dynamics

We present a new phase-field model including combined effects of edge diffusion, the Ehrlich-Schwoebel barrier, deposition and desorption to simulate epitaxial growth. A new free energy function together with a correction to the initial phase variable profile is used to efficiently capture the morphological evolution. The phase-field model is solved by a fully-implicit finite difference scheme with adaptive block-structured Cartesian meshes. The model is then use to investigate the evolution of small islands and step trains.

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MS82

Spiral and Mound Growth - A Phase Field Study

We use a phase field approach to solve the discrete-continuous Burton-Cabrera-Frank model for step dynamics. We are thereby interested in the interplay of Ehrlich-Schwoebel barriers and elastic effects. The phase-field model requires a degenerate mobility in order to approximate the jumps in the adatom density across the steps. We consider spiral and mound growth and propose an approach to grow regularly ordered trenches which can be used as templates to grow nanowires.

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MS83

Undulatory Swimming in Viscoelastic Fluids

We investigate the effects of fluid elasticity on the swimming behavior of a slender micro-organism (C. elegans, L 1mm) in experiments using particle image velocimetry, and by tracking the organism motion. Results show that the organism moves in highly periodic fashion and generate traveling waves which decay from head to tail. The organism velocity (U) decreases as the fluid elasticity is increased. However, the Strouhal number (St), defined as St=(fA)/U, decreases as the fluid elasticity increases. Here, f and A is the organism swimming frequency and amplitude, respectively. This suggests that the fluid rheology may have a strong effect on the organism swimming gait.

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MS83

Swimming Microorganisms in Viscoelastic Fluids and Gels

While the basic principles of swimming in Newtonian fluids are well understood, in many cases the natural environments which microorganisms navigate are non-Newtonian fluids or even gels, which result in different swimming behavior. For example, mammalian sperm swim through mucus in the female reproductive tract. I discuss how viscoelastic response affects swimming shapes and speeds of flexible swimmers such as sperm. Next, I describe issues that arise for swimmers moving through viscoelastic gels. First, swimming through solids such as gels requires altered boundary conditions on the swimmer, and unlike incompressible fluids, a gel can have compressional modes with relative motion between polymer and solvent fractions. In addition, many biological gels are heterogeneous on the

lengthscale of swimming microorganisms. I discuss the effect of microstructure heterogeneity in both continuum and microscopic models of swimming.

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MS83

Bio-locomotion Near Boundaries

We study the locomotive behavior of organisms in various fluidic environments to mimic complex natural habitat. To explore their behavior, we perform controlled experiments in the following scenarios: fluids with different viscosities, capillary tubes, and wet granular media. We find that, as organisms increase contact area with solid boundaries, they swim a greater distance per undulation without a significant change of their body stroke. Such high efficiency is typically not expected for the locomotion of small organisms in viscous fluid, but as we show, it is possible under the influence of boundaries.

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MS83

A Second Order Virtual Node Algorithm for Poisson Interface Problems on Irregular Domains

I will present a second order accurate, symmetric positive definite, geometrically flexible and easy to implement method for solving the variable coefficient Poisson equation with interfacial discontinuities. We discretize the equations using an embedded approach employing virtual nodes at interfaces and boundaries. A variational method is used to define numerical stencils near these special virtual nodes and a Lagrange multiplier approach is used to enforce jump conditions and Dirichlet boundary conditions. Numerical experiments indicate second order accuracy in L-infinty.

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MS84

Shear Banding and Interfacial Stability in Pressure Driven Flow of Wormlike Micellar Solutions in Straight Narrow Channels

We examine the linear stability of the steady, one-dimensional, pressure-driven channel flow of the VCM model (Vasquez, Cook, and McKinley, JNNFM 2007). The VCM model is a two-species, microstructural network model developed to describe flows of wormlike micellar solutions. The equations for each species are coupled and form a system of nonlinear partial differential equations. In addition to Rousian and reptative relaxation mechanisms, the VCM model incorporates the breakage and reforming of two micellar species (a long species 'A and a short species 'B). We consider effects of small perturbations of the base-state in both the flow and vorticity directions. Below a critical pressure drop the VCM model base solution is almost homogeneous across the channel, like the upper convected Maxwell model, but above this critical pressure drop the flow becomes inhomogeneous and shear bands. For the lower pressure the base solution is stable to the perturbations described above. We discuss the stability of the base flow to these perturbations above this critical pressure drop and contrast this with the behavior of other models.

