CP1
Percolation of Conductivity for Carbon Nanotubes

The problem of the percolation of conductivity that occurs from the suspension of carbon nanotubes in a nonconductive polymer matrix is of considerable interest for applications in the development of electronic devices at the nanoscale. The onset of conductivity awaits accurate prediction. This talk will examine models (Schramm-Loewner evolution [SLE], lattice-path walks, moduli space integration) that attempt to present this behavior. The advantages and disadvantages of these approaches will be discussed.

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CP1
Facet Evolution on Supported Nanostructures: the Effect of Finite Height

Nanostructures relaxing on a substrate consist of a finite number of steps and therefore have a finite height. We show that finite height effects play an important role in the structure's macroscopic evolution: for axisymmetric nanostructures relaxing under elastic/entropic repulsions and step line tension, we demonstrate a switch in the time behavior of the facet's radius from $O(t^{1/4})$ to $O(t)$.

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CP1
Simulation of Self-Organization in Surface Processes

Self-organization of components of two phase mixtures through diffusion is known as Ostwald ripening. This multiscale phenomenon is can be studied using mesoscopic models which are stochastic partial differential equations that have been derived directly from the underlying microphysics. In this talk, results from simulations using spectral schemes for stochastic partial differential equations are described. These simulation results are compared with theoretical results such as the Lifshitz-Slyozov growth law; the effect of adjusting the interaction length scale is also described.

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CP2
Mathematical Modeling of Heat-Shrinkable Thin Films

We present a mathematical model for simulating the behavior of thin films that undergo an irreversible deformation upon applying heat to their surface. We derive an asymptotic model, compare and relate to results obtained by using Γ-convergence techniques, and present numerical results. The problem is motivated by industrial attempts to deform originally flat, thin protective layers into shapes that can be easily applied onto car windshields. A typical material used in the simulations is PET.

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CP2
New PDEs from Polycrystal Plasticity

Several highly degenerate nonlinear PDE arising as Aronsson equations associated to variational principles for models in Polycrystal Plasticity obtained via Γ-convergence are introduced.

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CP2
High Contrast Homogenization in Dimension 2: Conduction Vs. Elasticity

We study the asymptotic behaviour of two-dimensional linear elasticity problems with equicoercive elasticity tensors. Assuming the L^1-boundedness of the sequence of tensors, we obtain a compactness result extending to the elasticity setting the divcurl approach of M. Briane and J. Casado-Daz for the conduction. We also show there is a gap, in the limit behaviour, between the very stiff problems of elasticity and those of conduction described by M. Briane and J. Casado-Daz.

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CP2

Variational Estimates for the Effective Conductivity of 3D Nonlinear Polycrystals

Bounds and estimates for the effective conductivity of nonlinear polycrystalline aggregates with isotropic crystallographic texture and two-point statistics are obtained by means of the "variational linear comparison" method of deBotton and Ponte Castaeda (1995). Use is made of the Hashin-Shtrikman (HS) bounds and of the "effective medium approximation" (EMA) for certain, suitably chosen classes of "linear comparison composites" to generate corresponding estimates for the nonlinear polycrystals. The new results are compared with the bounds of Garroni and Kohn (2003) for isotropic nonlinear polycrystals. As expected, it is found that the HS bound improves on the translation Garroni-Kohn bound for weakly anisotropic crystals, but is much weaker for strongly anisotropic crystals. However, surprisingly, it was found that the HS bound could be sharper than the linear comparison Garroni-Kohn bound, generated by making use of the linear conductivity bounds of Avellaneda et al. (1988), even for strongly anisotropic crystals (in some special situations). In addition, the linear comparison EMA estimates, not only satisfies all the bounds, including the translation Garroni-Kohn bound, but exhibits a scaling law that is strictly sharper than that predicted by the translation bound. The implications of these observations for the variational linear comparison methods, and for nonlinear homogenization, more generally, will be discussed.

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CP3

Complex Fluids in Microfluidic Devices: Purely Elastic Instabilities and Drop Breakup

Fluids with mesoscopic structure (e.g. polymeric liquids and DNA suspensions) often exhibit complex rheological behavior, particularly in response to applied external forces. Two examples are discussed here. First, we investigate the flow of viscoelastic polymeric fluids in an extensional flow, in which two flow instabilities are found. Next, the effects of elasticity on filament thinning and drop breakup in microchannels are investigated, in which the filament thinning shows two distinct temporal regimes: flow- and capillary-driven.

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CP3

Symmetry Properties of the Elastic and Bending Energy of a 2-Dimensional Fibered Network, with Applications to Soft Materials and Bio-Materials

In this work we study how the fine-scale geometry of a 2-dimensional network of deformable fibers affects the symmetry properties of the elastic and bending energy of the material. We focus on textiles that can be modelled as 2-dimensional networks of inextensible fibers, with a view to applications to biological tissues. For networks made by two families of fibers, four types of fine-scale structures are possible, corresponding to the simplest weave patterns in textiles as defined by the angle between the fibers and their material properties. The symmetry properties of the pattern determine the material symmetry group of the network, under which the deformation energy is invariant. In this work we derive representations for the elastic and bending energy of such materials, that are invariant under the symmetry group of the network. We also discuss the relation of these invariants with classical models in which the deformation energy depends from the shear and the curvature of the fibers only.

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CP3

A Model for Particle Size Segregation in Granular Flow under Nonuniform Shear

A hyperbolic conservation law in one space variable and time describes particle size segregation in the presence of nonuniform shear. This PDE generalizes the Savage-Lun (1988) and Gray-Thornton (2005) models of segregation in granular avalanches, which assume uniform shear. Size segregation is observed in a Couette cell experiment in which a bidisperse mixture of spherical glass beads is sheared by rotating the bottom boundary. Experimental results are compared to analysis of the PDE model.

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CP4

Inverse Elastic Electron Scattering with Adaptive Regularization and Meshes

To recover nanoscale material properties from the transmission electron microscope, inverse scattering is considered. Basically an accelerated electron considered as a plane wave propagates in empty space before interacting with a sample potential that is looked for. The measured and computed waves at the sample exit plane depend on this potential. Adaptive meshing methods regularizes the inverse scattering problem for both direct and adjoint states. Error estimators iteratively drive the refinement of the potential discretization.

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CP4

Data Parallel Block-Tridiagonal Divide-and-Conquer Eigensolver for Scf

In electronic structure calculation, solving non-linear eigenvalue problem using the SCF method is very time-consuming. As a matter of fact, in many cases it is not necessary to calculate eigen-solutions to full acccuracy. The block-tridiagonal divide-and-conquer algorithm calculates the eigen-solutions of a group of real symmetric matrices to pre-specified accuracy efficiently. We use trans-PA to demonstrate the efficiency of this algorithm and compare the advantages and disadvantages of data parallel and mixed data/task parallel implementations.

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CP4

First-Passage Monte Carlo for Materials under Irradiation

We present a principally new mathematical algorithm for Monte Carlo simulations of irradiated materials. Derived from the theory of first-passage processes and a time-dependent Green's function formalism, the new algorithm extends the simulated time horizon from minutes to tens and hundreds of years while retaining uncompromising accuracy. The new method presents an exciting opportunity to use accurate computer simulations for extrapolating material behavior observed in accelerated material tests to the much longer reactor material lifetimes. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. (UCRL-ABS-235912).

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CP4

Patch Dynamics: Macroscopic Simulation of Multiscale Systems

We discuss patch dynamics schemes as a means to perform simulation of an effective, macroscopic PDE, when the most accurate model of the system is given on a more microscopic scale. The schemes estimate the time derivative (for finite differences) or flux (for finite volumes) by performing a local simulation with the microscopic model in small patches around the macroscopic grid points. We discuss how to initialize this microscopic simulations, as well as how to choose the size of the patches and the boundary conditions and the simulated microscopic time. We present convergence results for classical homogenization problems and illustrate the method on a number of examples.

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CP5

Coherent and Incoherent Near-Resonant Dynamics in Biased Superlattices

We study electron dynamics in a biased undriven semiconductor ideal superlattice near energy level anticrossings in the presence of dissipation. In particular, we examine the dependence of wavepacket dynamical characteristics on electric field detuning and investigate mixed regimes involving superposition of energy level anticrossings and both Rabi oscillations and resonant Zener tunneling. Rabi and Zener resonances were shown to have same origin and a criterium for the occurrence of either was proposed.

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CP5

Absorbing Boundary Conditions for Atomistic-to-Continuum Coupling

When molecular dynamics (MD) models are coupled with continuum models, absorbing boundary conditions (ABCs) for MD region are required to prevent spurious heat-up due to phonon reflection. Many existing MD-ABCs are either accurate or efficient, but not both. By modifying an existing boundary condition for wave propagation problems, we present a new method that can effectively absorb high-frequency phonons. This talk will include formulation and numerical examples illustrating the superior performance of the proposed ABC.

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CP5

Using Kinetic Monte Carlo to Simulate Dendritic Growth

We consider the three dimensional growth of a dendrite into an undercooled melt. By combining standard Kinetic Monte Carlo for surface evolution, a temperature-dependent solidification rate, and the solution of the heat equation in the bulk we are able to exhibit the growth of dendrites on scales up to about a micron. This offers the potential to complement larger scale simulations based on continuum models.

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CP5

A New Method for Simulating Strongly

Anisotropic Cahn-Hilliard Equations

We present a new approach for modeling strongly anisotropic crystal and epitaxial growth using regularized, anisotropic Cahn-Hilliard-type equations as a model for the growth and coarsening of thin films. When the surface anisotropy is sufficiently strong, sharp corners form and unregularized anisotropic Cahn-Hilliard equations become ill-posed. Our models contain a high order Willmore regularization to remove the ill-posedness at the corners. A key feature of our approach is the development of a new formulation in which the interface thickness is independent of crystallographic orientation. In particular, we find excellent agreement between the computed shapes using the Cahn-Hilliard approach, with a finite but small Willmore regularization, with dynamical numerical simulations of a sharp interface model. The equilibrium shapes from our diffuse model are compared with an analytical sharp-interface theory recently developed by Spencer (2004) at the corners, and there is excellent match. Away from the corners there is an excellent agreement between the diffuse model with the classical Wulff shape. Finally, in order to model the misfit and displacement strains, we add the elastic energy and corresponding forces to our diffuse model. We analyze numerically the effect of elastic stress on the corner regularization in terms of two parameters: one parameter that describes the relative strength of the elastic energy to surface energy and the second that charactrastics the strength of the surface energy anisotropy.

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CP6

An Age Hardening Model for Interrupted Ageing of the Alloy Aa6061

A physically based model for interrupted ageing of the 6000 aluminum alloys has been developed which correlates the size, shape, and volume fraction of needle-shaped and spherical precipitates to the ageing parameters and yield strength. Simulation results demonstrate that the influence of interruption temperature on strength evolution can be related to size and shape distribution of the precipitates formed during interrupted ageing.

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CP6

Nonlinear Phase-Transformation Waves in Rechargeable Batteries

We present a general continuum model of phase transformation dynamics in rechargeable battery materials. It is based on a phase-field formulation and takes into account: (i) strong crystal anisotropy and (ii) surface Faradaic reactions, driven by chemical potential differences. Under certain conditions, the model admits nonlinear wave solutions, consistent with recent experiments on lithium iron phosphate, a promising material for high-rate applications. Wave-defect interactions also provide a new mechanism for power fade over many cycles.

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CP6

Structural Phase Transformations Studied by Molecular Dynamics Simulations in Some Binary Metal Systems

Applying the constructed n-body potential, the mechanism of martensitic phase transformation in the Ni-Ti, -Hf systems and physical origin of crystal-to-amorphous phase transformations of some binary transition metal systems were investigated through molecular dynamics simulations. It is shown that the intrinsic glass forming ability of metal systems could be directly estimated by MD simulations.

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CP6

Interfacial Reaction in Some Equilibrium Miscible and Immiscible Metal-Metal Multilayers Investi-

gated by Molecular Dynamics Simulations

Through molecular simulations, it is revealed that the interfacial amorphizations of metal-metal multilayers exhibits an asymmetric behavior in growth kinetics. The driving force of the interfacial reaction in the immiscible systems is the excess interfacial energy. The maximum thickness of the amorphous layer is calculated from thermodynamics model and the calculated results matches well with the MD simulation.

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CP6

The Effect of Material Properties of Interphase on the Bulk Modulus and Coefficient Thermal Expansion of Nanocomposites Containing Spherical Fillers

This work is to investigate the effect of the interphase on the Bulk Modulus and Coefficient Thermal Expansion (CTE) of nanocomposites containing spherical fillers. A mathematical model describing the material properties of the interphase is presented as a function of the thickness of the interphase between the filler and matrix. The Bulk Modulus and CTE of nanocomposites are obtained using the replacement method. The results agree well with the experimental and numerical results from literature.

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CP6

Molecular Dynamics Simulation of Acoustic Phonon Scattering from Particles Embedded in An Anisotropic Medium

Three-dimensional elastic wave scattering from isolated nanometer-scale impurity particles embedded in silicon is investigated using a new molecular dynamics simulation technique. The technique enables, for the first time, direct observation of the effects of mode conversion, lattice mismatch strain, elastic anisotropy, and atomistic granularity on acoustic phonon scattering from nanoparticles. The results will be useful for the design of novel nanoparticle-based thermal insulating materials, for example quantum dot superlattices for thermoelectric energy conversion.

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MS1

On the Definition of Stress in Molecular Dynamics

The ability to create and manipulate nanoscale structures has renewed interest in understanding the role of stress at the atomic scale. In particular, in a molecular dynamics setting, one would like to compute stress given a description of interatomic potentials, atomic coordinates, and momenta. Key concepts leading to the so-called virial stress were formulated by Clausius in 1870 in a study of the "effective force of heat," and have been adopted, more or less consistently, since then. Nevertheless, a rigorous derivation of atomic-level stress and proof of its validity has been somewhat elusive. In this paper, a derivation is given that is consistent with Cauchy's notion of the stress tensor and based upon the principle of virtual work. The result comprises four terms: the two well-known terms of the Virial Stress and two others. To understand the significance of each term and to establish the validity of this atomic-level stress, we have carried out a series of molecular dynamics simulations for heating of both harmonic and anharmonic crystals, with and without constraint. The calculated stresses are shown to agree both with physical intuition and continuum limits.

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MS1

Thoughts on the Concept of Stress

A rational analysis of the concept of stress must be based on a suitable mathematical infrastructure for continuum physics. It involves mathematical structures for understanding physical systems, the distinction between internal and external forces, and basic balance laws. In the special case of surface forces, one can prove the existence of a stress-contactor field, under reasonable conditions and with highly non-trivial proofs. Internal forces at a distance are often assumed to be absent in traditional continuum mechanics, but they should be included in a more general framework. One can then prove, under reasonable conditions, the existence of a lineon field that enters the local balance equations in the same way as the stress-lineon field. The adjective peridynamic has recently been used for such fields.

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MS1

Calculation of Local Stress and Elastic Constants Via Computer Simulation

I will discuss the calculation of local stresses and elastic constants using atomistic computer simulation. In particular, various local stress measures will be compared and contrasted by examining the stress field around an idealized defect. In addition, the use of displacement fluctutation formulae to obtain elastic response at different length scaled will be outlined.

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MS1

Microscopic Foundations of Continuum Mechanics: Overview and Current Directions

A great deal of attention is currently placed on the development of multiscale methods that couple discrete atomistics with continuum models. The correctness of such approaches hinges on the existence of definitions of continuum quantities at the microscopic scale. Despite this, a great deal of confusion and controversy still exists in this area. Examples include the lack of a clear microscopic definition for stress and controversies related to the principle of material-frame indifference. An overview of these issues will be presented along with some recent results.

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MS2

Fast and Ultrafast Dynamics of Magnetic Vortices in Confined Structures

Ferromagnetic thin-film elements have a natural tendency to form flux-closure magnetic domain patterns. Such flux-closure structures inevitably contain at least one magnetic vortex, i.e., a point around which the magnetization direction circulates in the film plane. In the core region of such vortices the magnetization aligns perpendicular to the surface. Remarkably, this tiny core region can have a decisive impact on the dynamic properties of vortices. The core magnetization, pointing either up or down, affects the orbit of the gyrotropic mode, a low-frequency excitation in which the vortex core rotates around its equilibrium position with a frequency of typically a few 100 MHz. The gyrotropic mode and other non-trivial dynamic properties of magnetic vortex structures have recently attracted much interest. By means of finite-element micromagnetic modelling, we have investigated the fast and ultrafast dynamics of vortices triggered either by external field excitations or by electric currents. We thereby discovered the fastest and probably most complicated micromagnetic switching process known to date. The simulations show that, if a vortex structure is excited above a well-defined energy threshold, it undergoes a dynamic transformation consisting of a series of vortex-antivortex pair creation and annihilation processes, which ultimately lead to the switching of the core region. This novel core switching process occurs within only a few tens of ps and is thus much faster than what was previously believed to represent the fundamental limit of magnetic switching speed. The three-dimensional simulations provide important insight into the complicated details of this micromagnetic process and allow for clear predictions for possible experimental studies.

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MS2

Thin-film Limits for Landau-Lifshitz-Gilbert Equations

Starting from the full micromagnetic model and a regime where the competition between stray-field and gyrotropic forces becomes singular, we derive an effective thin-film for the Landau-Lifshitz-Gilbert in form of a damped geometric wave equation. The analysis can be carried situations where exchange energy dominantes such as in microscopic models for domain walls and certain small particle models that exhibit boundary singularities. Finally we show applications to kinematic particle models for moving Neel walls.

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MS2

Spin Transfer Torques and Damping in Magnetization Dynamics

Current induced magnetization dynamics is routinely measured experimentally in both nanopillars and nanowires. In spite of the large theoretical effort addressing these experiments, much is still not known and more is difficult to treat computationally. In this talk, I describe what we think we know about the spin transfer torque and the magnetic damping in these systems. Then I discuss what aspects of the problem have been successfully modelled and some of the open questions.

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MS2

Dynamics of Domain Walls in Magnetic Nanostrips

Domain walls in ferromagnetic nanostrips can be moved by an applied magnetic field or spin current. Experiments and numerical simulations reveal a rich dynamics of the wall motion. In a weak field a wall moves steadily with a velocity proportional to the field strength. Above a critical field the steady motion breaks down and acquires an oscillatory character, which causes the drift velocity to drop significantly. We show that the root cause of this complex dynamics can be traced to the composite nature of domain walls. A wall typically consists of 2 or 3 elementary topological defects: vortices with integer and half-integer winding numbers. We model the motion of a wall using collective coordinates to parametrize soft modes. These modes exhibit an overdamped dynamics with topological terms due to a nonzero skyrmion charge carried by bulk vortices. The established framework describes wall motion with any number of collective coordinates. We apply our formalism to calculate the drift velocity of the vortex wall both below and above the breakdown. The results are compared to numerical simulations and available experiments.

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MS3

Overview of Coarsening in Networks

We briefly introduce and survey the issues to be discussed in this minisymposium. Network evolution or coarsening is a metastable process. This has consequences for what we can know about the system. New results in both theory and simulation bring us to a new level of understanding of the topological and statistical properties of materials evolution on a variety of levels, but the picture is far from

being complete. A broad perspective on current state of the art techniques and novel analytical, experimental and simulation results will be provided.

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MS3

The Geometry of Grains

This talk explores a good notion of the linear dimension of a 3 dimensional grain called the "mean width". The mean width is an essential component of the three dimensional analogue of the Neumann-Mullins law for the rate of growth of an individual grain, which is joint work with David Srolovitz. It should also be useful in other contexts.

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MS3

Effect of Crystal Symmetry on Stress-driven Grain Boundary Motion

A grain boundary (GB) can be moved by applied shear stresses and its motion produces shear deformation of the material. The coupling factor between the velocities of GB migration and parallel grain translation is a multi-valued function of the GB crystallography. We propose a theory predicting the complete set of coupling factors from the grain misorientation and the point-symmetry group of the crystal. The theory is tested by atomistic simulations of coupled GB motion.

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MS3

Grain Growth in Three-Dimensions: Exact and Simulation Results

We report on the extension of the famous two-dimensional von Neumann-Mullins law for the rate of growth of individual grains in a polycrystal to three (and all) dimensions. The exact three-dimensional result is based on the natural, linear measure of grain size. We present tests of the theory using Surface Evolver to model motion by mean-curvature in three-dimensions.

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MS4

Ferroelectrics for Actuator, Sensor and Optical Applications

Abstract not available at time of publication.

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MS4

Application of Multi-scale Modelling in Industry Needs and Challenges from a Mathematical Perspective

Abstract not available at time of publication.

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MS4

Multiscale Modeling of Crystalline Solids: Some Crucial Issues

I will discuss some of the most crucial issues on multiscale modeling of crystalline solids, including accuracy across atomistic-continuum interface, boundary conditions, treatment of thermal effects, etc. The new work presented here is joint with Xiantao Li and Pingbing Ming.

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MS4

Accelerating Materials Design with First Principles Calculations and Machine Learning

Concomitant advances in solid state physics and computing technology have opened the door for ab initio calculations to play a role in the design and discovery of new materials. In this talk we will highlight a framework in which ab initio methods are combined with machine learning techniques to discover materials with optimized properties. By combining the accuracy of ab initio calculations with the suggestive and self-learning character of machine learning techniques we have performed a large scale exploration of multi-component oxides and will discuss potential applications.