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MS84

Mathematical Models for Particle Laden Thin Films

We consider mathematical models for particle laden thin films and discuss various advances and challenges for this problem. We present experimental data for flow on a slope with particles and compare with the models. Relevant physics includes hindered settling, shear-induced migration, and surface tension.

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MS84

Dewetting of Thin Liquid Polymer Films

For films with a free surface, such as for the dewetting of a nano-scale thin polymer film on a hydrophobic substrate, the boundary condition at the substrate has been found to have a crucial influence on the dynamics and morphology of the film. Experimental studies of unstable thin films coating solids have shown significant differences in the dewetting rates and the patterns that develop after the formation of growing "dry regions' on the solid. The thin film models we derive allow systematic description of the film dynamics and profiles in time as the slip length is varied and used for direct comparison with experiments.

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MS84

Transient Stability Analysis for an Inertially-driven Extensional Motion of a Planar Liquid Sheet

We derive a time-dependent exact solution of the free surface problem for the Navier-Stokes equations describing the planar extensional motion of a fluid sheet driven by inertia. The linear stability with respect to one- and two-dimensional symmetric perturbations is examined within the framework of the slender body equations. Both transient growth and long-time asymptotic stability are considered. Analysis begins with one-dimensional perturbations

in the axial and transverse directions for viscous and inviscid sheets.

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MS85

Transformation Media Using Negative Refractive Materials

We will show that some transformation optics mappings can lead to many interesting optical illusion and wave manipulation effects. We will focus of those fold-geometry mappings that give negative refractive index materials. One interesting example is a conceptual device that can optically transform one object into another object[Y. Lai, J. Ng, H. Chen, D. Z. Han, J. J. Xiao, Z.-Q. Zhang, and C. T. Chan, Phys. Rev. Lett. 102, 253902 (2009)]. The device is itself invisible, and does not need to encircle the object. What we mean is that transformation optics can design a passive device that when placed near to (say) a spoon, will make look like (say) a cup for a far-field observer. The functionality is enabled by the fact that a negative index material can form part of a complementary media and at the same time, serves as a lens. Using similar ideas, we can achieve cloaking at a distance. Using negative index materials, we propose an invisibility cloak operating at a finite frequency that can cloak an object with a prespecified shape and size within a certain distance outside the cloaking shell [Y. Lai, H.Y. Chen, Z.Q. Zhang, C.T. Chan, Phys. Rev. Lett. 102, 093901 (2009)].

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MS85

Plasmonics Invisibility

Our work is at the frontier between the so-called plasmonics and metamaterials topics. We will report recent results on the use of transformation optics for surface plasmons waves propagating on a metallic interface. We will show how structuring the surface allows to control the propagation of light and, thus, from that propose structures to make an invisibility cloak for plasmons.

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MS85

Broadband Exterior Cloaking with Active Devices

We show how to make an object invisible from a known incident or probing field by designing wave emitting devices that simultaneously cancel out the incident field in a given region and radiate very little waves in the far-field. Thus the scattering from an object in this region is significantly reduced, rendering the object invisible. Our approach allows for cloaking over a broad range of frequencies, but it assumes the incident field is known.

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MS85

Acoustic and Electromagnetic Cloaking of Obstacles

In this talk, we shall consider virtually reshaping acoustic and electromagnetic obstacles by cloaking. First, we show that the cloaking medium must be anisotropic. Then, by using transformation media, we derive the cloaking devices. Finally, by scattering estimates corresponding to small obstacles, we show that the limit of virtual minification cloaking gives the invisibility cloaking. Our study are conducted in both homogeneous and general inhomogeneous background space.

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MS86

Force- and Energy-mixing Methods for Atomistic Multiscale Simulations of Solids

In the concurrent multiscale approach a small region is described with one method that is accurate but computationally expensive, while the larger surrounding region is described with a less accurate but much cheaper method. Despite the successes of this approach, the essential problem of how best to couple two different methods is still not resolved. In this talk I discuss some general issues in coupling atomistic methods, focusing on the tradeoffs between energy-based and force-based coupling. While the former allows a total energy to be defined, it necessarily gives rise to force errors at the boundary. The latter can produce accurate forces, but at the cost of having to give up defining a total energy. I present a comparison of various energy and force based methods for coupling quantum-mechanical and interatomic-potential descriptions of bonding for simple bulk crystalline systems. From this comparison we conclude that (at least for this system) force-based mixing and an abrupt transition produce optimal trajectories. I present our results for fracture in silicon using the force-mixing approach, where we have discovered low-speed instabilities in our atomistic simulation that we relate to experimentally observed micron-scale ridges. Finally, I discuss the prospects for a method that combines the best

features of the two approaches.