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MS4

Bulk Materials for Thermoelectric Energy Conversions

First principles prediction and tailoring of materials for thermoelectric energy conversion is a formidable task. Electrical and heat transport coefficients must satisfy contradictory requirements that depend on the details of the electronic structure, the anharmonic terms in the vibrations, and the effects of chemical disorder and defects. In order to capture the different length scale we have mapped the electronic structure on maximally localized Wannier functions and extended the predictive power of first principles methodologies to systems with hundreds of atoms. Approaches to screen thermoelectric materials based on their vibrational properties have also been devised in the framework of density functional perturbation theory. We show applications of our methodologies to prototypical silicon nanostructures, skutterudites, and germanates.

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MS5

Mathematical Problems of Q-tensor Theory

The talk will discuss various mathematical issues raised by the Q-tensor theory of de Gennes.

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MS5

Dynamics of Liquid Crystal Colloids Studied by 3D Microscopy of the Director Field

Liquid crystals colloids represent a fascinating class of soft matter, in which the equilibrium is often achieved by introducing topological defects in the director field, stabilized by surface anchoring at interfaces. In this report we present recent experiments on the dynamics of micron-size colloidal particles in a liquid crystal driven by an electric field. The director structures around the colloidal particles are determined using the recently developed techniques of 3D microscopy. We demonstrate that the applied electric field causes translational and rotational motion of the colloids and discuss the underlying mechanisms that include specific liquid crystal effects such as backflow (coupling of director reorientation and mass flow) and mechanisms of a general nature, valid in both anisotropic and isotropic fluids, such as electrorotation and hydrodynamic interaction between the particle and the confinig wall. The work has been supported by NSF DMR 0504516, Department of Energy, W.M. Keck Foundation, Ohio CMPND Program.

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MS5

Size and Shape Selection in Colloidal Liquid Crystalline Gels and Elastomers

Abstract not available at time of publication.

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MS5

Disorder Induced by a Perturbed Boundary in Nematic Liquid Crystals

When a nematic liquid crystal is bounded by a rough surface, the wrinkling of the surface induces a partial melting in the degree of orientation. This softened region penetrates the bulk up to a length scale which turns out to coincide with the characteristic wavelength of the corrugation. Within the boundary layer where the nematic degree of orientation decreases, the tilt angle steepens and gives rise to a non-trivial structure, which may be interpreted in terms of an effective weak anchoring potential. We will show how the effective anchoring strength is related to the microscopic roughness parameters and how the result can be rephrased in terms of a variational convergence for functionals.

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MS6

Overcoming Passive Transport Limitations: Concentration Enhancement Through Dynamic Loading

Studies have traditionally demonstrated that dynamic loading can increase the absorption rate of large molecules in hydrated tissue. Recently, it has been theoretically predicted that such loading may additionally yield higher steady state concentrations, beyond those achieved by passive diffusion. In this study we have implemented a dextran agarose model system to experimentally demonstrate this transport phenomenon, showing the biophysical potential of dynamic loading to overcome passive transport limitations and enhance nutrient supply.

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MS6

Modeling Swelling Porous Materials Accounting for Ionic and Hydrating Froces

For modeling swelling porous materials many models take

into account ionic interactions (especially models of biological tissues) or hydration forces (e.g. models for expansive soils). Here we consider a model based on hybrid mixture theory which accounts for both ionic and hydrating forces for flow and deformation.

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MS6

Multiscale Stiffness Prediction of Ionic Polymers

A multiscale modeling approach applied to the stiffness prediction of polymers with high crosslink density is presented. The approach applies the Mark-Curro approach to Rotational Isomeric State theory to develop a simulation model for Nafion polymer chain conformation; the resulting predicted chain lengths between crosslinks are used to generate probability density functions with the most appropriate Johnson family method. It is found that applying a simulation with chains having [50, 80] repeat units is sufficient to yield repeatable predictions.

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MS6

Mechano-chemical Models of Swelling in the Microscopic Environment of Articular Cartilage

Articular cartilage extracellular matrix can be modeled as a triphasic continuum mixture comprised of solid, fluid and ionic phases. Such models account, separately, for contributions of collagen fibers, fixed negative charges due to proteoglycans, interstitial fluid and dissolved ions to the apparent mechanical response of the tissue. In this talk, mechano-chemical models for osmotic swelling in the local environment of a single cartilage cell (chondrocyte) will be presented.

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MS7

The Stress in Periodic MD and Objective MD

Objective MD is a method of doing exact molecular dynamics that relies on the existence of an invariant manifold of these equations. It provides a simple way to simulate the behavior of diverse molecular structures, from carbon nanotubes to DNA to viral capsids. It also has fascinating links to known exact solutions of the Boltzmann equation (more precisely, to the equations for the moments) and to viscometric flows of non-Newtonian fluids. A similar question arises in these simulations as arises in periodic MD: what are the macroscopic forces and moments that correspond to such a simulation? We discuss this from a mathematical viewpoint.

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MS7

The StressTensor of a Molecular System: An Exercise in Statistical Mechanics

We prove that conservation of the stress tensor is a consequence of the invariance of the partition function under canonical diffeomorphisms. From this observation a simple and general derivation of the formula which gives the local expression of the stress tensor of a molecular system in terms of its microscopic degrees of freedom readily follows. The derivation is valid in the canonical as well as the micro-canonical ensemble. It works both in the classical and in the quantum mechanical setting and for arbitrary boundary conditions.

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MS7

Revisiting Quantum Notion of Stress

Existing notions of stress in a quantum mechanical framework are reviewed and discussed. Notwithstanding early fundamental work in this area since 1930s, the increasing availability of computational tools to perform ab initio quantum mechanical calculations with high accuracy and efficacy has renewed interest in this field especially in the context of computational mechanics and materials science. Although some unresolved issues remain, the subject has evolved considerably in the past two decades with various authors offering their own unique viewpoint. In the present review, we summarize the debate over the definition of stress in a quantum mechanical setting and discuss some controversial issues such as the uniqueness of the stress. Finally, we provide our own perspective.

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MS7

Atomic Level Stresses and Moduli in Condensed Matter Systems

Stresses at atomic level exist in any structure with non-equivalent atoms. However, an exact definition of both atomic level stresses and moduli has been elusive. We first discuss this problem within the density functional theory. However, when using potential schemes to describe bonding these quantities are well-defined and reflect local structural features. This will be illustrated on studies of structural relaxation of glasses, core structures of dislocations and local structures and properties of grain boundaries.

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MS8

Oscillating Cracks in Quenched Glass: Numerical Experiment

This talk presents a first attempt at providing a verification of the variational formulation of quasi-static brittle fracture using a quenching experiment of glass strips. For this problem, a large typology of crack evolutions has been identified in several experimental campaigns. The qualitative and quantitative properties of these evolutions depend on the experimental conditions and the materials used. I will briefly present the experimental setting and the variational model. I will discuss the numerical implementation of this model, and some details specific to this problem. Then, I will compare numerical and experimental results.

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MS8

Cohesive Zone Models

When cohesive forces act between the lips of an opening crack, the mathematical treatment of crack growth in the quasistatic regime shows serious mathematical difficulties. This talk presents some preliminary results when the crack path is prescribed. In particular, materials exhibiting a different behavior under loading and unloading are considered.

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MS8

Overview of Mathematical Issues in Damage and Fracture

I propose to review the so-called variational approach to quasi- static evolution, starting from basic principles in defect mechanics and demonstrating how the variational formulation naturally follows on both fracture and damage. I will then quickly review the state of the art, then describe various alternative models and gauge their performance when compared to the original theory. I will finally briefly evoke numerical approximating schemes, both in fracture and damage.

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MS8

Quasi-static Propagations of a Brittle Crack

We consider a brittle material under displacement control with a mode III crack running, in quasi-static regime, along a predefined path. Several definition of evolution, based on variational criteria, have been proposed in the last few years, essentially after the work of Francfort and Marigo. Our aim is to study these solutions, placing a special emphasis on energy, energy release rate and jump discontinuities, which may occur because of the non-convexity of the problem. The analysis is performed in a common framework, starting from the incremental formulation of problem, in such a way that similarities and differences appear clearly. Finally, we will present an ordering property of the evolutions.

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MS9

Mesoscale Modeling of Polycrystals: Interplay of Theory and Simulation

Facet interchange and grain deletion, coarsening induced variations in topology, introduce network level changes in the system which are stochastic in nature. Understanding these effects is crucial to the development of a complete theory of grain growth and is the focus of many investigations. We outline several recently developed theoretical approaches and summarize their advantages and difficulties. Key theoretical observations, such as time and space correlations, as well as steady-state solutions, are revealed, with theoretical predictions further compared to the results obtained via large-scale simulations and experiments. Newly discovered features of the dynamics underlying coarsening process discussed in this talk have implications for a wide class of physical applications.

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MS9

Modeling of Critical Events in Microstructure

We study critical events in a one-dimensional grain-boundary system in order to understand the role of topological reconfigurations during coarsening in polycrystalline materials. We introduce a stochastic framework for modeling texture evolution and formulate the model based on a master equation derived from numerically determined statistical properties of the system.

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MS9

Testing the MacPherson-Srolovitz Theory in Sim-

ulations of 3D Grain Growth

The theory by MacPherson and Srolovitz [Nature 446:1053 2007] provides an exact prediction of the growth rate of individual cells or grains in a space-filling network (microstructure). Testing the predictions of the theory requires measurement of (1) mean width (aka mean breadth) and (2) edge lengths where three cells meet at triple line junctions. This is most easily accomplished in networks that are discretized with a mesh. A Moving Finite Element (MFE) model was used to simulate the evolution (grain growth) over short times of a network discretized on a tetrahedral mesh and growth rates. Volumes, mean widths and edge lengths were measured. In this context, the times are short in comparison to the interval between topological changes in the network such as disappearance of a grain. The growth rates measured from the simulation were found to be in very good agreement with the predictions of the MacPherson-Srolovitz theory. The results from similar measurements in Monte Carlo and Phase Field models of grain growth will also be reported. In this case, measurement of mean width and edge length is complicated by use of a regular grid to discretize the network on a set of points or voxels. A modified algorithm by Ohser and Mcklich [Statistical analysis of microstructures in materials science, 2000] is used to measure mean width. Edge length measurement along triple lines requires conversion of the voxel image to a surface mesh. This work is supported by the National Science Foundation and by the Office of Naval Research. Extensive discussions with David Srolovitz are gratefully acknowledged.

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MS9

Challenges in Modeling Large Scale Interfacial Networks

Polycrystalline materials are in abundant use in most technologies ranging from microelectronic devices to structural components of airplanes. Their reliability and failure is of major concern in many engineering fields. In this talk we focus on modeling and simulation of large scale interfacial networks in polycrystals. We discuss mathematical formulations and their dissipative discretization schemes. We end with distribution functions that characterize the network at the mesoscale and point to approaches for constructing their equations.

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MS9

Morphology of Critical Nuclei in Solid-state Transformation and Relation to Microstructure Evolution

Predicting the shape of a critical nucleus in solids has been a long-standing problem in solid-state phase transformations. We show that a phase field model combined with a minimax algorithm is able to predict the 2D/3D critical nucleus morphology in elastically anisotropic solids without a priori assumptions. It is found that strong elastic energy contributions may lead to critical nuclei whose point group symmetry is below the crystalline symmetries of both the new and parent phases.

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MS10

Lipid and Protein Sorting during Membrane Tube Formation

Thin membrane tubes are common natural cellular structures and are also practically important for assays to measure membrane stiffness. Here we examine how the dependence of bending stiffness and surface tension on membrane lipid and protein composition affects tube formation. We show that drawing a tube from a vesicle leads to a rearrangement of composition in which the phase of higher flexibility segregates in the tube, the region of high mean curvature. The force vs. extension curve has a sharp drop just as the tube begins to form, consistent with experiments.

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MS10

A Path Integral Formalism of DNA Looping Probabilities

We derive a formula for the "semi-classical" approximation to the probability density function for looping of a stiff polymer such as DNA. The approximation includes fluctuations up to quadratic contributions about a local energy minimizer, and is based upon a path-integral formalism. The derived formula can always be evaluated in a straightforward fashion with a fast numerical computation. In simple cases the formula can be evaluated completely analytically. This is joint work with L. Cotta-Ramusino and R. Manning.

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MS10

Tethered Particle Motion: Theory and Experiment for Looped and Unlooped DNA

Tethered particle motion (TPM) is an experimental technique to monitor conformational changes in single molecules of DNA in real time, by observing the position fluctuations of a micrometer-size bead attached to the DNA. We present some recent work on theoretical problems inherent in the interpretation of TPM experiments, both in equilibrium and dynamical aspects. (1) The mean-square motion of the tethered bead can be used to report on the characteristics of its tether. We report on Monte Carlo simulation results, and compare them to experiments, relevant to bead diameters between 200–1000 nm and tether

lengths between 100–1000 nm. (2) Relatively long camera shutter times are sometimes convenient experimentally, but complicate the theory. We report a new correction scheme that compensates for this, and improves our agreement with new experimental data. (3) TPM is an attractive method for studying DNA loop formation by protein complexes such as LacI. We report a new Gaussian sampling Monte Carlo simulation method that roughly concurs with new TPM experimental data for loop sizes around 300 basepairs. (4) Experimental determination of looping kinetics is complicated by the near coincidence of the loop formation/breakdown lifetimes with the diffusion time of the bead in typical experiments. We present a new modification of Hidden Markov modeling that disentangles these two processes and hence yields rate constants from noisy experimental data.

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MS10

Fast High-Order Methods for Simulating the Dynamics of Inextensible Vesicles

Vesicle flows model numerous biophysical phenomena that involve deforming particles interacting with a Stokesian fluid. While conventional techniques can be used to simulate isolated vesicles, new approaches are needed for large number of interacting vesicles. We present a novel method for such problems. It incorporates a new time-stepping scheme that allows much larger time-steps than the existing explicit schemes. The associated linear systems are solved in optimal time using spectral preconditioners and fast summation techniques.

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MS11

Defect Effects in Smectics

The theory of smectic liquid crystals is notoriously difficult to study. Thermal fluctuations render them disordered through the Landau-Peierls instability, lead to anomalous momentum dependent elasticity, and make the nematic to smectic-A transition enigmatic, at best. I will discuss recent progress in studying large deformations of smectics which necessitate the use of nonlinear elasticity in order to preserve the underlying rotational symmetry. By recasting the problem of smectic configurations geometrically it is often possible to exploit toplogical information or, equivalently, boundary conditions, to confront these highly nonlinear problems. Specifically, I will discuss edge dislocations, disclination networks in three-dimensionally modulated smectics, and large angle twist grain boundary phases. Fortuitously, it is possible to make intimate comparison with experimental systems!

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MS11

Defects of Liquid Crystal Configurations and their Dynamics

Abstract not available at time of publication.

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MS11

Equilibrium Properties of Liquid Crystals in Confined Geometries

We study liquid crystal configurations within the continuum Landau-De Gennes theory. We obtain explicit upper bounds for the order parameters of equilibrium energy minimizing configurations in terms of the temperature, material constants, geometry and boundary conditions. These bounds show that the Landau-De Gennes predictions for the order parameters fail to agree with the statistical mechanics predictions in the low-temperature regime, far away from the nematic-isotropic transition point. Alternative approaches are discussed.

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MS11

Laser-controlled Molecular Orientation Patterns in Liquid Crystals and their Imaging with CARS Polarized Microscopy

Focused laser beams allow for a non-contact control of matter that can be applied to objects as diverse as atoms, biological molecules, and living cells. I will discuss their use for "shaping of multi-stable molecular orientation patterns in chiral liquid crystals. Starting from the underpinning physics phenomena, I will demonstrate that a focused beam can induce both axially-symmetric and linear localized structures of well-defined molecular orientation patterns. This, for example, allows for producing optically-controlled periodic crystal lattices on the scales ranging from hundreds of nanometers to hundreds of microns. I will show that the fine structure of these molecular orientation patterns is revealed by coherent anti-Stokes Raman scattering (CARS) polarized microscopy [A. Kachynski, A. Kuzmin, P. Prasad, and I. Smalyukh, Appl. Phys. Lett. 91, 151905 (2007).] and then conclude with an overview of potential applications.

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MS12

The Recovery Stroke of Myosin: Atomically Detailed Simulations by Milestoning

Milestoning is a technique to significantly extend the time scale of Molecular Dynamics simulations. It computes ex-

plicitly the time evolution of the system even if the process is not activated and exponential in time. The calculation is done in two steps. First, short time trajectories are used to compute Local First Passage Time Distributions (LFPTD) between nearby Milestones along a reaction coordinate. In the second step a stochastic non-Markovian integral equation that uses the LFPTD computes the overall time course of the reaction. I will briefly describe the technique and focus on an application for the recovery stroke in myosin. Myosin is a molecular machine that provides a power stroke in muscles at the cost of an ATP. Once the power stroke is completed the molecule recovers to its pre-stroke state. The relaxation step is called the recovery stroke. The recovery stroke does not require the investment of biological energy and is spontaneous and reasonably rapid in the presence of ATP. We computed a reaction coordinate for this process using a functional optimization that provides the minimum energy path. For a molecular machine that is designed for efficiency and minimal energy loss it might be expected that the process will follow a single well-focused reaction coordinate. Indeed the Milestoning calculation that uses the computed reaction coordinate (but included all degrees of freedom of an atomic and fully solvated myosin molecule) reproduces the time scale and the expected features of the free energy surface well. Joined work with Anthony West

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MS12

Transition Path Sampling

Abstract not available at time of publication.

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MS12

String Method for the Study of Rare Events

Abstract not available at time of publication.

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MS12

Recent Advances and Ongoing Challenges in Accelerated Molecular Dynamics Methods

Many important processes in chemistry, physics, materials science, and biology take place on time scales that vastly exceed the nanoseconds accessible to molecular dynamics simulation. Often, this long-time dynamical evolution is characterized by a succession of infrequent events. Over the last ten years, we have been developing a new class of methods, accelerated molecular dynamics, in which the known characteristics of infrequent-event systems are exploited to make reactive events take place more frequently, in a dynamically correct way. For certain processes, this approach has been remarkably successful, offering a view of complex dynamical evolution on time scales of microseconds, milliseconds, and sometimes beyond. Examples include metallic surface diffusion and growth, radiation damage annealing in ceramics, and carbon nanotube dynamics. After an introduction to these methods, I will present some recent advances and results, and then describe the major ongoing challenges and our current thinking on how to overcome them.

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MS13

Thermodynamically Consistent Generalized Hydrodynamics

The derivation of generalized hydrodynamic evolution equations(GHEE) attendant on the theory of irreversible processes in nonequilibrium fluids will be discussed. The GHEE consist of the evolution equations of conserved and non-conserved (e.g., stress tensors, heat fluxes, diffusion fluxes, etc.) variables. The making the GHEE materially objective will be discussed. Examples of applications of the theory will be presented, which include shock wave phenomena and rheology. The theory requires transport coefficients from statistical mechanics, and the density fluctuation theory to calculate them for liquids will be mentioned.

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MS13

Microscopic Origin of Stripes and Other Patterns

I will describe results about the formation of periodic structures in systems interacting via both short range attractive and long range repulsive or dipolar type interactions. The models studied include both microscopic ones as well as those described by mesoscopic free energies.

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MS13

Atomistic Scale-dependent Interpretations of Continuum Concepts and Balance Relations

Modelling molecules as interacting point masses whose motions are governed by Newtonian dynamics, it is shown how local balance relations can be established using spatial weighting function methodology. The intrinsic scale-dependence of field values and the concept of 'material point'is emphasised. Attention is drawn to the non-uniqueness of the stress tensor. Remarks are made on nanoscale modelling,material inhomogeneity, and further temporal averaging.

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MS13
A Step Towards Frame-Free Thermomechanics

In 1963 Walter Noll came up with the idea to use the second law of thermodynamics to restrict the form of constitutive equations. This process was first carried out by Coleman and Noll in their famous '63 paper for a specific class of materials and since then has been carried out for various other constitutive assumptions. This process became so standard that it was dubbed the "Coleman-Noll procedure". In my talk I will discuss how this procedure can be carried out without the use of a frame of reference. Extending the ideas in Noll's New Theory of Simple Materials, I will show how all of the familiar concepts in thermomechanics, such as stress and heat flux, can be given meaning when no explicit frame of reference is used. The Clausius-Duhem inequality also has a frame-free counterpart which plays a fundamental role in carrying out the Coleman-Noll procedure in this context. I will also talk about how material symmetry, in the frame-free setting, can place further restrictions on constitutive relations. In order to describe the action of the environment on a body a frame of reference must be used. When the frame-free constitutive equations are placed into such a frame they automatically satisfy the principle of material frame indifference. This is the primary advantage of doing mechanics frame-free; no additional work is required to guarantee that this principle is satisfied.

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MS14
Instabilities in Aluminium Alloys with PLC Effect: Mathematical and Numerical Aspects

Abstract not available at time of publication.

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MS14
Quasi-static Brittle Fracture Evolution and Local Minimality

We give a new definition of stability, ε-stability, that implies local minimality and is robust enough for passing from discrete-time to continuous-time quasi-static evolutions, even with very irregular energies. We use this to give the first existence result for quasi-static crack evolutions that both predicts crack paths and produces states that are merely local minimizers at every time. A new ingredient is the physically reasonable property, absent in global minimization models, that whenever there is a jump in time from one state to another, there must be a continuous path from the earlier state to the later along which the energy is almost decreasing.

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MS14
Dynamic Fracture: An Example of Convergence Towards a Discontinuous Quasi-static Solution

Considering a one-dimensional problem of debonding of a thin film in the context of Griffith's theory, we show that the dynamical solution converges, when the speed of loading goes down to 0, to a quasi- static solution including an unstable phase of propagation. In particular, the jump of the debonding induced by this instability is governed by a principle of conservation of the total quasi-static energy, the kinetic energy being negligible. Some applications of that result to the determination of the effective toughness of a composite material will be investigated.

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MS14
The Loewner Equation and the Critical Stability of a Mode III Crack Configuration

Quasistatic crack evolution is essentially governed by two conditions: critical equilibrium and stability. The first one gives the well-known energy balance equation involving the energy release rate and the Griffith constant. In the Griffith-Irwin formulation, this is a scalar equation involving the stress intensity factor. The second condition did not receive too much attention in the literature. Starting from a critical configuration we consider a family of optimal "trial paths" generated by the so-called Loewner equation in complex analysis. By writing the energy released as a functional over a set of conformal maps, we are able to obtain a second scalar equation for quasistatic crack evolution in Mode III.

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MS15
Numerical Methods for Landau-Lifshitz-Gilbert Equations

The Landau-Lifshitz-Gilbert equation describes magnetic behavior in ferromagnetic materials. The construction of numerical strategies to approximate weak solutions for this equation is made difficult by its top order nonlinearity and nonconvex constraint. Various numerical schemes are now availabe that satisfy the constraint exactly at the nodes of a triangulation. We discuss robustness of the algorithms in the regime of small damping parameters, address the necessity of angle conditions on triangulations, and numerically study the occurrence of finite-time blow-up in two dimensions.

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MS15
Ferromagnetic Nanowires

We present monodimensional models of ferromagnetic nanowires obtained by Gamma-convergence method. For infinite wires, we discuss the stability and the controlability of walls configurations. For finite wires, we explain the hysteresis phenomena by stability arguments.

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MS15
Bifurcation of the Concertina Pattern

The Concertina Pattern is a metastable stage in the switching-process of elongated thin-film magnetic elements. During the switching-process this quasi-periodic structure undergoes a cascade of coarsening events, at which the mean periodicity grows.
We investigate a reduced model rigorously derived from the micromagnetic energy functional:

1. Convexity of the energy in terms of the mean periodicity leads to destabilization.
2. The secondary bifurcations are related to symmetry breaking. The symmetries of the Concertina Pattern determine the number of branches and the type of bifurcation. The branches are computed numerically.

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MS16
A Computational Rod Model to Siumulate the Mechanics of DNA Looping

We employ a rod model to simulate the nonlinear dynamics of loop/supercoil formation in DNA. Our formulation accounts for the structural stiffness of the DNA, its intrinsic curvature, chiral construction and has provisions for its physical interactions with itself, proteins and the surrounding medium. The simulations of an example protein-mediated DNA looping illustrate how the mechanical properties of DNA may affect the chemical kinetics of DNA-protein interactions and thereby regulate gene expression.

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MS16
Mechanics of Gene Regulatory DNA Loops

DNA loop formation in one of several mechanisms used by organisms to regulate genes. The free energy of forming a loop is an important factor in determining whether the associated gene is switched on or off. In this presentation we use an elastic rod model of DNA to determine the free energy of forming short (50-100 basepair) protein mediated DNA loops. We employ the analytical solutions for a non-linearly elastic Kirchhoff rod to determine the shape of the loop and the elastic energy stored in it while also accounting for the superhelical stress in the DNA of living cells.

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MS16
The Fluid Dynamics of Active Suspensions

An active suspension is a fluid whose microstructure is motile, and the roiling dynamics of a bacterial bath is one example of the macroscopic dynamics found in such systems. We have developed micro-mechanical models of simple rod-like swimmers in Stokesian fluids, and simulated the hydrodynamically mediated interactions of several thousand in three-dimensional domains. Our numerical methods build directly on tools, such as fast summation strategies, recently developed for rigid rod suspensions. I will discuss various instabilities found in this system, and demonstrate that individuals act as random walkers over large-times while collectively creating large time- and space-scale coherent structures and dynamics. These active suspension also demonstrate very strong mixing dynamics that may be beneficial to efficient distribution of nutrients in biological populations. This is joint work with David Saintillan.

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MS16
Instabilities in Elastic Springs with Applications to Multistability of Helical Ribbons in Biophysical Systems

We derive new equilibrium equations governing the deformation of helical strips of inextensible material. For certain values of the elastic parameters we find instabilities and associated hysteresis behaviour for end-loaded helices of sufficiently large ratio of radius to pitch. The results may help explain the existence of helices of two different pitches in certain biophysical systems, for instance the self-assembled helical ribbons formed by cholesterol crystallisation in gallbladder bile as a precursor to gallstones.

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MS17
Non-Extensive Statistical Thermodynamics of Swelling Media

By relying upon the concept of Tsallis entropy, I provide an introduction to the non-extensive thermodynamics of swelling polymers which possess a fractal substructure. Central limit theorems which are equivalent to a renormalization group formalism are employed to upscale from the macromolecular scale to higher scales in fractal media. I use -stable Levy motions in the analysis where the stability constant is the fractal dimension of the polymeric matrix. Power law scaling results are obtained and used to explain many interesting properties of the upscaled system.

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MS17
A Reaction-Diffusion Model of Cartilage Regener-

ation using a Level Set Approach

Articular cartilage is a connective tissue lining bony surfaces in diarthrodial joints. Cartilage exhibits defects due to osteoarthritis that can be filled using biocompatible hydrogel scaffold materials. We present a reaction-diffusion model of an in vitro cartilage regeneration experiment in which the core of a cylindrical explant is replaced with hydrogel. A level set method is used to model the advancing gel-tissue interface and estimate tissue regeneration times as cell-synthesized matrix proteins degrade the hydrogel.

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MS17

Two-scale Modeling of Clays

A two-scale asymptotic analysis for a viscous flow in an elastic porous medium, with electrokinetic surface effects is considered. The microscopic behavior is upscaled by using homogenization. More precisely, we consider the flow of a univalent electrolyte in the presence of an elastic solid with surface charges, that generates a double layer. The presence of the double-layer introduces slip conditions on the solid boundaries.

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MS17

Using Pseudospectral Methods to Solve a Nonlinear Transport Equation

A transport model for a swelling porous material is proposed and numerically solved. A pseudospectral method is implemented for the spatial derivatives while the time-stepping is executed by separating the equation into linear and non-linear parts. The linear part is solved exactly while the nonlinear part is solved using numerical quadrature. Results are presented for various diffusion coefficients input into the model. The scheme's strengths, weaknesses and algorithmic implementation are also discussed.

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MS18

Free Energies and Kinetics of Molecular Systems from Coarse Master Equations

Coarse master equations and diffusion models provide powerful tools to study the equilibrium and non-equilibrium properties of molecular systems. Maximum likelihood and Bayesian approaches have been used successfully to construct such models from the observed dynamics projected onto discrete and continuous low-dimensional sub-spaces. By using a Green's-function based formalism, issues arising from fast non-Markovian dynamics can be circumvented. The general formalism for the construction of coarse master equations and diffusion models will be illustrated with applications to peptide and protein folding.

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MS18

Hidden Markov Models (HMM) in the Context of Rare Events

Abstract not available at time of publication.

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MS18

Spatial Warping and Temperature-accelerated Dynamics Methods for Enhancing Conformational Sampling in Complex Systems

One of the computational grand challenges is the sampling of conformational equilibria of systems such as biomolecules and polymeric materials that are characterized by rough energy landscapes. If met, the impact on important problems, including protein and nucleic acid structure prediction, would be substantial. In this talk, two approaches to the conformational sampling problem will be described. First, it will be shown how to devise novel variable transformations for the statistical mechanical partition function that effect a warping of the conformational space, effectively removing barriers and enhancing attractive regions without altering thermodynamic and equilibrium properties (Z.W.Zhu, M.E. Tuckerman, S.O. Samuelson and G. J. Martyna. Phys. Rev. Lett. 88, 100201 (2002); P. Minary, M.E. Tuckerman and G. J. Martyna. SIAM J. Sci. Comput.(2008)) 1,2. This approach is compared to the popular replica-exchange technique and is shown to outperform it by several orders of magnitude. It will also be shown that variable transformations used within a temperature-accelerated approach leads to a scheme for mapping out multi-dimensional free-energy surfaces(L. Rosso, P. Minary, Z.W. Zhu and M. E. Tuckerman. J. Chem. Phys. 116, 4389 (2002); L. Rosso, J. B. Abrams and M. E. Tuckerman. J. Phys. Chem. B 109, 4162 (2005); J. B. Abrams and M. E. Tuckerman)(in preparation). Finally, it will be demonstrated that explicit variable transformations can be circumvented by the introduction of driving variables that couple to collective coordinates of interest and are, themselves, subject to the effect of temperature acceleration, thereby yielding a more flexible scheme for mapping out multi-dimensional free-energy surfaces.(

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MS19

Strain-alignment Coupling: Discrete and Continuum Models

In the framework of linear elasticity, we study the limit of a class of discrete free energies modeling strain-alignment-coupled systems by a rigorous coarse-graining procedure, as the number of molecules diverges. We focus on three paradigmatic examples: magnetostrictive solids, ferroelectric crystals and nematic elastomers, obtaining in the limit three continuum models consistent with those commonly employed in the current literature. We also derive the correspondent macroscopic energies in the presence of displacement boundary conditions and of various kinds of applied external fields.

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MS19

Strongly Coupled Multiferroic Oxides by Design

The rational design of new materials with emergent properties is a challenge today in materials physics. It begins with formulating a mechanism to control the interplay between diverse microscopic degrees of freedom in order to create targeted macroscopic phenomena and ends with the discovery or design of new material realizations. When combined with first-principles theoretical techniques, this approach provides an efficient strategy to survey the vast space of possible materials to target for synthesis. As an example, in this talk I will discuss recent work on designing materials rarely found in nature - multiferroic oxides in which a spontaneous magnetism not only coexists with but also is strongly coupled to a spontaneous electric polarization. By manipulating the competition between different ordered phases in real materials, I will show how in one case the interplay between spins and phonons can be exploited to produce a colossal magnetoelectric effect while in a second case, a polar lattice distortion can be designed to induce ferromagnetism.

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MS19

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 nongeneric 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 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.

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MS19

Soft Elasticity of Liquid Crystalline Elastomers

Soft elasticity is a property of ideal liquid crystal elastomers that have undergone a phase transition from a higher-symmetry phase. Materials that exhibit soft elasticity can be strained along certain directions with zero stress. This talk will present general phenomenological models for nematic and smectic elastomers and discuss their soft elasticity.

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MS20

Threshold Based Model for Damage

We will first consider a variational model for damage proposed by Francfort and Marigo, and then give an existence result (for a quasi-static version) by Francfort and Garroni. A case for a strain-threshold damage model will be made, and precise definitions for both an unrelaxed (i.e., the damage region is a set at each time) and relaxed (i.e., the damage set is given by a density function, together with an effective tensor that stores the microstructure of the damage) quasi-static evolution will be given. It turns out that solutions of the unrelaxed variational problem are solutions to the unrelaxed threshold problem, but there is an interesting issue in showing the same for the relaxed problems. This issue is related to a question regarding G-closure and the relative scalings of damage microstructure at different times. A new variational formulation, arguably more physical than the existing one, will be given, and we will show that relaxed solutions of this variational problem are solutions of the relaxed threshold problem.

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MS20

Supersonic Rupture of Rubber

I will present a theory for the rupture of rubber. Unlike conventional cracks, ruptures in rubber travel faster than the speed of sound, and consist in two oblique shocks that meet at a point. Physical features of rubber needed for this phenomenon include Kelvin dissipation and an increase of toughness as rubber retracts. After describing the experiments that led to these studies, I will present an approximate continuum theory, an exact analytical solution of a slightly simplified discrete problem, and numerical method that permits solution of realistic and fully nonlinear equations of motion.

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MS20

Dynamics of Propogating Phase Boundaries in NiTi

We describe experiments where propagating phase boundaries have been generated in polycrystalline NiTi specimens under a tensile impact loading condition. The time evolution of the strain at different spatial locations in the specimen is monitored. Nucleation and propagation of multiple phase fronts were detected in these experiments. The driving force for the motion of the phase front was evaluated from the measurements in order to establish the kinetic relation.

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MS20

The Role of Local Minima in Fracture Mechanics: An Example

We consider a one dimensional model of a body with decohesions with the energy functional represented by the sum of two terms, convex bulk and general cohesive. The cohesive energy penalizes jump discontinuities of the displacement field. Already for rather simple cohesive energies the elastostatic solution of the problem based on local minimization can not be extended beyond certain values of the loading parameter. To continue the solution beyond such points we propose two dynamic extensions of the model: both non-inertial and over-damped. In the first one the dissipative mechanism is viscous which leads in the quasi-static loading to dissipation being localized in time on discontinuous transitions between equilibrium branches (brutal damage). In the second, we interpret the cohesive energy as irreversibly dissipated. The latter augmentation of the model leads to the incremental reformulation of the variational problem which preserves the overall response of the first model in quasi-static loading but provides a more realistic description of the unloading. The two dynamic reformulations allow one to reproduces a broad class of inelastic behaviors from brittle fracture and damage to rate independent plasticity. Joint work with G. Del Piero.

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MS21

The Use of Gamma-convergence in the Analysis of Multiscale Problems

Gamma-convergence is a very useful tool for the description of complex variational problems involving small parameters (homogenization, phase transitions, atomistic systems, etc.). The underlying idea of the Gamma-convergence approach is to substitute an energy with a small parameter by another one where the dependence on this parameter has been averaged out (Gamma-limit), or simplified (Gamma-development). The resulting energy 'justified by Gamma-convergence' may however fail to represent the relevant behaviour of the original energy in its sensitiveness on relevant external parameters (boundary conditions, forcing terms, etc.) or be of a type different from a desired form commonly used by practitioners. I will present some proposals on how to use Gamma-convergence to overcome (some of) those drawbacks. On the one hand Gamma-convergence may be used as an equivalence relation (so that a wide range of energies may be equivalent to the same Gamma-limit, or Gamma-development, even if defined on different function spaces). On the other hand we may focus on the 'singular' external parameters where the description given by the Gamma-convergence approach is not 'uniformly close' to the original one. Those parameters may be singled out by simple necessary conditions and in many situations constitute a simple set of isolated points. Close to those values a finer analysis is necessary by the computation of a family of Gamma-limits. Once this analysis is performed, the issue of the construction of 'uniformly-equivalent theories' can be addressed. Joint work with Lev Truskinovsky.

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MS21

Multiwell Rigidity in Nonlinear Elasticity

I discuss quantitative rigidity estimates for multiwell problems in nonlinear elasticity which include surface energy. In particular, I shall show that low-energy states of materials undergoing a solid-solid phase transition are locally approximately affine, in a large part of the volume. Precisely, if a ball contains little interface, then on a smaller ball only one phase is present. The talk is based on joint work with Milena Chermisi and Ben Schweizer.

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MS21

Calculus of Variations with (a) twist: Defects in Pattern Formation

Roll Patterns in Rayleigh-Benard convection are described by the minimizers of the Cross-Newell (Aviles-Giga) en-

ergy, which generically have line defects, if the minimization is over "single-valued" functions. Natural patterns have a more interesting defect structure, in that they generically have coexisting line-like and point like defects. We explain this behavior (in an idealized setting) by deriving a rigorous scaling law for the minimizers of the Cross-Newell (Aviles-Giga) energy over a larger class of test functions "multi-valued" phases. This is joint work with Shankar Venkataramani

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MS21

Equilibrium Configurations of Epitaxially Strained Cristalline Films: Existence, Regularity and Qualitative Properties of Solutions

We shall discuss a variational model for strained epitaxial films grown on a relatively thick substrate. In this model the total free energy of the system is assumed to be the sum of the energy of the free surface of the film and the strain energy. Because of the lattice mismatch between film and substrate, flat configurations are in general energetically unfavourable and a corrugated or islanded morphology is the preferred growth mode of the strained film. We present some recent results on the existence problem and some new regularity results for volume constrained local minimizers leading, as a byproduct, to a rigorous proof of the zero contact-angle condition between islands and wetting layers. Finally we shall also discuss qualitative properties of critical points of the energy functional with positive second variation. As a result, we shall give necessary and sufficient conditions for the flat configuration to be the unique minimizer and necessary conditions which prevent the formation of cusp-like singularities.

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MS21

Phase Field Models of Reactive Wetting

The addition of hydrodynamics to diffuse interface models of phase transformations has now been well studied in some relatively simple systems. However, properly coupling such flows to a description of an elastic solid remains an area where the models need substantial improvements. In recent years we have been interested in the problem of reactive wetting, where a droplet disolves the substrate upon which it spreads. Describing this system mathematically, with a firm grounding in the laws of thermodynamics, and applying it to a realistic material (such as Sn-Bi) in a manner that admits numerical solution in reasonable time scales is the focus of this work. We will also discuss related approaches, including phase field crystal models, of the same phenomenon.

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MS22

String and Beam Models of Propulsion of Sperm Flagellum

We describe two models of flagellar motion based on the equations corresponding to a slender beam and a flexible string in the low-Reynold's number regime. Comparisons are made between the string and beam models and laboratory observations; our results suggest that accurate predictions of the waveforms of flagella are obtained with the string model rather than the beam model, unless the bending rigidity of the microtubules is lowered significantly from measured values.

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MS22

Computational Modeling of Arterial Platelet Thrombosis

Arterial blood clots (thrombi) that form as a consequence of artherosclerotic plaque rupture are comprised largely of aggregates of platelets. These thrombi form under conditions in which the flow changes substantially both in space (initially because of the plaque, later also because of the clots) and in time (as the thrombi develop). We present a continuum model that describes platelet thrombosis initiated by a ruptured atherosclerotic plaque in a coronary-artery-sized vessel. It includes full treatment of the fluid dynamics, and the aggregation of platelets in response to the plaque rupture and further chemical signals. In the model, the growing clots influence the fluid motion by a distribution of forces that act on the fluid rather than by an explicit change in fluid domain geometry. Among the behaviors seen with this model are the growth of wall-adherent platelet thrombi to occlude the vessel and stop the flow, and the transient growth and subsequent embolization of thrombi leaving behind a passivated injured surface. The model will be the basis for an exploration of the interactions among flow, biology, and vessel geometry during arterial thrombosis.

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MS22

Nonlocal and Nonlinear Hydrodynamics of Swimming Microorganisms

Microorganisms that are swimming in viscous fluids inhabit a world quite different from the one we are used to experiencing. In this talk, we will discuss some properties and recent results of fluid-based locomotion on very small scales in fluids and geometries where nonlinear behavior naturally arises. First, we will present theoretical work on locomotion in viscoelastic fluids, for two types of actuation: waving and flapping. We will then present experimental and theoretical results on the hydrodynamic attraction of swimming cells by solid surfaces.

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MS22

Computational Implementations of Entropic Correction to DNA Cyclization

Recent work by Zhang and Crothers proposed a computation for DNA J-factors, including the entropic part, within a discrete model. Recently, Cotta-Ramusino and Maddocks have developed the appropriate computation for this problem in the continuum rod setting. Here we present a computational implementation of the Cotta-Ramusino/Maddocks method, including examples with rod intrinsic shapes designed to model short DNA segments.

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MS23

Computational Field Theory of Block Copolymer Assembly

I will discuss current challenges and limitations in the field-based approach to modeling block copolymer assembly, and highlight applications to a few contemporary topics in academic experiment and industry.

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MS23

Self-Consistent Field Theory Simulations of Block Copolymer Assembly on a Sphere

We describe a self-consistent field theory (SCFT) model of block copolymers for the study of self-assembly in thin block copolymer melt films confined to the surface of a sphere. In this model, we assume that the composition of the thin block copolymer film varies only in longitude and colatitude and is constant in the radial direction. Using this approach we are able to study the formation of defects in the lamellar and cylindrical phases, and their dependence on sphere radius. Specifically, we compute ground-state configurations on the sphere for both the cylindrical and lamellar phases.

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MS23

Ostwald Ripening in Dilute Copolymer Systems

The evolution of microstructure in block copolymer mixtures can be described by a modification to the usual Cahn-Hilliard equation in the form of a nonlocal interaction energy. A competition between surface energy that promotes coarsening and long ranged energy that inhibits it leads to a wide variety of stable microstructures. This talk focuses on the Ostwald ripening regime where one phase has a low volume fraction. An analog to the classical LSW approximation can be developed to describe the crossover between intermediate-time coarsening and late stage pattern development. We take advantage of the notion of screening in the LSW approximation to derive a homogenized effective system that describes both intermediate "polydisperse" configurations and their evolution toward equilibrium.

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MS23

Phases and Phase Transitions of Block Copolymers

Spontaneous formation of ordered structures from amphiphilic molecules has attracted tremendous attentions in the last decades. Among the many different amphiphilic systems, block copolymers with their rich phase behaviour and ordering transitions have become a paradigm for the study of structural self-assembly. For the simplest case of diblock copolymers, which are linear polymers composed of two different sub-chains (A and B blocks), a variety of ordered bulk phases, including lamellae, hexagonally-packed cylinders, body-centered-cubic spheres and a bicontinuous network structure called gyroid, are observed. Understanding the structures and phase transitions in block copolymers has been one of the most active research areas in polymer science in the past two decades. One of the achievements is the self-consistent field theory, which provides a powerful framework for the study of ordered phase of block copolymers. I will present our recent development of self-consistent field theory for block copolymers and its applications to triblock copolymers and gradient copolymers.