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MS86

Interface Conditions for Coupling Molecular Dynamics to Continuum Models

Simple coupling of molecular dynamics (MD) simulations with continuum models result in spurious reflections at the MD-continuum interface. We develop a coupling procedure to reduce these spurious reflections by incorporating the recently developed Perfectly Matched Discrete Layers (PMDL) technique into a domain-decomposition based multiscale framework, and adapting PMDL for finite temperature heat baths. Through numerical examples, we show that this method shows promise to be an efficient and accurate alternative to existing coupling strategies.

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MS86

Coupling Molecular Dynamics and Peridynamics

Our presentation considers the coupling of molecular dyanmics and peridynamics via the fluxes in balances laws. The peridynamic momentum and energy balances laws are derived using the principles of statistical mechanics. In particular, we show that the peridynamic force density integral operator is the phase space expected value of internal force density given by a general multibody interatomic potential. The derivations generalize the seminal work of Irving-Kirkwood (1950), and build upon the elegant ideas due to Noll (1955) that generalized the former work.

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MS86

Atomistic-based Boundary Element Method

We present a dimension reduction method to reduce the number of degrees of freedom associated with atomistic models. The model retains atoms in critical areas, e.g. around crack tips, and a boundary element representation is used to remove the surrounding atoms. We will discuss the formulation in both 2D and 3D.

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MS87

Lamination Mirostructure in a Copper Single Crystal Shear Experiment

We investigate the formation of microscopic patterns in a copper single crystal deformed in a shear experiment. Using high-resolution electron backscatter diffraction imaging, we find a band-like microstructure consisting of confined areas in the sample with rotated lattice. Digital image correlation allows us to exactly determine the macroscopic state of deformation of the sample. This data can be used as a side condition to calculate the lamination parameters from the theory of kinematically compatible lamination of separate material regions, each deforming in single slip. The parameters given by the theory agree with the measured properties, i.e., a lattice rotation of 3 degrees and a lamination normal rotated 7 degrees counterclockwise from a ¡111¿ direction.

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MS87

Several Applications of the Level-set Approach to Dislocation Dynamics

In this talk, we will present results obtained in collaboration with Nicolas Forcadel and Regis Monneau about the dynamics of dislocation lines in a slip plane. First we will explain how the motion of several dislocation lines can be described at the microscopic scale by solving a non-local eikonal equation. We will next present homogenization results to derive elasto-visco-plastic law at the macroscopic level. To finish with, we will present results about the level-set approach in the case of singular interactions.

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MS87

Surface Effects in the Inelastic Response of Molecular Crystals

Understanding the mechanisms of deformation of molecular crystals is critical in processing of pharmaceutical products as well as in tailoring key drug properties such as dissolution rate and stability. The inelastic response of these crystalline materials is mediated by dislocation motion and their interaction with defects, such as second phase particles, dislocations, grain boundaries and stress free surfaces. This is particularly important when the scale of the volume of analysis approaches the microstructure scale as in micron and submicron size particles. Here we propose a model to study the transition from a high dislocation density crystal to an amorphous material during the process of milling of molecular crystals. In particular we analyze the effect of grain and particle size in this transition with 3D phase field dislocation dynamics simulations.

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MS87

A Stochastic Model for the Propagation of Cracks

in Heterogeneous Solids

Crack propagation is the fundamental process leading to the failure of brittle solids. However, if one goes beyond the failure of a continuum homogeneous medium and considers more realistic situations, i.e. solids with inhomogeneous failure properties, various aspects of its dynamics become unclear, in particular about the intermittent dynamics of cracks or the variations of its growth velocity with the external driving force. In this work, we show how one can extend the classical theory of Fracture Mechanics to inhomogeneous media, and propose a stochastic equation of motion to describe the propagation of a crack. Our analysis shows that the quasi-static failure of inhomogeneous solids corresponds to a dynamical critical transition also referred to as a depinning transition: critical failure occurs when the driving force is sufficiently large to depin the crack front from the material heterogeneities. Another remarkable prediction of this crack growth model is a highly intermittent crack dynamics close to the failure threshold. We show that propagation occurs through sudden jumps, with power law distributed sizes and durations. These predictions compare quantitatively well with the direct observations of the propagation of interfacial cracks in heterogeneous solids. These results show that the depinning transition of cracks in heterogeneous solids is revealed both by the average crack dynamics and by its velocity fluctuations. Such an interpretation of failure of brittle materials opens new perspectives in the design of stronger solids with increased lifetime that will be finally discussed.

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