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MS24

A Novel Mechanism for the Onset of Step-bunching Instabilities During the Epitaxy of Single-species Cystalline Films

We present a thermodynamically consistent, discrete-

continuum theory for step-flow epitaxy that extends the classical BCF framework. In it, a novel expression for the step chemical potential that holds far from equilibrium is derived. A stability analysis of the resulting free-boundary problem yields an unexpected result. Namely that, in contrast with the predictions of the BCF model, a deposition regime exists for which step bunching occurs if the equilibrium adatom coverage is sufficiently high. The physical origin of this instability and its relevance to, e.g., the MBE of GaAs is discussed.

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MS24

KMC Simulations of the Meandering Instability and Pyramid Formation During Step Flow of Cu Vicinals: Intrinsic vs Impurity Effects

An effective way of patterning a substrate over mesoscopic lengthscales is to exploit the spontaneous tendency of out-of-equilibrium systems towards formation of long-range structures. In particular, vicinal, or stepped, surfaces, often organise spontaneously in non-trivial patterns during atom deposition and step flow growth. In the present work, we have performed kinetic Monte Carlo simulations of deposition of two kinds of particles (atoms and impurities) on a vicinal crystal suface. We have chosen parameters in such a way that growth proceeds by step flow, and that spontaneous patterning of the surface takes place in the absence of impurities, in the form of long ridges separated by deep channels. Adding impurities, nanopyramids form spontaneously on top of the ridges, the impurities acting as nucleation centers. The density of the nano-pyramids may be tuned by varying the impurity concentration. A detailed comparison of the surface morphology with that of vicinal copper surfaces will be made.

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MS24

Numerical Studies of Step Instabilities in the Nonlinear Regime

We discuss numerical approaches for step flow models and apply them to study step instabilities. Examples are spiral growth under the influence of an Ehrlich-Schwoebel barrier, step meandering as a result of an Ehrlich-Schwoebel barrier and the formation of columnar structures and the influence of an applied electric field on step structures.

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MS24

Lattice Gas Model for Phase Transitions and Asymmetric Boundary Fluctuations in Acridine-9-carboxylic Acid (ACA) Thin Films

Experiments show that ACA molecules form chain-like monolayers on Ag(111). However boundary fluctuations along and normal to the chain direction show little asymmetry, contrary to predictions of a simple lattice model with stronger interactions along the chains. Accounting for the effects of different substrate interactions on differently oriented molecules leads to a generalized model that gives good agreement with experiment. This work has been supported by NSF-MRSEC under Grant DMR05-20471.

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MS25

The Effect of Nearest Neighbor Pb-O Divacancy Pairs on the Ferroelectric-relaxor Transition in $Pb(Sc_{1/2}Nb_{1/2})O_3$ (PSN)

Molecular dynamics simulations were performed on a first-principles-based effective Hamiltonian for $Pb(Sc_{1/2}Nb_{1/2})O_3$ (PSN) with nearest-neighbor Pb-O divacancy pairs. Simulations were performed for PSN with ideal chemical order, chemical short-range order, and random chemical disorder. Divacancy-concentration vs. temperature, $X_{[Pb-O]}$ vs. T, phase diagrams were calculated. They are shown to be topologically equivalent to the previously calculated hydrostatic pressure vs. temperature diagram. In PSN with ideal chemical order, the Burns temperature, T_B, defines an isotherm, analogous to the "Griffiths Temperature," T_C^0, which defines the high-temperature limit of the "Griffiths Phase" in the magnetic dilution problem.

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MS25

Computational Modeling of Multifunctional Materials

Multifunctional materials, such as multiferroic materials, offer numerous desirable physical properties and characteristics in a single system. The ability to understand, predict and optimize such properties, and to develop new multifunctional materials, has the potential to improve the portability and performance of a variety of existing and potential devices and thus drive future technological innovation and even facilitate the emergence of entirely new industries. Computational methods may lead to design of improved multifunctional materials for specific applications. The challenge is twofold: the first is the development and implementation of an appropriate mathematical model; the second is the structural complexity of many multifunctional materials. Here we illustrate the efficiency of our computational methods to multiferroic bismuth ferrite in providing understanding of the fundamental physics and predicting novel phenomena in advance of synthesis.

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MS25

Ferroelectric Superlattices from First Principles

With recent advances in the synthesis of complex oxides, it has become possible to produce superlattices of perovskite ferroelectrics with layers as thin as a single unit cell. Using models with parameters determined from first-principles calculations on a database of selected systems, the structure and functional properties of arbitrary superlattices can be predicted and interpreted. This provides valuable guidance for the analysis of experimental measurements and for the "materials by design" identification of promising new superlattice sequences.

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MS25

Use of First Principles Methods to Develop Design Rules for New Polar Materials

The use of first principles calculations to design new materials with improved functionality is a subject of ongoing interest. One approach to this problem is to use calculations to map out chemical and structural trends at an atomic level. These can be summarized in so-called design rules, which can then be used in formulating new compositions. Here this is illustrated using the example of perovskite ferroelectrics. Design rules are formulated and are applied to find perovskite compositions that combine polar behavior and ferromagnetism. This work was supported by the Department of Energy, Division of Materials Science and Engineering.

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MS26

Rigidity Problems in Fracture Mechanics

I will discuss some issues related to the quasistatic theory of fracture growth, and in particular of the structure of fractured materials with finite energy, when the stored elastic energy vanishes.

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MS26

Numerical Simulation of Dynamic Crack Propagation with X-FEM: Control of Energy a Key for Predictive Comptations

Predictive dynamic crack propagation simulations still remains a difficult challenge. This paper shall present a robust numerical strategy adopted to compute dynamic crack propagation using X-FEM Level set technique. It will be shown that a carefull formulation which exactly preserves energy produces very predictive results when compared with experiments. Two computed predicted crack paths and crack length histories shall be compared to two experiments performed by the team. The first one shows a brittle fracture complex path with rotating crack arrest and restart. The second is associated with plastic state and also has a complex mixed mode loading: for this case the loading is quasi static and the propagation speed is decreasing from 800m/s et zero, and it will be shown that a quasistatic analysis cannot predict the crack path and arrest. The main limitation of this work is that the presented results are 2D and that the crack propagation physical criteria are very simple and may be criticized by material scientists who find them too crude. The proposed method has the main advantages to be predictive, numerically efficient, and to compare well with experiments.

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MS26

Quasistatic Evolution in Plasticity with Softening

In this talk a quasistatic evolution problem in plasticity with softening is considered in the framework of small strain associative elastoplasticity. The presence of a nonconvex term due to the softening phenomenon requires a nontrivial extension of the variational framework for rate-independent problems to the case of a nonconvex energy functional. In this case the use of global minimizers in the corresponding incremental problems appears to be not justified from the mechanical point of view. Thus, a different selection criterion for the solutions of the quasistatic evolution problem is proposed, which is based on a viscous approximation. This leads to a generalized formulation in terms of Young measures.

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MS26

Fracture Dissipations Based on Fronts: Relaxation and Rate-Independence

Crack fronts play a fundamental role in engineering models for fracture: they are the location of both crack growth and the energy dissipation due to growth. However, there has not been a rigorous mathematical definition of crack front, nor rigorous mathematical analysis predicting fracture paths using fronts as the location of dissipation. In this talk, I will present a natural weak definition of crack front and front speed, and consider models of crack growth in which the energy dissipation is a (non-linear) function of the front speed, i.e., the dissipation rate at time t is of the form

$$\int_{F(t)} \psi(v(x,t)) d\mathcal{H}^{\mathcal{N}-\epsilon}(\S)$$

where $F(t)$ is the front at time t and v is the front speed. In general, dissipations of this type must be relaxed. I will present a general relaxation formula that gives the surprising result that the effective dissipation rate is always rate independent, meaning it depends linearly on the front speed.

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MS27

Title Not Available at Time of Publication

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MS27

Wetting on Rough Surfaces

Roughness enhances considerably the hydrophobic properties of a hydrophobic surface, and it decreases substantially contact angle hysteresis. I will report on recent progress on this topic based on the tools of calculus of variations and on joint work with G. Alberti, N. Grunewald, and F. Otto.

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MS27

Homogenization of Mumford-Shah Type Energies in Periodically Perforated Domains

The homogenization of Mumford-Shah type energies in periodically perforated domains is studied in case of both Dirichlet and Neumann conditions on the boundary of the set of perforations via a Γ-convergence approach.

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MS27

Gamma Convergence for Local Minimizers

It is well known that if E_n Gamma-converges to E, it is not generally true that local minimizers of E_n converge to local minimizers of E. We give a new definition of convergence, s-Gamma convergence, with the property that stable states, in a sense, of E_n converge to stable states of E. We illustrate with an example how this can be used to capture all strict local minimizers of E. This is joint work with A. Braides.

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MS28

Complex Fluids in Microfluidic Devices: Purely Elastic Instabilities and Drop Breakup

Fluids with mesoscopic structure (e.g. polymeric liquids and DNA suspensions) often exhibit complex rheological behavior, particularly in response to applied external forces. Two examples are discussed here. First, we investigate the flow of viscoelastic polymeric fluids in an extensional flow, in which two flow instabilities are found. Next, the effects of elasticity on filament thinning and drop breakup in microchannels are investigated, in which the filament thinning shows two distinct temporal regimes: flow- and capillary-driven.

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MS28

A Rigorous Approach for Modeling the Effective Response of Muscle Myofibrils

Muscles have a hierarchical structure that spans several scales. We present a theoretical framework for predicting the collective behavior of biologically relevant ensembles of sarcomeres, the basic contractile unit. The analysis is accomplished by transforming the non-linear dynamics of an assemblage of sarcomeres into a partial differential equation for the probability distribution function of sarcomere lengths in the presence of stochastic fluctuations and biological variability. It reproduces experimental results and

explains some puzzling observations.

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MS28

A New View of the Mechanism for Actin-polymerization-driven Motility

An important component of the cellular cytoskeleton is F-actin, a biopolymer whose non-equilibrium self-assembly is key to the process of cell crawling. We use Brownian dynamics to study this driven self-assembly process and to determine how it leads to motion. We find that the creation of new polymerizing filaments by the branching process leads to a steady-state density profile of actin away from the moving surface. This non-equilibrium concentration profile is associated with a chemical potential profile that moves the leading edge of the crawling cell forwards; this is analogous to an effect known as "self-diffusiophoresis."

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MS28

Momentum-transfer Mechanisms for Millimeter-sized Swimmers

We use a heaving foil as a simple model for the propulsive appendage of a millimeter-sized swimmer, and present a framework for splitting the fluid forcing due to this foil into contributions from a zoology of coherent wake structures. Under conditions of symmetrical actuation we show that the thrust developed by the propulsor comes from two sources: transfer of momentum to vortices shed from the foil edges, and viscous drag from slowly overturning coherent eddies.

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MS29

Morphological Characterization of Diblock Copolymer Problem

We apply computational homology to characterize the complex transient morphology during the phase transition dynamics in diblock copolymer problems. Our topological characterization reveals the transient perforated lamellar state in the lamellar-hexagons transition and the t^{-1} law of the Betti number in the late stage of phase-ordering process.

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MS29

Hexagonal Patterns of Di-Block Copolymer Melts

We consider the functionals containing a small parameter and a long-range interaction arising in the models for the phase separation in di-block copolymers. We take the singular limit of the properly rescaled functional to obtain the sharp interface problem and present a mathematical account of a hexagonal pattern selection observed in di-block copolymer melts.

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MS29

Droplet Solutions of a Two-Dimesnional Free Boundary Problem from Diblock Copolymer Morphology

The Ohta-Kawasaki density functional theory of diblock copolymers gives rise to a nonlocal free boundary problem. In a proper parameter range an equilibrium pattern of many droplets is proved to exist in a general planar domain. A sub-range is identified where the multiple droplet pattern is stable. Each droplet is close to a round disc. The boundaries of the droplets satisfy an equation that involves the curvature of the boundary and a quantity that depends nonlocally on the whole pattern. The locations of the droplets are determined via a Green's function of the domain. In constructing the droplet pattern we overcome three obstacles: interface oscillation, droplet coarsening, and droplet translation.

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MS29

A Variational Model for Patterns in Diblock Copolymer-Homopolymer Melts

In a diblock copolymer two mutually repelling types of polymer molecules are chemically bonded together, thereby limiting the distance they can separate. This leads to pattern formation on a length scale between system and molecules. We investigate a model for an extension of this system: a diblock copolymer-homopolymer blend. This variational blend-model, is now well-understood in one dimension. In higher dimensions we find energy bounds and study the stability of specific morphologies in two dimensions.

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MS30

Energetically Driven Alloy Segregation in Heteroepitaxy

Strain in a heteroepitaxial system can drive the formation of nontrivial geometry and structures. We consider a substrate of material A containing a prescribed number of atoms of material. We optimize the location of the B atoms, by minimization of the elastic strain energy, using simulated annealing. The results show lateral alloy segregation that may be significant in determining the location and size of subsequent surface features.

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MS30

Step-flow Instabilities During the Epitaxy of Binary Compounds and Alloys

A BCF-type model for the step-flow growth of a generic binary compound film is presented, the purpose of which is to investigate the influence of chemical kinetics on the onset of step bunching. The resulting free-boundary problem consists of a system of reaction-diffusion equations augmented by coupled nonlinear boundary conditions along the steps, one of which generalizes the classical Gibbs–Thomson condition. Explicit stability criteria for the onset of one-dimensional instabilities are obtained, and the resulting phase diagrams are presented. Comparisons with existing experiments are discussed.

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MS30

Unification of Step Bunching Phenomena on Vicinal Surfaces

A unification is presented of step bunching (SB) instabilities occuring under various conditions on crystal surfaces. We show that when attachment-detachment at steps is the rate-limiting process, the SB of interacting, concentric circular steps is equivalent to the commonly observed SB of interacting straight steps under deposition, desorption or drift. We derive a Lagrangian partial differential equation that describes the onset of instabilities for circular steps.

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MS30

Dewetting of Solid Films on Vicinal Surfaces

Thin solid films on crystal surfaces are often unstable. We report on the dynamics of the dewetting instability. We focus the case of vicinal substrates (i.e. misoriented with respect to a facet orientation). Experimental results have shown that islands formed during the dewetting process migrate "downhill" on vicinal surfaces. We solve the dynamics of the migration process for various types of kinetics. We consider both the surface energy, and the misfit elastic energy. Important shape changes are observed during migration.

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MS30

Step Bunching in Growth Models: Scaling and Universality

The talk is centered around the study of two models of (unstable) vicinal growth: the model of growth in the presence of an inverse Ehrlich-Schwoebel effect [Sato, M. and Uwaha, M., Surf. Sci. 493, (2001) 494] and the recently introduced "C+ - C-" model [Ranguelov, B. et al., CR de l'Acad Bulg.Sci. 60, 4 (2007) 389]. Step bunching is studied in the long time limit and the qualitative differences between the two models are outlined. Both size- and time-scalings for the step bunches are obtained for a broad range of model parameters. The resulting universality classes are compared with the predictions of generalized continuum [Pimpinelli, A. et al., PRL 88, (2002) 206103 and Krug, J., et al., PRB 71, (2005) 045412] and discrete minimal models [Ranguelov, B. et al., Nanoscience and Nanotechnology 6, Balabanova, E., Dragieva, I.(eds.), Heron Press, Sofia, 2006, 31 and Popkov, V and Krug, J., EPL 72, 6 (2005) 1025].

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MS31

Electronic Structure Calculations at Macroscopic Scales

Abstract not available at time of publication.

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MS31

Efficient and Accurate Linear Scaling Quantum Mechanics Algorithms for Materials and Molecules

A status report will be presented on two classes of linear scaling electronic structure methods we have developed, where the emphasis is on achieving algorithmic efficiency while retaining accurate physics. The first topic is a new linear scaling ab initio many-body wavefunction code that provides accurate treatment of electron correlation in molecules. This is founded on multi-reference configuration interaction (MRCI) theory, in which we systematically eliminate significant algorithmic bottlenecks to linear scaling, reducing the inherent N6 scaling down to N, for molecules with more than 10 heavy atoms. The second topic is on a new parallel, linear scaling code for non-local orbital free density functional theory (OFDFT), which provides accurate physics for main group metal alloys and some semiconductor properties. OFDFT solves directly for the electron density without introducing wavefunctions and can be made to scale linearly provided a number of algorithmic tricks are employed. However, it should only be used with non-local density functionals for the kinetic energy in order to retain accuracy. Local functionals are trivially O(N) but do not contain accurate physics, whereas non-local functionals are much more accurate but are more challenging to render O(N) scaling. We focus on the latter approach, and again show how systematic elimination of bottlenecks can render all aspects of the algorithm linear scaling.

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MS31

Sub-linear Scaling Algorithms for the Study of the Electronic Structure of Materials

Abstract not available at time of publication.

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MS31

Density Functional Calculations with Fractional Occupation Numbers

Abstract not available at time of publication.

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MS32

Coarsening of Island Distributions on Surfaces: Ostwald vs Smoluchowski vs Anomalous Ripening

Evolution of distributions of 2D islands in homoepitaxial systems provides an ideal testing ground for 2D coarsening theories. Surprisingly, Ostwald ripening (OR) dominates in some systems but Smoluchowski ripening (SR), i.e., diffusion and coalescence of islands, in others. We provide an analysis to assess the dominant mechanism in specific systems. For SR, this involves consideration of the unusual size-dependence of island diffusion (and also prompts analysis of coalescence dynamics). For evolution of 3D islands in heteroepitaxial systems, we describe anomalous coarsening kinetics due quantum size effects (where factors other than island radii drive evolution).

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MS32

Generic Two-phase Coexistence and Coarsening in the Quadratic Contact Process: A Stochastic Spatial Model for Epidemics or Autocatalysis

First-order transitions in nonequilibrium systems exhibits many novel phenomena that are fundamentally different from their more familiar equilibrium counterparts. It has been found that for a wide variety of systems, phase transitions occur over a finite measure of the parameter space. Using the quadratic contact process on a square lattice as an example, we demonstrate effects of this generic phase coexistence on orientational dependence of equistability, propagation of interfaces, and coarsening.

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MS32

Evolution of Interfaces During Coarsening: Topology and Morphology

The three-dimensional interfacial structure of materials is examined through large-scale simulations of spinodal decomposition and phase ordering. While both transformations yield complex interconnected structures, the interfacial morphologies, as measured by the probability of finding a patch of interface with a given pair of principal curvatures, are quite different. By contrast, the topology of the interfaces is nearly independent of the volume fraction or mass transport process. A discussion of these results will be given.

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MS32

Morphometrics Through Singular Limits and the Maximum Dissipation Principle

We consider the coarsening dynamics of solutions to dissipative singularly perturbed PDE which model faceted crystal growth. We characterize the associated singular-limit dynamics via asymptotic expansions of Onsager-Rayleigh-type maximal dissipation principles. We predict scaling laws $\mathcal{L} \sim \sqcup\surd$, for the growth in time, t, of the characteristic morphological length scale, $\mathcal{L}$. Scaling pre-factors C,

$\mathcal{L}_{\mathcal{M}} = \mathcal{C}\tau^{\surd}$, and a variety of scale-invariant morphometrics are then identified through direct simulation with the computational geometry tool $\mathcal{PAGE}$.

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MS33

Composites with Unexpected Values of the Homogenized Hall Coefficient

This work with G. Milton deals with the homogenization of the Hall effect in dimension three. The effective Hall coefficient preserves the bounds of the local Hall coefficient in dimension two. This is not the case in dimension three. We present three-dimensional composites for which the homogenized Hall coefficient has opposite sign to the local Hall coefficient, and composites for which the homogenized Hall coefficient is arbitrarily large compared with the local Hall coefficient.

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MS33

Homogenization of Monotone Graphs

This is joint work with Francois Murat and Luc Tartar. Having previously proved existence of solutions to $-div\ a(x, \nabla u) = f$, together with appropriate boundary conditions, whenever, for every fixed x, $a(x, e)$ belongs to a certain class of maximal monotone graphs in e, we derive the corresponding homogenization result by letting $a(x, e)$ depend upon $\varepsilon \searrow 0$, and imposing adequate ε-uniform boundedness and coercivity properties. Our results do not assume any kind of periodicity.

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MS33

Magnetism and Homogenization of Microresonators

Arrays of metal micro-resonators embedded in a dielectric matrix were proposed by Pendry, et. al., as a means of creating a bulk medium that exhibits magnetic reponse at frequencies not realized in nature. Homogenization analysis reveals that one must pay special attention to the appropriate method of averaging the electromagnetic fields. The effective material coefficients obtained via these averages characterize a bulk medium that produces the same scattering data as the micro-structured composite.

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MS33

Homogenisation of High-contrast Periodic and Perturbed Periodic Composites and Applications

We review recent work on the use of "non-classical" (high-contrast) homogenization for various problems involving periodic and perturbed periodic composites, and some relevant applications. The employed mathematical techniques include a high-contrast version of two-scale asymptotic expansions and the two-scale convergence with associated operator convergence, compactness, etc, due to some recent ideas of V.V. Zhikov. The resulting effective properties are described by a two-scale limit operator often displaying unusual physical effects. Applications include asymtotics for band gaps and localised modes in the gaps due to defects with relevance to photonics, and slowing down of waves. (Joint work with I. Kamotski, M. Cherdantsev, N. Babych and P. Kuchment).

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MS34

Mathematical Validation and Algorithms for the Quasicontinuum Method

The quasicontinuum approximation is a method to reduce the atomistic degrees of freedom of a crystalline solid by piecewise linear interpolation from representative atoms. The coarsened triangles can be further approximated by a strain energy density based on the Cauchy-Born rule to obtain the finite element approximation in the continuum region. The forces on all of the representative atoms are determined except for those representative atoms in an atomistic-continuum interfacial region, where it is not known how to model the forces to simultaneously satisfy conditions of accuracy, efficiency, and conservation. We will present a theoretical framework for evaluating the goal-oriented accuracy of the atomistic-continuum interface, and we will apply this theory to analyze several quasicontinuum approximations. We will also present an a posteriori goal-oriented error estimator and a corresponding adaptive atomistic-continuum modeling and mesh refinement algorithm to enable a quantity of interest to be efficiently computed to a predetermined accuracy.

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MS34
Benchmarking Multiscale Methods

In recent years there has been a multitude of new methods developed to couple an atomistic model to a continuum-based approximation (such as finite elements). The goal of these methods is to be able to reproduce the results of a fully atomistic simulation at a reduced computational cost. Naturally each of these methods has associated with it an inherent accuracy and efficiency, however it is difficult to compare these attributes between methods for three reasons. First, it is necessary to spell out what is a suitably rigorous yet sufficiently simple and controllable test problem to study as a benchmark for these methods. Second, it is necessary to implement all these methods within a unified overall framework. This eliminates any differences between elements that are common across methods (such as, for instance, routines to compute atomic forces or solver algorithms), and thus permits a fair comparison. Third, a common numerical analysis of the methods is required to clearly identify the differences between the methods and how their accuracy and efficiency can be controlled. In this work, we move towards overcoming these difficulties. We present a 2D implementation of a large number of the methods taken from the literature. This allows quantitative comparison between their accuracy and efficiency in modeling a problem involving the structure and motion of a dislocation dipole in a single crystal. A final goal is to develop a complementary numerical analysis to guide methods of improving the efficiencies in the 2D implementation. For example, the analysis may suggests way to control errors in the methods, to understand how the error converges with model size or to improve solver algorithms.

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MS34
Stability of Atomistic Models and the Quasicontinuum Method

Linear stability can often by used to control the quality of approximation in nonlinear problems. In this talk, I discuss some details of this approach for atomistic material models and the Quasicontinuum approximation. In particular, I will discuss the following closely related questions: (i) Given an exact solution of the atomistic model, is there a 'nearby' QC approximation? (ii) Given a 'good' QC solution, does there exist a 'nearby' exact solution of the atomistic model? (iii) Given a sufficiently regular local mimimizer of the Cauchy–Born equations, does there exist a 'nearby' atomistic local minimizer?

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MS35
Homogenization with Nonseparated Scales and Generalized Cauchy-Born Rule

We discuss a novel mathematical approach that allows to construct discrete finite dimensional approximations with a controlled error estimate in continuum PDE models with non-separated scales. This approach is based on approximation of gradients of H^2 functions in L^2 norm by a linear combination of M divergence free vector fields from $(L^2(\Omega))^n$ with coefficients that are piecewise linear on a partition of the domain $\Omega \subset R^n$ of a given resolution h with an error of the order h. Here M is any integer greater than n. We apply this approach to elasticity problems and, in particular, derive a generalized Cauchy-Born rule for non-monoatomic solids.

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MS35
Ginzburg-Landau Theory for the XY Spin Model: A Variational Approach

The XY model is a two-dimensional vector spin model that posses circular symmetry and whose stable configurations include vortices. This lecture present a variational approach to the Ginzburg-Landau theory of the XY model and of some of its variants. From a mathematical perspective this involves the Gamma-convergence analysis of the discrete-to-continuum limit of a proper scaling of the potential energy of the XY system.

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MS35
Thermodynamic Needs Versus Capabilities of Micro-macro Transitions

Lattice models serve as simple models that allow to simulate the dynamics of macroscopic bodies on an atomistic scale, where their microscopic discrete structure is described by structureless atoms interacting with each other by given forces. In this setting the ODE system is given by Newton's equation of motion for N atoms. One expects that possible limiting cases $N \to \infty$ lead to a small PDE system for macroscopic quantities within the framework of the laws of thermodynamics. We shall focus on some selected aspects of these micro-macro transitions and we shall show that the limit $N \to \infty$ must simultaneously be carried out by a corresponding scaling of time and space. This can be done in various ways, leading to different PDE systems. On the other hand thermodynamics provides a general setting of those PDE systems that are in accordance with the

physical laws and in particular with the 2nd law of thermodynamics. In this setting the evolution of deformation and heat in physical bodies on the macroscopic scale relies on equations of balance, which are closed by constitutive equations obeying an extended Gibbs equation. We apply to the atomic chain in 1D several scalings to illustrate that some properties of thermodynamics can be described by micro-macro transitions and others are currently out of reach.

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MS35

Continuum Limit of Quantum Mechanics Models

We will discuss the continuum limit of models from quantum mechanics, namely the density functional theory models and tight-binding models. This is joint work with Jianfeng Lu.

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MS36

The Continuum Elastic and Atomistic Viewpoints on the Formation Volume and Strain Energy of a Point Defect

We discuss the roles of continuum linear elasticity and atomistic calculations in determining the formation volume and the strain energy of formation of a point defect in a crystal under stress. The elasticity treatment is based on the Green's function solution for a center of contraction or expansion in an anisotropic solid. It makes possible the precise definition of a formation volume tensor and leads to an extension of Eshelby's result for the work done by an external stress during the transformation of a continuum inclusion.

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MS36

Electronic Structure Calculations at Macroscopic Scales

This talk presents a seamless multi-scale scheme to perform electronic structure calculations at macroscopic scales, paving the way to an accurate electronic structure study of defects in materials. The key ideas that constitute the multi-scale scheme are (i) a real-space variational formulation of orbital-free density-functional-theory, (ii) a nested finite-element discretization of the formulation, and (iii) a systematic means of adaptive coarse-graining retaining full resolution where necessary, and coarsening elsewhere with no patches, assumptions or structure.

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MS36

Understanding Electrical and Optical Effects of Dislocations in III-V Semiconductors

Dislocations provide strain relief in GaN and GaAs, but they also affect optical and electronic properties due to electron trapping by dangling bonds, and the bandstructure shift due to the dislocation strain field. Here we develop a multiscale atomistic-continuum model that accounts for these factors and quantitatively predicts the reduction in photoluminescence intensity and electron mobility with increasing dislocation density, the presence of dislocation-related radiative recombination, and the difference in dislocation sensitivity in various materials.

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MS36

Multiscale Simulations of Complex Materials for Engineering and Biological Applications

A variety of physical phenomena involve multiple length and time scales. Some interesting examples of multiple-scale phenomena are: (a) mechanical behavior of crystals and in particular the interplay of chemistry and mechanical stress in determining the macroscopic brittle or ductile response of solids; (b) molecular-scale forces at interfaces and their effect in macroscopic phenomena like wetting and friction; (c) alteration of the structure and electronic properties of macromolecular systems due to external forces, as in stretched DNA nanowires or carbon nanotubes. In these complex physical systems, the changes in bonding and atomic configurations at the microscopic, atomic level have profound effects on the macroscopic properties, be they of mechanical or electrical nature. Linking the processes at the two extremes of the length scale spectrum is the only means of achieving a deeper understanding of these phenomena and, ultimately, of being able to predict and control them. While methodologies for describing the physics at a single scale are well developed in many fields of physics, chemistry or engineering, methodologies that couple scales remain a challenge, both from the conceptual point as well as from the computational point. In this presentation I will discuss the development of methodologies for simulations across disparate length scales with the aim of obtaining a detailed description of complex phenomena of the type described above. I will also present illustrative examples, including hydrogen embrittlement of metals, DNA conductivity and translocation through nanopores, and the use of surface chemical modification to control the

wettability of surfaces for biological applications.

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MS37

Dislocation Dynamics and Plasticity of Sub-Micron Metal Pillars

In compression experiments of single crystal micro-pillars, the flow stress is found to increase dramatically as the pillar diameter decreases below one micron. To clarify the fundamental mechanisms, we develop a Dislocation Dynamics (DD) model with an efficient algorithm to compute the image stress from the cylindrical surface. The DD simulations reveal a new self-replication mechanism for dislocations in BCC pillars, which leads to important differences in the size-dependent plasticity between BCC and FCC pillars.

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MS37

The Physics and Mechanics of Plasticity in Micro-pillars

Plastic flow in small volumes is caharcteristically different from its counter-part in polycrystalline materials. One of the interesting systems which exhibits remarkable characteristics of plastic flow is the plasticity of micro-pillars. We present results of Dislocation Dynamics computer simulations that show that the strength and rate of hardening in these systems are sensitive to the system size, that plastic flow is intermittent and not continuous, that the dynamics of stress/strain exhibit a limit cycle, and that plastic instabilities are geometric in origin, and are generated as a result of finite deformation and lattice rotations. We also discuss the roles of several dislocation mechanisms, including cross-slip, in engendering these unusual characteristics.

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MS37

Coupling Discrete Dislocation to Continuum Crystal Plasticity

We present a multi-scale approach combining discrete dislocation plasticity and conventional continuum crystal plasticity. Our formulation is for plane strain and, for this class of problems, greatly extends the range of plastic zone sizes and therefore the loading range that can be analyzed using discrete dislocation plasticity. The key to this approach is the treatment of the interface between the two regions. The interface formulation used will be described and example problem solutions presented.

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MS37

Level Set Simulations of Dislocation Dynamics in Multilayered Heteroepitaxial Film Systems During Growth

We develop a level set method-based, three-dimensional simulation method to describe the motion of dislocations during growth of heteroepitaxial multilayered thin film systems. The simulations accurately describe the elastic interactions of the dislocations, stress fields throughout the film and substrate, dislocation annihilation, and dislocation reactions. Systematic parametric studies are performed to investigate the effects of cross-slip, energetic and kinetic barrier formation and system geometry on strain relaxation and reduction of threading dislocation density.

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MS38

Daubechies Wavelets for Density Functional Electronic Structure Calculations

A basis set of Daubechies scaling functions and wavelets is well suited for density functional electronic structure calculations since it is orthogonal and localized both in real and Fourier space. The various contributions to the total energy such as the kinetic and potential energy can be calculated efficiently. Our implementation in the ABINIT software package outperforms plane wave basis sets and allows the calculation of very large and complicated molec-

ular systems.

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MS38

Domain Decomposition and Electronic Structure Calculation: A New Approach

Electronic structure calculations are a well known challenging problem of computational chemistry. Such calculations consist of nonlinear eigenvalue problems of large size, which have several specificities in comparison with other eigenvalue problems arising in other engineering sciences. The talk will first introduce the context, and point out the peculiarities of the problem under consideration. Then, a recently developed approach, based on the domain decomposition paradigm, will be presented. The talk is based upon joint works with Maxime Barrault, Guy Bencteux (Electricite de France), Eric Cances (ENPC-INRIA) and William Hager (University of Florida).

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MS38

Locality in Quantum Mechanics: Theory and Applications

The locality is of crucial importance in quantum mechanics. It is the underlying principle for linear scaling and even sublinear scaling algorithms for density functional theory. In this talk, we will discuss the construction of localized basis for the eigen-subspace, linear scaling algorithms based on localization and also the Cauchy-Born rule for quantum systems which yields sub-linear algorithms.

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MS38

Solving Large Scale Eigenvalue Problems in Electronic Structure Calculations

Density Functional Theory (DFT) is a successful technique used to determine the electronic structure of matter which is based on a number of approximations. It converts the original n-particle problem into an effective one-electron system, resulting in a coupled one-electron Schrödinger equation and a Poisson equation. This coupling is nonlinear and rather complex. Specificially, the eigenfunctions are solution of an eigenvalue problem whose coefficients depend nonlinearly on the charge density. This gives rise to a non-linear eigenvalue problem which is solved iteratively. The challenge comes from the large number of eigenfunctions to be computed for realistic systems with, say, hundreds or thousands of electrons. We will discuss a parallel implementation a finite difference approach for this problem with an emphasis on diagonalization. We will describe the algorithms used and illustrate them with our in-house code, called PARSEC. This code has evolved over more than a decade as features were progressively added and the diagonalization routine, which accounts for the biggest part of a typical execution time, was upgraded several times. We found that it is important to consider the problem as one of computing an invariant subspace in the non-linear context of the Kohn-Sham equations. This viewpoint leads to considerable savings as it de-emphasizes the accurate computation of individual eigenvectors and focuses instead on the subspace which they span. Results with a technique based on Chebyshev filtering which implements this strategy will be reported.

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MS39

Gradient Flow of the Aviles-Giga Functional

Aviles and Giga proposed an energy functional which has appeared in various guises, ranging from thin film blistering to epitaxial growth and modulational theories of pattern formation. The associated gradient flow has an intriguing phenomenology, including the appearace of diffuse interfaces and interface junctions whose dynamics can be ascertained in a particular singular limit. The structure of the evolutionary problem can be characterized variationally by showing a connection to the conjectured Gamma-limit of the singularly perturbed energy. The long-time coarsening behavior can be explained by dimensional analysis of the reduced problem.

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MS39

Self-similar Solutions to Coagulation Equations

The "dynamical scaling assumption" predicts that solutions with finite total volume to coagulation equations (with homogeneous coagulation kernels) should behave in a self-similar way for large times. This prediction has been thoroughly investigated for three particular kernels for which explicit self-similar solutions are known. The picture is yet not so complete for other kernels and, as a first step, results on the existence and local properties of self-similar solutions will be presented.

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MS39

Infinite Divisibility and the Scaling Attractor for Models of Coagulation

Dynamic scaling is a central feature in clustering. In mean-field models, this problem is often degenerate– there is a one-parameter family of self-similar solutions whose domains of attraction are rigidly determined by the tails of the initial data. What happens if the initial data does not have regular tails? A complete description of scaling limits (self-similar solutions and beyond!) may be obtained for some solvable models of coarsening. This talk is a description of this *scaling attractor*. The key idea is to pursue an

analogy with the probabilistic notion of *infinite divisibility*.

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MS39

Rigorous Bounds on Coarsening Rates in Nonlocal Interfacial Systems

Interfacial systems with nonlocal energies arise in a variety of models from phase segregation to biological aggregation. In particular Giacomin and Lebowitz have derived a nonlocal Cahn–Hiliard type equation as a limit of lattice-gas dynamics approximating phase segregation in binary alloys. On long time scales the interfaces between the phases evolve to reduce a measure of interfacial area. This leads to coarsening of length scales present in the system. The rate of coarsening can be investigated using the energy based approach introduced by Kohn and Otto. We will describe a geometric viewpoint, which unites the coarsening results in a variety of interfacial models.

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MS40

The Yield Strength of Composites and Polycrystals. Examples from a Toy Model

We study, by means of simple analysis and examples, a toy model to compute the yield strength of composites and polycrystals. Our goal is to understand the dependence of the effective yield strength of the material on the microgeometry and the properties of the pure phases that compose the material.

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MS40

Stress Amplification Inside Random Two-phase Composites

In this talk we discuss methods for bounding the higher L^p norms, $2 \leq p \leq \infty$, of the rotational invariants of the local stress and strain inside random media. Here optimal lower bounds are given in terms of the applied loading and phase volume fractions for random two phase composites. Such bounds provide the means to measure load transfer across length scales relating the excursions of the local fields to the applied boundary loading.

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MS40

Realizable Response Matrices for Discrete Networks at Given Frequency

Homogenization of composite built from high contrast constituents can lead to a macroscopic behavior entirely different from those seen in nature. A crucial step when characterizing all possible materials is the study of possible response of discrete networks. Here we study the response, at a given frequency, of dicrete networks in the linear frameworks of electricity, acoustics or elasticity. We prove that all response matrices are possible, provided they respect the second principle of thermodynamics.

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MS40

Incremental Variational Principles with Application to the Homogenization ofNonlinear Dissipative Composites

This study is devoted to the overall response of nonlinear composites comprised of phases which have a partly reversible and partly irreversible behavior. After time-discretization, the evolution equations describing the constitutive behavior of the phases are reduced to the minimization of an incremental energy function. This minimization problem is rigorously equivalent to a nonlinear thermoelastic problem with a nonuniform transformation field. Two different techniques for approximating the nonuniform eigenstrains by piecewise uniform eigenstrains and for linearizing the nonlinear thermoelastic problem will be presented.

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MS41

Coupling of Length Scales for Mechanical Properties: Quantum-mechanics, Empirical Potentials, and Continuum Elasticity

Quantum mechanical methods provide the most accurate description of atomic interactions, but they are computationally expensive. Empirical interatomic potentials are a much faster approach to atomistic simulation, but still much less efficient than continuum descriptions of matter. By applying each method only in the region where it is required, we can combine the best features of each. I will discuss some general issues in concurrent coupling of different computational methods, and in particular how they manifest themselves in continuum and atomistic descriptions of solid mechanics. I will then present several ways we have applied the coupling of length scales approach. One example couples a quantum-mechanical total energy method to the quasi-continuum method to study fracture in silicon with the accuracy of a quantum-mechanical de-

scription of bonding at the crack tip. The other example shows how we coupled a finite temperature atomistic simulation to a finite element solution of continuum elasticity to simulate contact and friction for self-affine surfaces.

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MS41

Coarse-graining the Free Energy of Atomistic Systems: A Simple Case

Molecular dynamics is a classical method to compute constant temperature thermodynamical averages. For instance, the evolution of a material science system according to the Langevin equation is simulated, while some relevant observables are averaged along the trajectory. 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, called repatoms, following the QuasiContinuum terminology. In this case, it is natural to try and design a dynamics on these repatoms that can be used to compute more efficiently the canonical averages under study. A way to design such a dynamics is to compute, for any position of the repatoms, the free energy of the system. In this talk, we first consider a 1D chain of atoms, and we present some methods to rigorously and efficiently compute this free energy. Our approach is based on a thermodynamic limit procedure. We will consider the NN and the NNN cases and illustrate the obtained theoretical results with numerical simulations. We next report on ongoing works for the 2D case.

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MS41

A Study of a Coarse-grained Approximation for Dynamics of an Atomic Chain

In the talk I will briefly introduce results for the convergence analysis of the quasicontinuum approximation in the steady state case. I will then focus more on a simple generalization of the quasicontinuum idea to a dynamical atomic chain and then obtain a coarse-grained approximate dynamical model. We then numerically and analytically study the convergence of the coarse-grained model in a time-average sense assuming the nearest neighbor interaction. The corresponding PDE of the dynamical atomic chain is a nonlinear wave equation of mixed type. We can construct the solution of its Riemann problem under an admissible condition. We then explain how this Riemann solution may be used to justify the coarse-grained dynamical solution.

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MS41

Multiscale Simulations of Flow and Friction Using Hybrid Atomistic/continuum Methods

Atomic scale interfacial processes dominate friction, fracture, adhesion and nanoscale flows. However, interfacial conditions are determined by deformation and flow at much larger scales. Integrating an atomic-scale treatment of bond breaking, sliding, and flow at interfaces, with a continuum description at larger scales poses major challenges. The talk will describe algorithms for simultaneous multiscale modeling that have been developed by our group. An atomistic description is used in regions of rapid change in stress, strain or composition, such as interfaces. Continuum descriptions are used in regions of slow change, with the spatial and temporal resolution coarsening as gradients decrease. Closely related algorithms have been developed for fluids and solids. They allow flow of particles and heat between atomistic and continuum domains. The two domains are coupled via an overlap region where the fluxes or displacements from one description provide boundary conditions for the other. Results from the fluid algorithm will be presented for slip at rough walls, singular corner flows in cavities, contact line motion and heat transport. The analogous algorithm for solids has been applied to contact of rough surfaces and the resulting friction. The methods have allowed us to span up to six orders of magnitude in length scale.

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MS42

From Interatomic Potentials to Wulff Shapes, via Gamma Convergence

We present recent progress on analysing the behaviour of ground states of N particles interacting via interatomic potentials as N becomes large. In a 2D model system, the emergence of crystalline structure, elastic energy, and surface energy are all seen to emerge in a natural way.

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MS42

From Discrete Stochastic Lattices to Continuum Theories

(joint work with X. Blanc (Univ. Paris 6) and PL. Lions(College de France)). We study the continuum (macroscopic) limit for some atomistic models for crystals. The purpose is to derive densities of mechanical energies from microscopic models. In contrast to previous studies , where the microscopic structure was assumed to be periodic, we consider the case of a microstructure modelled by a stochastic lattice. We also show the relation between this type of questions and questions of stochastic homogeniza-

tion.

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MS42
Homogenization of Networks with Bar Interactions

We describe the equilibrium of an elastic lattice made of nodes (or atoms) and of bars (or bonds) that can be a living tissue – for instance the myocardium – as well as a carbon network. The energy of the large deformation frame-indifferent model takes into account both the bar lengths and the angles between bars. By passing to the limit, we derive from the discrete model a continuous model, which is a membrane model.

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MS42
Discrete-to-continuum Limits of Magnetic Forces in Dependence on the Distance Between Bodies

Force formulae for two magnetic bodies in dependence on their mutual distance are derived as continuum limits of atomistic dipole-dipole interactions. For atomistically large distances we recover a classical formula for magnetic forces. For distances comparable to atomistic units, however, we discover a new term explicitly depending on the underlying crystal lattice structure, thus linking the classical force formula and the case of two bodies being in contact. (Joint work with A. Schloemerkemper, Leipzig)

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MS43
On the Choice of Coarse Variables for Dynamics

A methodology for developing dynamical equations for coarse variables representing time-averaged behaviour of a fine-scale autonomous dynamics is presented. Given the fine dynamics with some idea of what time-averaged coarse variables one might be interested in, an augmentation with a singular perturbation structure emerges that is perhaps amenable to mathematical treatment by work of Artstein and Vigodner (1996). A coarse dynamics can then be constructed by calculating suitably generalized solutions to an "invariance PDE".

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MS43
Nucleation and Kinetics of Phase Boundaries in Peridynamics

Classical continuum models of active materials are not closed, and require nucleation and kinetic information as additional input. We examine this in peridynamics, a non-local integral continuum model. Our analysis shows that kinetics is inherent to the theory. The perspective of nucleation as a dynamic instability leads to interesting results that are consistent with simulations, and not with the traditional view. We also find an unusual mechanism for a phase boundary to bypass an inclusion.

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MS43
Coarse-graining Molecular Dynamics

In practice, molecular dynamics is usually limited to small systems and short time period. I will discuss a dimension reduction technique to coarse-grain molecular dynamics. A new system of equations, governing only a small number of variables will be derived. I will also discuss practical implementations under this framework.

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MS43
The Relative Role of Dispersion, Dissipation and Inertia in Dynamics of Martensitic Phase Boundaries

We study the kinetics of a martensitic phase boundary in a one-dimensional lattice with long-range interactions and its dependence on the degree of discreteness. We find that the viscoelastic and viscosity-capillarity quasicontinuum models provide an upper and lower bound, respectively, for the kinetic relation linking the driving force and the phase boundary velocity. The quasicontinuum approximations work best at near-sonic velocities but cannot be trusted near the depinning threshold.

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MS44
The Translational Gauge Theory of Dislocations

We investigate the T(3)-gauge theory of static dislocations in continuous solids. We propose and use the most general linear constitutive relations for the force and pseudo moment stresses for isotropic solids. The constitutive relations contain six material parameters. In this theory both the force and pseudo moment stresses are asymmetric. The theory possesses four characteristic lengths. We derive the three-dimensional Green tensor of the master equation for

the force stresses in the translational gauge theory of dislocations. We investigate the situation of generalized plane strain (anti-plane strain and plane strain). Using the stress function method, we found new gauge theoretical solutions for screw and edge dislocations. The solution of the screw dislocation is given in terms of one independent length. For the edge dislocation we obtain a solution in terms of two characteristic lengths. Thus, this theory possesses only two independent lengths for generalized plane strain.

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MS44

Atomistic Simulation of Surface Dislocation on Au (001) Surfaces

Recent high resolution electron microscopy investigations of Au (001) surface show the existence of highly mobile surface dislocations. We examined the thermodynamic and kinetic properties of this novel surface structure using atomistic simulations. Two different types of stable surface dislocation structures are obtained and are consistent with experimental observations. Minimum energy path calculations using the string methods were also performed to study the migration kinetics of surface dislocations. We are also going to present preliminary results from temperature accelerated dynamics simulations

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MS44

Non-planar Dislocation Cores: A Ubiquitous Phenomenon Affecting Mechanical Properties of Materials

Non-planar dislocation cores lead to strong temperature and orientation dependencies of yielding, the breakdown of the Schmid law and various anomalies in plastic flow. We show that such dislocation cores are prevalent in elemental metals, with an exception of FCC ones, ordered alloys, ionic crystals, molecular crystals and, presumably, other materials. Our discussion of the core structures and their effect on dislocation glide and thus yielding behavior is based on the results atomistic computer modeling.

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MS44

A Generalized Peierls-Nabarro Model for Curved Dislocations in FCC Materials

We present a generalized Peierls-Nabarro model for curved dislocations in FCC materials, in which the anisotropic elastic energy is obtained efficiently using the Fast Fourier Transform method, and the generalized stacking fault energy is used for the interplanar potential across the slip plane. Simulation results are reported on core structures and activation energies of dislocation loops in Al and Cu, incorporating both the elastic anisotropy and the full disregistry vector in the slip plane.

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MS45

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS45

Real-time Dynamics of Electrons and Ions in Nanostructures and Biomolecules

I will discuss a new methodology for applying real-time dynamics to study the evolution of excited states in nanostructures and biomolecules, with applications to dye-sensitized nanowires for photovoltaics and to biomolecules such as the constituents of melanin. The real-time dynamics offers accurate and insightful description of the system evolution and reproduces realistically interesting mechanisms for de-excitation and light absorption.

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MS45

An Orbital-Free Density Functional Based QM/MM Methodology for Metals

We present a QM/MM formalism for coupling density functional theory (DFT) based quantum simulations to classical atomistic simulations for metals. The multiscale methodology is applicable to systems where important quantum phenomena are confined to a small region, but their impacts could be felt over much larger scales. The concurrent coupling between QM and MM regions is treated quantum mechanically via the orbital-free density functional theory (OFDFT). We propose two energetic formulations for the QM region: one is based on OFDFT and the other based on the Kohn-Sham (KS) DFT. In the first case, the degree of freedom is the electron charge density in the QM region, and the total energy functional is directly minimized with respect to the charge density. In the second case, the degrees of freedom are KS orbitals in the QM region. An embedding potential representing the influence

of the larger MM region onto the QM region, is included in the KS Hamiltonian for the QM region, which is solved self-consistently. Calculations for a perfect lattice and vacancy clusters of aluminum demonstrate that the present QM/MM approaches yield excellent results both in terms of energetics and electron density.

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MS45

Partition-of-unity Finite-element Approach for Large, Accurate Ab Initio Electronic Structure Calculations

Over the past few decades, the planewave (PW) pseudopotential method has established itself as the dominant method for large, accurate, density-functional calculations in condensed matter. However, due to its global Fourier basis, the PW method suffers from substantial inefficiencies in parallelization and applications involving highly localized states, such as those involving 1st-row or transition-metal atoms, or other atoms at extreme conditions. Modern real-space approaches, such as finite-difference (FD) and finite-element (FE) methods, can address these deficiencies without sacrificing rigorous, systematic improvability but have until now required much larger bases to attain the required accuracy. Here, we present a new real-space FE based method which employs modern partition-of-unity FE techniques to substantially reduce the number of basis functions required, by building known atomic physics into the Hilbert space basis, without sacrificing locality or systematic improvability. We discuss pseudopotential as well as all-electron applications. Initial results show order-of-magnitude improvements relative to current state-of-the-art PW and adaptive-mesh FE methods for systems involving localized states such as d- and f-electron metals and/or other atoms at extreme conditions. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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MS46

Aggregation During a Thermal Quench

The creation of clusters in the context of a quench is studied. Two model problems are considered. First, undersaturated vapor is cooled at a prescribed rate. After a time-lag, the nucleation rate rises exponentially. A short burst of nucleation decreases the super-saturation and ends the creation of new clusters. We find asymptotic descriptions of the resulting distribution of cluster sizes and the total amount of clusters generated. The time-lag is related to the quench rate by an implicit formula. Next, the flow of a warm gas onto a cold wall is examined. The creation and growth of clusters in the boundary layer next to the cold wall are the natural extension of the first problem. We find the total amount of clusters generated, the concentration of monomers in the gas and the size of the clusters as functions of the distance to the wall. We also determine the distance from the wall at which the nucleation happens, and the length of the "growth layer", during which the growth of clusters brings the gas to equilibrium.

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MS46

A New Variant of Becker-Doering Equations

The Becker-Doering equations are a well-known model for cluster formation in a set of identical particles, where clusters can grow or shrink only by gaining or loosing a single particle, respectively. Usually, the transfer equations are closed by certain standard assumptions for the transitions rates, and this give rise to an infinite-dimensional nonlinear dynamical systems. Recently, Dreyer and Duderstadt proposed a modified Becker-Doering equation, which is based on a different closure procedure and leads to a different long time behavior. We focus on the mathematical properties of the modified model and compare with the standard model.

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MS46

Long Time Behavior of a Modified Becker-Doering System

A modification, based on asymptotic behavior, of the Becker-Döring system is introduced in which the concentration of monomers is slaved to the concentrations of the other clusters. This modified system has the same continuum limit as the usual Becker-Döring system. For one member of the modified systems it is proved, for compact initial data, that all solutions will converge to the same self-similar form as time tends to infinity.

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MS46

Similarity Solutions for Size-dependent Aggregation

We consider the pure aggregation form of the Becker-Döring equations, with time-dependent monomer input and in which the aggregation rates have an algebraic size-dependence. We show that such systems possess a range of behaviours which can be classified by the exponents of the input rate and aggregation rates. By considering the large-time asymptotics of the cluster size distribution functions, we find a variety of self-similar solutions, whose shapes can be explicitly quoted.

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MS47

Phase Boundary Motion by Surface Diffusion Flow with Triple Junction

The surface diffusion flow is a fourth order geometric evolution law for an evolving hypersurface which has the property that the perimeter of an enclosed domain decreases whereas the volume is conserved. In this talk, the motion of phase boundaries with triple junction is studied. Our goal is to derive the criteria of the linearized stability of the equilibrium states and to apply it to the analysis of the nonlinear stability.

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MS47

Coupled Surface Diffusion and Motion by Mean Curvature

A variety of phenomena occur when grain boundaries evolving within a crystalline specimen connect up to an external surface which evolves by surface diffusion. Because of the difficulties involved in treating these coupled motions, we have focused on a number of special 2D and 3D geometries with certain symmetries. We employ a variety of analytical, numerical, and asymptotic tools, and report on some surprising effects, some of which can be confirmed experimentally.

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MS47

Numerical Analysis of a Steepest-descent PDE Model for Surface Relaxation Below the Roughening Temperature

We study the numerical solution of a PDE describing the relaxation of a crystal surface to a flat facet. The PDE is a singular, nonlinear, fourth order evolution equation. It can be seen as the gradient flow of a convex but non-smooth energy with respect to the H^{-1} inner product. Our numerical scheme uses implicit discretization in time and a mixed finite-element approximation in space. The singular character of the energy is handled using regularization, combined with a primal-dual method that remains robust as the regularization parameter tends to zero. We study the convergence of this scheme, both theoretically and numerically.

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MS47

Modeling and Simulation of Crystalline Surface Evolution by Surface Diffusion with Anisotropic Surface Free Energies

We present a mathematical model and computational method for the surface evolution of crystalline material by surface diffusion with anisotropic surface free energy. We study the evolution path to equilibrium and examine the effect and treatment of different levels of anisotropy. We show that a polyhedron Wulff shape is the limit of Wulff equilibrium crystal shapes with smooth surface energies. An application of the model and simulation to grain boundary grooving with tungsten is demonstrated.

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MS48

Atomic-to-continuum (AtC) Coupling Using Peridynamics

My presentation describes a coupling of peridynamics with molecular dynamics and classical elasticity. In direct analogy with molecular dyanmics, peridynamics uses a nonlocal model of force, does not employ stress/strain relationships germane, and does make any assumptions on the displacement field in constrast to classical elasticity.

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MS48

Boundary Condition and Surface Stress Effects on the Resonant Properties of Metal Nanowires

We utilize the recently developed surface Cauchy-Born model, which extends the standard Cauchy-Born theory to account for surface stresses due to undercoordinated surface atoms, to study the influence of boundary conditions and surface stresses on the resonant properties of $\langle 100 \rangle$ gold nanowires with $\{100\}$ surfaces. The focus of this work is on quantifying variations in the nanowire resonant frequencies due to surface stresses depending on whether fixed/free (cantilevered) or fixed/fixed boundary conditions are utilized, and in quantifying the variation as compared to the corresponding bulk material that does not observe surface effects. The key finding of this work is a strong dependence of the resonant frequencies on the stress state of the nanowires resulting from the boundary conditions and surface stresses. In particular, we find that while the resonant frequencies of fixed/fixed nanowires are elevated as compared to the corresponding bulk material, the resonant frequencies of fixed/free nanowires are reduced as a result of compressive relaxation caused by the surface stresses. Furthermore, we find that for a diverse range of nanowire geometries, the variation in resonant frequencies for the

fixed/free nanowires due to surface stress effects is a geometric effect that is characterized by the nanowire aspect ratio.

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MS48

On the Control of the Position and Size of the Overlap Region in an Atomistic-to-Continuum Coupling Method

In this research, we present an adaptive approach based on the control of modeling error for an atomistic-to-continuum coupling method. The method is based on the Arlequin framework that introduces an overlapping region to couple the continuum and atomistic models. A goal-oriented adaptive strategy is then extended to this problem in order to predict the position of this interface so as to reduce the modeling errors within preset levels of accuracy.

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MS48

Replica Asynchronous Variational Integrator

We develop a novel computational approach, to be referred to as Replica-AVI or RAVI for short, that effectively bridges molecular dynamics and irreversible continuum thermodynamics. The essential idea behind RAVIs consists of overlaying replicas of the coarse elements, with the element replicas sharing the same spatial domain. The replicas are each run at its own slow time step and are out-of-phase with respect to each other by one fast time step. In this manner the thermal phonons can be transmitted losslessly from the fine to the coarse-grained regions of the mesh. RAVIs provide a natural and effective accounting device for tracking thermodynamic measures, such as heat and temperature, in the coarse-grained region.

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MS49

Step-flow Growth of a Crystal Surface by Levy Flights

Step-flow growth of a vicinal crystal surface is considered in the case when the surface diffusion of adatoms is governed by anomalous diffusion, namely, Levy flights. The step-flow velocity is found as a function of the terrace length and the Levy flights exponent. It is shown that with the decrease of the anomalous diffusion exponent (i.e. increase of the diffusion rate) the step-flow velocity decreases due to the possibility of long jumps over the steps.

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MS49

The Effect of the Rayleigh Instability on Anisotropic Crystalline Rods

Properties of strength, toughness, ductility, and hardness of materials are greatly influenced by the conditions of solidification. We study the effect of anisotropic surface energy on the stability of a solidifying crystalline rod, both free-standing and on a surface. The study is partially motivated by the apparent stability of elongated nanowires in a bridge configuration or grown epitaxially on a heterogeneous surface. The rod is assumed to be smooth with a uniform cross-section given by a two-dimensional equilibrium shape. We apply the analysis to examples with uniaxial or cubic anisotropy and showed that the anisotropic surface energy played a significant role in establishing the stability of the free standing rod or rod on a surface.

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MS49

A Tangent-plane, Marker-particle Method for the Computation of 3D Solid Surfaces Evolving on a Substrate

I will describe a particle method for computing morphological evolution by surface diffusion. The method does not rely on gridding or numerical differentiation, and applies to surfaces with finite slopes and overhangs. Moreover, the method is capable of explicit and accurate tracking of the contact lines. Large time steps are allowed due to the meshless nature of the method. The method is low cost, partially because it operates in the local tangent plane,

where the surface Laplacian has simpler form. The method is demonstrated by computing the decay and growth of perturbations to cylindrical wires (rods) pre-grown on a substrate (Rayleigh instability).

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MS49
Asymmetric Transition States in Quantum Dots

We present a model for the shape transitions in strained solid films with strongly anisotropic surface energy. In the absence of substrate miscut, it is known that a truncated pyramid minimizes the energy at small volume while a dome minimizes the energy at larger volume. Here we demonstrate the existence of an asymmetric "half-dome" shape which acts as a low-barrier metastable transition state in the transition from the truncated pyramid to dome. Thus, in a system with moderate fluctuations, half-dome quantum dots should be observed, if only rarely. We also determine that in the presence of a miscut substrate, "half-pyramid" and "half-dome" shapes can be stable equilibrium states. This work is in collaboration with Jerry Tersoff.

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MS50
Growth of Objective Structures by Self-assembly

Objective structures are molecular structures consisting of identical molecules, such that corresponding atoms in each molecule see the same environment up to orthogonal transformation. These structures are common in viruses – capsids, necks, tails and baseplates. Following the intuitive arguments of Caspar and Klug (Cold Spring Harbor Symp. Quant. Biol. 27 (1962), 1-24), a possible reason for their widespread appearance is that they are the natural structures for self-assembly. That is, the addition of a molecule to a partly built structure tends to complete the environment of the molecules present, and also of the one added. But one has to explain why, given a finite number of molecules in the invaded cell, full capsids (baseplates, tails, etc.) are formed rather than many bonded pairs of molecules. We discuss these issues from a mathematical viewpoint.

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MS50
Geometry and Elasticity of Leaves and Flowers

Many structures in biology consist of thin sheets that naturally form rippled surfaces. These can be explained by viewing them as surfaces in which growth processes create target metrics that are not flat. The surface ripples in an attempt to bring its metric to the target. I will discuss a combination of analytical, experimental, and numerical results that show how geometry and elasticity work together to create these structures.

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MS50
Emergence of Patterns During Tissue Morphogenesis

The morphogenetic patterning that generates three-dimensional (3D) tissues requires dynamic concerted rearrangements of individual cells with respect to each other. We have developed lithography-based 3D culture models that recapitulate the architecture of epithelial ductal trees, enable micrometer-resolution control of tissue geometry and microenvironment, and provide quantitative 4D data in a physiologically relevant context. This approach has revealed that tissue patterns emerge from complex social interactions between the epithelial cells comprising the duct, which are directed by tissue mechanics.

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MS50
Hidden Symmetries in Virus Architecture and their Implications on Virus Assembly

It is shown that the structures and radial extensions of the material boundaries in simple RNA viruses, from the protein capsid that encapsulates the viral genome down to the innermost RNA, are collectively constrained by symmetry. This structural correlation between the genomic material and the capsid proteins is used to model the constraints implied by the viral RNA on the assembly of the protein containers as discussed in detail for the example of bacteriophage MS2.

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MS51

Euler-Lagrange Equations and Smoothness Properties of Minimizers of Kirchhoff's Plate Functional

Kirchhoff's theory rules the behaviour of nonlinearly elastic plates, whose mid-plane deformations are isometric immersions defined on a flat reference configuration. We develop techniques which allow to modify generic isometric immersions locally while essentially preserving their energy. We apply these techniques firstly to prove that generic deformations with finite Kirchhoff energy can be approximated by smooth ones. Secondly, we derive the Euler-Lagrange equations for Kirchhoff's energy functional and use them to study the smoothness of minimizers.

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MS51

Convergence of Equilibria of Thin Elastic Beams

In a series of recent papers a hierarchy of lower dimensional theories for nonlinearly elastic thin beams has been rigorously derived, starting from three-dimensional elasticity, by means of Gamma-convergence. This approach guarantees convergence of minimizers of the 3d elastic energy to minimizers of the reduced problem. In this talk we will discuss the convergence of (possibly non-minimizing) stationary points of the 3d elastic energy. These are joint works with S. Mueller and M.G. Schultz.

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MS51

Folding and Deployment of Ultra-thin Structures

The motivation for this work is the design of novel radar structures for earth-observation satellites that do not require any mechanical hinges and can be manufactured in a single piece. We consider singly-curved structures, with the shape of a cylinder or a box with straight or curved edges. These structures can be folded inextensionally into a nearly flat configuration and then into a concertina. In each case, we are interested in determining the folded shape in sufficient detail to estimate the maximum strain and stress in the material, and the dynamic deployment behaviour when a constraint that holds the structure packaged is released.

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MS51

Theory of Inextensible Elastic Sheets with Application to the Moebius Strip

We derive a new set of geometrically-exact equilibrium equations for the deformation of thin inextensible strips of finite width. The equations are the Euler-Lagrange equations for a geometrical variational problem with a functional in terms of the curvature and torsion of the strip's axial curve as well as their derivatives with respect to arclength. The equations are used to solve the long-standing problem of finding the characteristic shape of a Moebius strip.

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MS52

Heteroepitaxy and Other Free-boundary Problems: From Phase-fields to the Phase-field Crystal Method

The vast majority of naturally occurring or synthetic materials are not in equilibrium and contain complex spatial structures across a multitude of length scales. This is particularly important since these morphologies often determine the mechanical, electrical, and optical properties of the material. Traditionally, the temporal evolution of morphologies has been modeled through numerically solving either a set of physically-based sharp-interface or diffuse-interface (phase-field) models. While such approaches have proven to be very useful in elucidating the physics behind the evolving morphologies in, e.g., phase transformations and thin film growth, incorporating plastic effects and other atomistic features in these models becomes quite cumbersome. As an alternative approach, in this talk I will describe a simple continuum model which is capable of modeling both elastic and plastic deformation under non-equilibrium conditions. This so-called phase-field crystal method introduces a continuous atomic mass density field in which fast atomic vibrations have been integrated out. The free energy functional of the system supports spatially periodic states, and naturally incorporates elastic and plastic effects, grain boundaries, free surfaces, and arbitrary crystal orientations. Dissipative dynamics can be constructed to govern the temporal evolution of the density field at mesoscopic time scales, inaccessible by direct Molecular Dynamics simulations. I will illustrate the utility of this approach with specific examples from epitaxial growth of ultrathin alloy films and ferroelectric nanostructured materials.

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MS52

A New Approach for Modeling Strongly Anistropic Crystal Systems

We present a new approach for modeling strongly anisotropic crystal and epitaxial growth using regularized, anisotropic Cahn-Hilliard-type equations. Such problems

arise during the growth and coarsening of thin films. When the surface anisotropy is sufficiently strong, sharp corners form and unregularized anisotropic Cahn-Hilliard equations become ill-posed. Our models contain a high order Willmore regularization to remove the ill-posedness. A key feature of our approach is the development of a new formulation in which the interface thickness is independent of crystallographic orientation. We also have added strain energy to this model to study the effect of elasticity. We present 3D numerical results using an adaptive, nonlinear multigrid finite-difference method. In particular, we find excellent agreement between the computed equilibrium shapes using the Cahn-Hilliard approach, with a finite but small Willmore regularization, and an analytical sharp-interface theory recently developed by B. J. Spencer [2004].

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MS52

Heteroepitaxy of Magnetic Thin Films: Connecting Ab Initio Calculations to Continuum Modeling

We present a dislocation model based on the Peierls-Nabarro formulation to study dislocation structures within heteroepitaxial Fe films grown on Mo(110) and W(110) substrates. The continuum model calculates the elastic field originating from the misfit dislocation array within a film of finite thickness. We use the stacking fault energy of the Fe/Mo and Fe/W systems from ab initio calculations as an input to the model. The parametric studies and equilibrium dislocation energy calculations are presented.

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MS52

Rapid Computation of Elastic Energy Differences with Application to Heteroepitaxy

When simulating heteropitaxial growth using kinetic Monte Carlo one needs to compute the elastic energy difference between two simliar configurations a vast number of times. This talk will describe several tools to allow one to accomplish this efficiently. A Fourier-multigrid method which allows one rapidly compute the displacement field for an arbitrary film profile coupled to semi-infinite substrate will be discussed. Next, the principle of energy localization will be stated which combined with the expanding box method allows one to accurately compute changes elastic energy using local calculations. Finally some results showing the formation of self-assembled stacked quantum dots will be shown. This is joint work with Giovanni Russo and Tim Schulze.

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MS53

Strain and Stress Fields in Shape-memory and Rigid-perfectly Plastic Polycrystals

The study of polycrystals of shape-memory alloys and rigid-perfectly plastic materials gives rise to problems of nonlinear homogenization involving degenerate energies. We present a characterisation of the strain and stress fields for some classes of problems in plane strain and also for some three-dimensional situations. Consequences for shape-memory alloys and rigid-perfectly plastic materials are discussed through model problems (again, in two and three dimensions). In particular we explore connections to previous conjectures characterizing those shape-memory polycrystals with non-trivial recoverable strain.

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MS53

Modeling the Macroscopic Behavior of Two-phase Nonlinear Composites by Infinite-rank Laminates

A new approach is presented for estimating the macroscopic behavior of two-phase nonlinear composites with random, particulate microstructures, based on infinite-rank sequential laminates. The resulting estimates incorporate microstructural information up to the two-point correlation functions, and are guaranteed to be convex, to satisfy all pertinent bounds, and to be exact to second order in the heterogeneity contrast. Comparisons are presented with earlier homogenization estimates, as well as with numerical simulations available from the literature.

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MS53

Bounding the Recoverable Strains in Polycrystalline Shape-memory Alloys

New upper bounds are proposed for a generic problem of geometric compatibility, which covers the problem of bounding the effective recoverable strains in composite shape memory alloys (SMAs), such as polycrystalline SMAs or rigidly reinforced SMAs. Both the finite deformation and infinitesimal strain frameworks are considered. The methodology employed is a generalization of a homogenization approach introduced by Milton and Serkov (2000) for nonlinear composites in infinitesimal strains. Some analytical and numerical examples are given to illustrate the method.

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MS53

Localizing Limit of Vanishing Porosity in Strongly Anisotropic, Compressible, Linear Lattices of Voids, by Combined Mellin Transforms and Lattice Sums Techniques

The so-called "second-order" homogenization methods, aimed at predicting the overall nonlinear behavior of composites, use an underlying anisotropic homogenized linear medium whose anisotropy is determined consistently by variances of the (strain or stress) fields. Recent works suggest that plastic localization in a perfectly plastic porous medium implies the appearance of non-integer powers of the volume fraction of voids, f, in expansions at small f of effective quantities such as the overall plastic limit. To investigate this phenomenon at the level of the underlying linear homogenized medium, a model of a strongly anisotropic linear medium containing a two-dimensional periodic array of pores is considered. We show how the appearance of non-integer powers of f in the overall elastic moduli is connected to a cross-over phenomenon between individual and collective response of the voids (tantamount to localization), confirmed by FFT calculations. This behavior involves a porosity- and anisotropy-dependent cross-over length scale, very much like phase transitions in statistical physics. The transition is investigated mathematically using Mellin transform and lattice sum techniques, and the cross-over length is explicitly exhibited. This work is part of a collaboration with P. Ponte Castañeda and M. Idiart.

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MS54

Fluctuations of Fields and of Effective Properties in Random Media

From numerical simulations, the average effective properties and their fluctuations are studied by a geostatistical approach, involving the experimental determination of the integral range of the fields of interest. This is illustrated for the dielectric permittivity of 2D autodual random sets and of a 3D Boolean model of spheres. The permittivity and the corresponding RVE are estimated for an increasing contrast, and related to the behaviour of the covariance of the dielectric displacement field.

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MS54

Mathematical and Statistical Methods for the Coarse-Graining of Many-Particle Stochastic Systems

In this talk we discuss recent work on coarse-graining methods for microscopic stochastic systems. The emphasis is both on the numerical analysis of the schemes focusing on error quantification, as well as on developing improved algorithms capable of operating in wide system parameter regimes. Furthermore we develop adaptive coarse-graing schemes with the capacity to automatically adjust during simulation once substantial deviations are detected in a derived error indicator. The methods employed in the analysis and algorithm development rely on one hand on statistical mechanics methods such as renormalization and cluster expansions, while on the other make use of ideas from the numerical analysis of PDE, e.g a posteriori error estimation, as well as statistics tools such as importance sampling. Finally, we discuss the connections and extensions of the work on lattice systems to the growing engineering literature on coarse-graining of polymers.

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MS54

Failure Initiation and Uncertainty Inside Multiscale Random Media

In this talk we discuss the problem of resolving the location of high stress zones inside composite media using coarse-grained field measurements together with statistical descriptions of the microstructure. We show how to apply the statistics and measurements to assess the extent of high stress zones inside heterogeneous structures under suitable assumptions on the size of the heterogeneities.

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MS54

Towards a Systematic Time Coarse Graining of KMC Models

We study a hierarchy of successively time coarse-grained stochastic processes. These processes include pure jump processes arising in kinetic Monte Carlo models and approximations that are less expensive to compute, namely Ito diffusions and deterministic differential equations. We discuss the approximation error associated with coarse graining and numerical discretizations. We also present a framework to produce hybrid models automatically based on a posteriori error estimation.

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MS55

Step Dynamics Modeling of Multilayer Growth

Atomistic modeling of unstable multilayer growth in specific homoepitaxial systems has been very successful in predicting the formation and evolution of mounds.* However, an understanding of the essential features of mound dynamics is potentially enhanced by development and analysis of appropriate continuum evolution equations. Derivation directly from atomistic models has proved problematic, but some progress has been made starting from 'intermediate' step dynamics models. We describe such analyses designed to capture mound slope slection due to downward funneling, and indicate remaining challenges related to incorporation of nucleation of new layers at mound peaks and fluctuation effects. Finally, we show how the step dynamics approach is valuable in treating more complex heteroepitaxial multilayer growth systems where behavior is impacted, e.g., by strain and quantum size effects. *J.W. Evans, P.A. Thiel, M.C. Bartelt, Surf. Sci. Rep. 61 (2006) 1.

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MS55

Kinetic Hierarchies and Continuum Limit for Stepped Crystal Surfaces

Below roughening crystal surfaces consist of distinct steps whose motion is described by discrete schemes and drives morphological evolution. The connection of such schemes to continuum laws is not well understood. In this talk I will present progress and challenges in tackling two interrelated issues: (i) The formulation and closures of kinetic (BBGKY-type) hierarchies for step correlation functions. (ii) The homogenization (continuum limit) of step laws in settings of physical importance, particularly faceting, surface reconstruction and long-range step interactions. This work has been supported by NSF-MRSEC DMR0520471 at the University of Maryland.

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MS55

Coarsening Versus Non Coarsening of Nonequilibrium Surfaces

Several nonequlibrium systems exhibit patterns characterized by a lengthscale. The lengthscale may be fixed in time (at least its average over time, or in the statistical sense). It may alternatively, perpetually increase in time (typically as a power law). The perpetual increase of the lengthscale is a process which is called coarsening. An intermediate stage may occur : interrupted coarsening. We present a class of nonlinear equations that exhibit these three typical scenarios (no coarsening, coarsening, or interrupted coarsening). We provide a simple criterion on which scenario prevails by just inspecting the portrait of *steady-state solutions*. This is made possible thanks to the extraction of analytical results based on phase diffusion equation of the pattern. We further provide a straightforward manner to evaluate the coarsening exponent by using information from phase diffusion. We exemplify the method on typical examples. We discuss how these results, which are obtained in one dimension, can be generalized to higher dimensions.

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MS55

Surface Dynamics from Chemical Potential Gradients: Step

The dynamics of crystal surfaces at low temperatures is dominated by the motion of steps, which move by the attachment or detachment of adatoms at the step edge. The associated change in free energy given by a small step displacement defines a local step chemical potential and many features of surface dynamics can be understood as arising from gradients in these step chemical potentials. We extend this general perspective to describe the dramatic effects of impurities in solution growth of crystals. Impurities that impede the motion of surface steps typically produce step-bunching instabilities during vapor growth, and reduce the growth rate. However Land, et. al [T. N. Thomas,T. A. Land, W. H. Casey,and J. J. DeYoreo, Phys. Rev. Lett. 92, 216103/1-4 (2004)] showed that during solution growth of KDP crystals impurities can induce very different behavior. In particular, under appropriate conditions, while single steps are blocked by impurities, large coherent bunches of steps emerge that can move much faster than single individual steps. These "supersteps" dominate the subsequent crystal growth. We introduce a new and general model of impurity effects during crystal growth that describes both steps and impurities using effective chemical potentials. Essential features of model account for the effective impurity strength, the different mechanisms of mass transport during vapor or solution growth, and the effect of step repulsions. The latter can produce an increased driving force on the first step in the bunch and lead to superstep motion. Good agreement with many features of the experiments is found.

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MS56

Size Effects in the Vapor-Liquid-Solid Growth of Alloy and Heterostructured SixGe1-x Nanowires

This presentation will address several size-dependent growth phenomena in the synthesis of nanowires by the vapor-liquid-solid mechanism. Experimental evidence for size-dependent growth rates and composition in Si1-xGex nanowires composition will be discussed. Then the ability to produce chemically abrupt interfaces in Si-Si1-xGex axial heterostructures will be examined. Finally, the criteria that govern the growth of epitaxial, defect-free axial or radial heterostructures in the nanowire geometry will be addressed along with the prospects for enhaning carrier mobility.

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MS56
Experimental Studies of Nanowire Nucleation and Growth Kinetics

Nanowires (also known as whiskers) are one-dimensional, typically single-crystalline, high aspect ratio structures. In the recent years, nanowires have gained attention owing to their potential applications in the areas of catalysis, optoelectronics, energy storage, and sensors. Nanowires are most commonly grown via vapor-liquid-solid (VLS) process. The VLS method involves dissociative adsorption of the material from the vapor phase via a liquid catalyst, commonly a low-melting alloy. Preferential incorporation of the material at the solid-liquid interface, leads to growth in the form of cylindrical pillars or "wires." Over the past 40+ years, several classes of materials (including simple elemental metals, semiconductors, and complex compounds) have been synthesized as wires and characterized. To-date, several recipes exist for controlled growth of wires with desired diameters (from 10 nm to ¿100 nm) and lengths (from 100 nm to ¿10 m). For large-scale device applications, however, wires with precisely controlled morphology (shape, length, and size), crystalline structure, chemical composition, and abruptness of the heterointerfaces are desirable. This can only be achieved through fundamental understanding of the factors influencing these characteristics, for example, the state of the catalyst (solid or liquid), nucleation and growth mechanisms. Here, we present recent in situ transmission electron microscopy (TEM) studies of Au-catalyzed growth of Si and Ge nanowires. All our experiments are carried out in an ultra-high vacuum TEM equipped with in situ physical and chemical vapor deposition facilities. Si and Ge nanowires are grown on clean Au-covered Si substrates using Si and Ge containing precursor gases. TEM images of the wires and the catalyst droplets are collected at video rate as a function of growth pressure, temperature and gas environment. From direct observations of the nanowire nucleation and growth process, we find new insights into the factors affecting the morphological and structural evolution in nanowires. In case of Si wires, we observe Ostwald ripening of liquid catalysts on top of the wires. From the measurements of wire growth rates, we suggest that the rate-limiting process is the incoming flux of Si from the vapour phase. In the Au-Ge system, we find that Ge wires grow both in the presence of solid as well as liquid catalysts, although at different rates. The stability of the liquid AuGe catalyst is governed by the Ge supersaturation in the liquid phase. Both Si and Ge wire morphologies and growth orientations can be controllably varied with deposition flux, gas ambient, and temperature. *Work done at the IBM T. J. Watson Research Center, Yorktown Heights, NY

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MS56
Modelling the VLS growth of Silicon Nanowires

Thermodynamic and continuum aspects of modelling the growth of nanowires via the Vapour-Liquid-Solid mechanism (VLS) are discussed. A framework for modelling the effects of surface energy, surface stress, elastic effects and diffusion in multicomponent alloys is presented and used to find a solution to a steadily-growing straight nanowire with isotropic surface energies.

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MS56
Phase Equilibrium and Nanowire Growth

The phase equilibrium of liquid catalyst in the VLS method of nanowire growth is examined incorporating the effects of surface stress and surface energy. The modification to the liquidus lines are calculated and discussed.

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MS57
Peridynamic Modeling of Damage Propagation in Composite Materials

In this paper, we present our modeling and analysis work on predicting residual compressive strength after hail induced impact damage in composite materials. Furthermore we demonstrate that Peridynamics correctly predicts the failure mode in large-notch composite coupons with different stacking sequences under tensile loading, as well as in biaxially loaded cruciform-shaped composite plates. The simulation results agree fairly well with our experimental data.

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MS57
Adaptivity, Convergence, and Multiscale Modeling

with Peridynamics

In peridynamics, cracks are part of the solution, not part of the problem. We discuss the implementation of adaptive methods in peridynamics and show results for dynamic crack propagation, including crack branching, using adaptive refinement techniques. Multiscale modeling and grid adaptivity are closely related in peridynamics. The peridynamic method offers the promise for a seamless implementation of multiscale models, since it can represent, without changes in the form of its equations, different scales.

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MS57

Peridynamic States

Early development of the peridynamic method relied on forces between independent pairs of particles. To help overcome the resulting restrictions on material response, the theory has been generalized using peridynamic states. These allow forces within each bond to depend on the collective deformation of all the bonds connected to a given material particle. This talk will outline motivation for using peridynamic states and where the theory currently stands.

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MS57

Peridynamic Analysis of Elastic, Viscoelastic, Viscoplastic Deformations of Thin Sheet

The method of Peridynamics is applied to the study of large strain, high strain rate deformations of thin sheets. The model accounts for large strain, rate sensitivity, yielding and hardening, and fracture. This is based on a simple adaptation of the so-called mechanical sub-layer model for uniaxial response. The method is particularly well suited to implementation within the framework of Peridynamics. It is used to simulate ballistic impact and perforation of a metallic film.

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MS58

Pattern Formation in Epitaxial Systems

Abstract not available at time of publication.

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MS58

Phase Field Crystal Modeling of Mound Formation and Dislocation Nucleation during Epitaxial Growth

The growth of coherent epitaxial films is often compromised by elastic strains that give rise to various instabilities such as buckling and dislocation nucleation. In this talk I would like to discuss an analysis of strained film growth as described by a simple phase field model that models atomic structures on diffusive time scales. Analytic and numerical results are presented to predict the mound size as a function of strain. Contrary to standard continuum elasticity theory (i.e., the Asaro-Tiller-Grinfeld instability), the results indicate that the average mound size is inversely proportional to the strain, consistent with recent experiments on SiGe. When the height of the mounds reaches a critical value dislocations nucleate and the film is no longer coherent with the substrate. It is found that this critical height decreases with strain and is consistent in form with the Matthews-Blakeslee equation.

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MS58

Self Assembly of Quantum Dots in Thin Epitaxial Films Wetting an Elastic Substrate

The evolution of quantum dots (QDs) resulting from the Asaro-Tiller-Grinfeld instability of an epitaxially strained thin solid film deposited on a solid elastic substrate is considered. For a film that wets the substrate, a non-local integro-differential equation is derived that describes the evolution of QDs in the long-wave limit. The contribution of a wetting stress that accounts for the change in elastic energy due to variation of the film thickness caused by the film wetting interaction with the substrate is considered. It is found that wetting interactions can damp the long-wave perturbations and lead to the Turing-type instability. By means of weakly nonlinear analysis, general conditions for the wetting potential are found for which the formation of spatially-periodic arrays of QDs is possible. It is shown that in the case of two-layer and glued-layer wetting potentials, the spatially regular arrays of QDs are unstable. The numerical simulations show that the QD's evolution exhibits a power-law coarsening, with different characteristics described by different coarsening exponents.

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MS58

Morphological and Compositional Patterning in Strained Quantum Dots

Knowledge of composition profiles within self-assembled SiGe and InGaAs quantum dots is critical for applications in optoelectronic and memory devices as variations in composition at the nanoscale can substantially influence their electronic properties. Obtaining the quantitative description of composition profiles in the quantum dot is a challenging task due to the coupling between composition variations, shape of the quantum dots and long-range elastic interactions. In this talk, we present an efficient scheme that combines the finite element analysis with an optimization scheme based on a quadratic programming method to determine equilibrium profiles in strained quantum dots. Composition profiles are found to strongly depend on the shape of the quantum dots, as strain relaxation in dots with steeper sidewalls allows for segregation of the larger alloy component in the regions near the apex. Based on these observations, we have developed a phase diagram that shows the degree of segregation of the alloy components in the phase space spanned by the temperature (which governs chemical mixing) and the shape of the dot. Further, we find that the segregation of the alloy components can substantially reduce the critical dot size for the transition between the shapes with different facets.

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MS59

Motion by Curvature in Heterogeneous Media

We study the motion of a discrete interface (or, equivalently, of a continuous interface in a heterogeneaous medium) following the minimizing movement approach. Its macroscopic behavior is described by an effective crystalline (continuous) motion with pinning, velocity quantization and non-uniqueness effects.

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MS59

Onset of Cavitation in Compressible, Isotropic, Hyperelastic Solids

In this work, we derive a *closed–form* criterion for the onset of cavitation in *compressible*, isotropic, hyperelastic solids subjected to *non–symmetric* loading conditions. The criterion is based on the solution of a boundary value problem where a hyperelastic solid, which is infinite in extent and contains a single vacuous inhomogeneity, is subjected to uniform displacement boundary conditions. By making use of the "second–order" variational procedure of Lopez-Pamies and Ponte Castañeda (2006), we solve this problem approximately and generate *variational estimates* for the critical stretches applied on the boundary at which the cavity suddenly starts growing. The accuracy of the proposed analytical result is assessed by comparisons with exact solutions available from the literature for radially symmetric cavitation. In addition, applications are presented for a variety of materials of practical and theoretical interest, including the harmonic, Blatz-Ko, and compressible Neo-Hookean materials.

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MS59

Failure Surfaces for Finitely Strained Porous Elastomers Under Arbitrary In-plane Loading

The present work studies 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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MS59

Composites with One and Two Families of Fibers

It can be shown that for any deformation gradient $\mathbf{A}$ and a unit vector $\hat{\mathbf{N}}$ there is a coordinate system where $\mathbf{A}$ can be represented as a product $\mathbf{RA}_c$, where $\mathbf{R}$ is a rotation and $\mathbf{A}_c$ is expressed in terms of the TI invariants λ_n, λ_p, γ_n, γ_p and ψ_γ [deBotton et al, J. Mech. Phys. Solids, **54**:533, 2006]. Physically, these invariants correspond to particular deformation modes. By application of sequential lamination technique we determine the strain energy function of fiber composites with neo-Hookean phases

$$\tilde{W}^{TIH}(\mathbf{A}) = \tfrac{1}{2}\left(\bar{\mu}(\lambda_n{}^2 + 2\lambda_p{}^2 - 3) + \tilde{\mu}_n\gamma_n{}^2 + \tilde{\mu}_p\gamma_p{}^2\right). \quad (1)$$

Next, this is extended to the class of orthotropic composites with two families of fibers. Comparisons of the response predicted by these effective potentials with estimates of Lopez-Pamies and Ponte Castañeda [Math. Mech. Solids, **9**:243, 2004], phenomenological models for biological tissues, and finite element simulations reveal good agreement.

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MS60

Rise of Correlations of Transformation Strains in Laminated Random Polycrystals

We present a model of a laminated polycrystal with n grains. The orientation of each grain is given by an uncorrelated random sequence of the orientation angles. Under the imposed boundary conditions each grain undergoes stress free transformation, that depends on its orientation angle and result in random sequence of transformation strains obtained as the solution of of a nonlinear optimization problem. While the orientation angles are uncorrelated random variables, the transformation strains may or may not be correlated – this is the central issue of our analysis. We investiogate this rise of correlations in three different scaling limits. Our proofs use the de Finetti's Theorem as well as the Riesz rearrangement inequality. This is a joint work with O. Bruno and A. Novikov.

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MS60

A Coupling Method to Perform Monte-Carlo Simulations at Atomic Scale

We develop a coupling method that enables to perform Monte-Carlo simulations on random systems described at the atomic scale. It is based on the Arlequin framework and concepts used in the Stochastic Finite Element Method. The coupling, performed with a compatible stochastic continuum model defined far away from the region of interest, allows a dramatic reduction in computational cost while providing relevant information on the probability density for specific local quantities of interest.

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MS60

Uncertainty Quantification Using Multiscale Numerical Models

In this talk, I will describe the use of coarse-scale (upscaled) models in uncertainty quantification. The problem under consideration is posed as a sampling problem from a posterior distribution. The main goal is to develop an efficient sampling technique within the framework of Markov chain Monte Carlo methods that uses coarse-scale models and gradients of the target distribution. The purpose is to reduce the computational cost of Langevin algorithms for dynamic data integration problems. We propose to use inexpensive coarse-scale solutions in calculating the proposals of Langevin algorithms. To guarantee the correct and efficient sampling of the proposed algorithm, we also intend to test the proposals with coarse-scale solutions. Comparing with the direct Langevin algorithm based on fine-scale (direct) solutions the proposed method generates a modified Markov chain by incorporating the coarse-scale information of the problem. Under some mild technical conditions we show that the modified Markov chain converges to the correct posterior distribution. Our numerical examples show that the proposed coarse-gradient Langevin algorithms are much faster than the direct Langevin algorithms but have similar acceptance rates. Applications to subsurface flows will be presented. This is a joint work with A. Datta-Gupta, P. Dostert, T. Hou, and B. Mallick.

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MS60

Scale-dependent Homogenization of Elastic and Plastic Random Polycrystals

Scale-dependent bounds on the constitutive response of both 3D random elastic and plastic polycrystals are obtained by setting up Dirichlet and Neumann boundary value problems. This methodology enables one to estimate the size of the Representative Volume Element in polycrystals. For the plastic material, one also can estimate the scale dependence of dissipation potentials in the velocity and force spaces. In general, the RVE is attained at

smaller scales for plastic than for elastic polycrystals.

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MS61

Application of the Wigner Surmise to Stepped Surfaces: Theoretical and Practical Issues

By virtue of the Calogero-Sutherland model for fermions in 1D, we can relate the distribution of spacings between steps on vicinal surfaces (i.e. misoriented from high-symmetry directions) to the Wigner surmise of random matrix theory. We generalize this result to allow application to steps with arbitrary repulsion strength and discuss the advantages over competing approaches. One can also consider pair correlation functions of steps, in principle a simpler problem that might allow the consideration of "non-instantaneous" interactions. Other open questions remain, particularly for vicinal surfaces having, also, in-plane misorientation producing forced kinks. We have obtained a good accounting for the step-stiffness anisotropy in models of such steps, but it is not clear how such anisotropy affects the interactions between steps or the kinetic coefficients. Also, finite-size and discreteness can complicate comparisons with these continuum-model predictions.
Work supported by NSF-MRSEC DMR 05-20471.

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MS61

Non-Gaussian Distributions in Physics and Mathematics: A Universal Paradigm

Gaussian, or normal distributions pop up in many descriptions of natural phenomena, mainly as a consequence of the Central Limit Theorem. However, more and more situations are known, in which non-Gaussian distributions appear to be the rule. These include the distribution of spacings of energy levels of atomic nuclei, as well as the spacing distributions of energy levels of quantum chaotic Hamiltonians, the distribution of domain sizes in 1D Potts and Ising models, the distribution of step spacings on crystal surfaces at equilibrium, the spacings between parked cars and the intervals between arrival of buses in Cuernavaca, Mexico, the distribution of capture zone areas in atomic and molecular deposition on surfaces, and the distribution of the spacings between zeros of the Riemann zeta function. The latter are considered the consequence of the ubiquity and universality of the description that Random Matrix Theory (RMT) gives of fluctuating quantities. However, the relation with RMT is often far from obvious. After describing several examples among those listed above, I will discuss how a simple argument based on a simple stochastic differential equation may help understanding why such distributions are so common, and what is their relation with RMT.

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MS61

Thermal Fluctuations of Facet Edges

We argue that the thermal fluctuations of a facet edge have the same statistics as the uppermost world line of the Calogero-Sutherland (CS) model. For the Ising model at low temperatures this property can be verified through an explicit computation. In this case the CS model is at parameter beta = 2 (Gaussian Unitary Ensemble - GUE).

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MS61

Multiscale Theory of Fluctuating Interfaces: Renormalization of Atomistic Processes

We describe a methodology for the multiscale analysis of atomistic models of fluctuating interfaces. Beginning with an exact analytic formulation of kinetic Monte Carlo simulations in the form of a lattice Langevin equation, we derive stochastic partial differential equations for the smoothed lattice models by regularizing the transition rules. Subsequent coarse-graining is accomplished by calculating renormalization-group (RG) trajectories from initial conditions determined by the regularized atomistic models. Our general microscopic continuum equation is applicable to a wide class of solid-on-solid type lattice models. The RG analysis of this equation shows that the morphological manifestation of a given atomistic relaxation mechanism can depend qualitatively on the length and time scales considered as well as on the dimensionality of the fluctuating interface. Moreover, our analytic theory allows the systematic study of the interplay between different atomistic processes for general experimental input parameters. We will illustrate these ideas with several examples of two-dimensional systems, including surface diffusion with random deposition, the Wolf-Villain models, and variations thereon. Numerical integrations of the equations corresponding various points along the RG trajectory will be shown to illustrate the morphological evolution in real space. Time permitting, we will also discuss our efforts at deriving equations for the morphological evolution of heteroepitaxial films.

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MS62

Simultaneous Matrix Secant Algorithms for Density Functional Calculations: Broyden's "Bad" Method Not So Bad After All

We study the general problem of mixing for ab-initio quantum-mechanical problems. We propose a multisecant form of Broyden's second method for solving the self-consistent field equations of Kohn-Sham density functional

theory. The algorithm is robust, requires relatively little fine-tuning and appears to outperform the current state of the art, converging for cases that defeat many other methods. We compare our technique to the conventional methods for problems ranging from simple to nearly pathological. This is joint work with Laurence Marks.

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MS62

Inverse Problems for Ultrafast High Resolution X-ray Imaging

The most successful routine to image macro-molecular structures is by numerically processing the diffraction pattern of a structure replicated in a periodic system: X-ray crystallography. The next challenge, imaging entire cellular organisms with billions of resolution elements requires the solution to a large scale nonconvex problem. A nonconvex fixed point iteration has demonstrated practical solutions to giga-element nonlinear phase retrieval problems, escaping local minima and producing images at resolutions beyond the capabilities of lens-based optical methods. These methods have been applied to image object as complex as biological cells, nanotubes, quantum dots, nanaocrystals, and nanoscale aerogel structures. Other test patterns were captured in the fastest flash image ever recorded at suboptical resolution. With a 10^{10} increase in peak brightness of upcoming light sources, more powerful algorithms will be required to tackle problems of increasing scale. Acceleration strategies for the fixed point iteration using lower dimensional Newton and quasi-Newton methods will be discussed.

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MS62

Robust and Fast Mixing for DFT methods

One of the rate-limiting steps in ab-initio density functional calculations is what is called mixing. This is the iterative solution of the Kohm-Sham equations, usually by using Broyden's second method for non-linear equations or similar algorithms. Unfortunately in many cases these methods can be unstable and only converge for a limited set of parameters which have to be found by trial and error. This paper will focus on the physics behind this, and discuss how this suggests a multisecant Broyden method with an implicit trust region which in practice is both faster, 2-3 times or more in many cases, and more stable requiring minimal or no user intervention. Evan for relatively large calculations (1000 atoms) with the all-electron Wien2k code convergence is achieved in about 30 iterations and sometimes less only very weakly dependent upon the number of atoms/electrons and more dependent upon how well the physical problem is posed.

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MS62

Shake-and-Bake Algorithm for Structure Determination

The crystallographic phase problem is formulated as a problem in constrained global minimization. The minimal function, based on probabilistic and statistical properties of the structure invariants, serves as the foundation of the Shake-and-Bake optimization procedure that automatically and repetitively alternates reciprocal-space phase refinement with a complementary real-space density modification to impose the atomicity constraints. Shake-and-Bake is capable of solving structures containing as many as 2000 atoms. Research support from NIH grants EB002057 and GM072023 is gratefully acknowledged.

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MS63

Equilibrium Shape of Nanocrystals Computed within a Phase Field Crystal Model

We use an atomistic phase field crystal (PFC) model to compute equilibrium shapes of nanocrystals for various temperatures and observe a transition from more or less isotropic situation to a fully faceted hexagonal shape if the temperature is decreased. Macroscopic anisotropy functions for a free energy are fitted to the computed shapes. As a numerical method to solve the 6th order nonlinear PFC model we use an adaptive semi-implicit finite element discretization which allows orders of magnitude larger time steps than typical explicit discretizations.

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MS63

The Dynamics of Heteroepitaxy via Lattice Phase Field Computations

Using a lattice phase field method we examine the effects of an applied stress on the stability of a solid-liquid interface. We find that stress leads to cusp formation and the nucleation of dislocations. We have extended the model to examine thin film growth. Using this approach we observe steps on surfaces, dipolar stress fields at step edges, and step-flow growth of the film from the vapor.

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MS63

Large-Scale Coarsening of Four-Fold Facetted Surfaces

We investigate the coarsening of thin-film systems wherein the surface energy pre-selects the slopes that appear on the film surface during coarsening. In particular, the energy may select for facetted surfaces. We study the coarsening of such systems numerically using energy-stable algorithms that allow for large time-stepping, which permits an understanding of coarsening in the very-long-time regime. Specifically, we describe the effect that corner rounding has on the dynamics of facetted surfaces in the long-time regime.

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MS64

Magnetostrictive Controller with an Inverse-Compensator for Milling Applications

Magnetostrictive materials, such as Terfenol-D, have great potential as solid-state actuation devices in control, variation suppression and machining applications. However, their highly non-linear and hysteretic behaviors are detrimental to their direct use in these applications. Several control strategies have been devised to overcome these limitations. One such approach solves the non-linear optimal control problem offline for a trajectory that is known apriori [Oates, W.S., Evans, P.G., Smith, R.C., and Dapino, M.J., Experimental Implementation of a Hybrid Nonlinear Control Design for Magnetostrictive Actuators]. In this work, the calculated control input cannot compensate for inaccuracies in plan modeling or estimation and disturbances that occur in real-time. Hence, a closed loop PI controller is employed for small perturbations about the designed operating condition, to improve tracking. Another approach involves using an inverse compensator that was implemented using the inverse Preisach operator [Tan, X., and Baras, J., Modeling and control of hysteresis in magnetostrictive actuators, Automatica, vol. 40, pp. 14691480, 2004]. In this paper, an attempt is made to solve the entire non-linear problem online. The inverse compensation is achieved by an efficient inverse implementation of the Homogenized Energy Model (HET) for magnetostrictive materials [Oates, W.S., Evans, P.G., Smith, R.C., and Dapino, M.J., Experimental Implementation of a Hybrid Nonlinear Control Design for Magnetostrictive Actuators]. The open-loop response of this compensator-plant system for a sinusoidal input used to machine elliptical piston-heads is studied. Further, to compensate for errors in estimation of plant behavior and high frequency disturbances (such as higher harmonics that commonly occur in machining applications) an LQR observer-controller is designed over the linearized compensator-plant system. An attempt is also made to design a narrow-band controller to reject higher harmonics with minimal control effort.

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MS64

Continuum Thermodynamic Model for Magnetostrictive Galfenol Alloys

Magnetostrictive iron-gallium (Galfenol) alloys exhibit significant magnetostriction and have structural-grade mechanical properties. The design of anisotropies through manufacturing and post-processing methods made possible with Galfenol could enable load-bearing adaptive systems with 3-D functionality and superior dynamic response. We present an anisotropic 3-D model for magnetization and magnetostriction of Galfenol alloys subjected to magnetic fields and mechanical stresses. We formulate the model in state-space form to simplify the computational implementation for device design and control.

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MS64

Homogenized Energy Modelling of an SMA Wire Actuator

Shape memory alloys are a part of the class of so-called smart materials, which can take advantage of changes in external fields to generate motion. Actuators designed from smart materials display significant hysteresis nonlinearity, which must be accounted for in controller design if their full potential is to be harnessed. In this work, we explore the use of the Homogenized Energy Model in modelling the behaviour of an SMA wire actuator.

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MS64

An Energy Derivation for Classical and Extended Preisach Models

Preisach models formulated in terms of density or measure-based expansions have proven highly successful for characterizing hysteresis and constitutive nonlinearities in materials where the underlying physics is difficult to quantify. This provides a rich mathematical framework for characterizing nonlinear material behavior as well as a framework which facilitates either full or approximate inversion for linear control design. However, the lack of an energy basis for Preisach representations yields models which often have a large number of parameters and are difficult to update to accommodate changing operating conditions (e.g., temperature) since the model parameters are not correlated with physical quantities. Moreover, it is difficult in general to incorporate the frequency-dependence exhibited by essentially all smart materials without resorting to vector-valued parameters or measures which much be identified throughout the range of operation for the system. In this paper, we develop an energy formulation for certain extended Preisach models through consideration of appropri-

ate Gibbs and Helmholtz free energy representations. This permits the incorporation of frequency and temperature-dependence in the underlying basis, rather than in parameters identified for a specific system which expands significantly the flexibility of the technique.

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MS65

Critical Failure Volume for Fiber Reinforced Composite Systems

Critical failure volume (CFV) method is proposed. CFV is defined as a finite subvolume in material with general nonuniform stress distribution, which has the highest probability of failure, i.e. loss of load carrying capacity. The evaluation of the probability of failure of the subvolumes is performed based on the lowest stress and thus provides an estimate of the lower bound of the probability of local failure. An algorithm for identifying this region, based on isostress surface parameterization is proposed. It is shown that in the case of material with strength following Weibull weak link statistics such a volume exists and its location and size are defined both by the stress distribution and the scatter of strength. Moreover the probability of failure predicted by using CFV method was found to be close to that predicted by using traditional Weibull integral method and coincide with it in the case of uniform stress fields and in the limit of zero scatter of strength. CFV method allows for simple and robust extension to phenomena with nonlocal failure models, such as fibrous composites. The method was modified to account for presence of limit scaling size, consistent with recent Monte-Carlo simulations by Landis et al. (Landis, C. M., I. J. Beyerlin, and R. M. McMeeking. (2000). "Micromechanical Simulation of the Failure of Fiber Reinforced Composites. Mechanics and Physics of Solids, 48 (621-648).), and was able to describe the experimentally observed magnitude of the hole size effect on composite tensile strength in the examined range of 0.1 to 0.6 hole diameters. The predictions were based solely on statistical distributions of composites strength properties measured on standard tension specimens containing no holes.

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MS65

Simulation of Diffusion Through Disordered Media: Coarse Scale Equations from Experimental or Monte-Carlo Data

Within many disordered media, diffusion displays transient subdiffusive effects, which means that is not governed by Fick's laws, and cannot be described accurately by the traditional diffusion equation. Such a situation can be encountered, for example, within materials composed of polymers. In this talk, we present some methods to obtain standard linear reaction-diffusion equations that can be used to model and simulate diffusive transport in such media without sacrificing the transient nature of the behavior. We also show how to obtain computationally the parameters of such a system starting from Monte Carlo data or single particle tracking experiments.

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MS65

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MS65

Uncertainty in Multiscale Modeling of Materials

In this talk recent developments in multiscale simulation will be reviewed. Developments from our work on coarse-grained Monte Carlo simulations and various types of hierarchical multiscale simulation will be discussed. Examples of multiscale modeling will be presented from materials self-organization for pattern formation leading to quantum dots (e.g., Pb on Cu) and catalytic processes. Special emphasis will be placed on the role of uncertainty in top-down and bottom-up multiscale modeling of materials.

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MS66

Grain Growth Kinetics in the Presence of Second-Phase Particles

Grain growth is perhaps the most common process that takes place during materials processing, and a number of computational approaches are now available to model the grain structure evolution kinetics. This presentation will discuss recent progresses in advancing the phase-field method for grain growth in single- and two-phase systems. Although the first phase-field model for grain growth was proposed more than a decade ago, large-scale, three-dimensional, coalescence-free grain growth simulations became possible only recently thanks to a number of computationally intelligent implementations that significantly improve the efficiency and at the mean time reduce the memory requirement. We will present an implementation for grain growth in the presence of a second phase by combining the semi-implicit spectral method and the active order parameter tracking algorithm. The effect of second-phase volume fraction as well as its particle morphology and wetting conditions at grain boundaries on grain growth kinetics will be discussed.

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The Numerical Solution of a Crystalographically-Aware Phase Field Model

We describe the development and implementation of a numerical algorithm for the solution of a 3D phase field model of polycrystalline microstructure evolution. Our approach incorporates a Newton Krylov method of lines formulation for the implicit integration of a system of equations for a phase order parameter and quaternion representation of grain orientation. Efficient resolution of interfaces is achieved using adaptive mesh refinement. Results obtained by the model for solidification problems will be presented. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Phase Field Approach to Homogeneous and Heterogeneous Crystal Nucleation in Alloys

Recent work on applying the phase field (PF) approach for calculating the nucleation barrier and for simulating homogeneous and heterogeneous crystal nucleation in undercooled melts will be reviewed. This incorporates a quantitative testing of a PF model of homogeneous nucleation based on a Ginzburg-Landau expanded free energy for the hard-sphere system, where all the input data and the barrier height are known from atomistic simulations, and its application for binary eutectic systems [G. I. Tth, L. Grnsy: J. Chem. Phys. 127, 074709 (2007)] including crystal nucleation in the metastable liquid immiscibility region [G. I. Tth, L. Grnsy: J. Chem. Phys. 127, 074710 (2007)]. Recent methods for incorporating heterogeneous crystal nucleation on surfaces of given contact angle into PF modeling [L. Grnsy, T. Pusztai, D. Saylor, J. A. Warren: Phys. Rev. Lett. 98, 035703 (2007)] are reviewed and generalized for binary alloys. Numerical simulations will be presented that illustrate the potential of these methods for addressing heterogeneous nucleation on complex surfaces.

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Three Dimensional Phase-field Simulation of Grain Growth in Dual-phase Structures

Three dimensional phase-field simulations of grain growth in dual-phase structures have been performed on the condition that the volume fraction of the second-phase grains (SPGs) f_α is larger than 0.1. The dependence of the grain growth kinetics and the topological evolution on the value of f_α has been investigated. The simulation results reveal that almost all the SPGs are situated at corners of the matrix grains. The pinning effect of the mobile particles is much stronger than that of the immobile particles.

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Three-dimensional Phase Field Simulations of Grain Growth in Anisotropic Systems

Phase-field modeling has proven to be a valid tool for simulating the evolution of the grain structure in polycrystalline materials. However, its computational requirements pose severe limitations on the number of grain orientations that can be considered in a practical simulation. In this talk, we discuss the mathematical and computational aspects of large-scale three-dimensional phase-field simulations of the evolution of grain structures with misorientation dependent grain boundary properties.

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A Visual Editor for EMU with Applications

This presentation provides a description of Visual EMU, a graphical user interface developed for the peridynamic EMU code. Visual EMU allows a user to interactively create an EMU model, visualizing the material regions, peridynamic grid, and resulting nodes. Using Visual EMU, we perform analyses of several standard problems (fracture specimen, hole in plate, etc.) and compare the results with recognized solutions.

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Micro-Peridynamics for Fiber Reinforced Composites

We discuss multi-scale techniques for modeling the peridynamic fluctuations inside fiber reinforced plys subjected to dynamic load conditions. We introduce two-scale asymptotic expansions that provide a framework for multi-scale analysis. The asymptotic expansions capture the multi-scale response of the local deformation field. Explicit error bounds between the expansions and the actual deformation are obtained for different classes of initial data and body forces. The expansions are used in numerical simulations for dynamically driven fiber reinforced laminates in the presence of residual forces.

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Peridynamics via Finite Element Analysis

This paper describes how peridynamics can be implemented in and coupled to conventional finite element analysis (FEA) using truss elements and constraint equations. With this approach different subregions of a model can be solved with either the classical partial differential equations or the peridynamic equations in the same calculation thus combining the efficiency of FEA with the generality of peridynamics. Several examples show the equivalency of the FEA and the meshless peridynamic approaches as well as demonstrate the utility and robustness of the method for problems involving fracture, damage and penetration.

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Mesoscale Simulations with Microscale Tools: Peridynamics in a Molecular Dynamics Code

In the discretized peridynamic model, a continuum body is modeled by discrete particles, where each particle's motion is determined by summing interaction forces with neighboring particles. The discretized peridynamic model thus has the same computational structure as molecular dynamics. We discuss our implementation of the peridynamic model within the massively parallel molecular dynamics code LAMMPS, and demonstrate example problems. We also discuss approaches to connect atomistic and mesoscopic models within this framework.

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