IP1
Motility at Microscopic Scales

Motility of cells is at the root of many fundamental processes in biology: from sperm cells swimming to fertilize an egg cell, to metastatic tumor cells crawling to invade nearby tissues. We will discuss the mechanical bases of cellular motility by swimming and crawling. Special emphasis will be placed on the connections between low Reynolds number swimming and Geometric Control Theory, and on the geometric structure of the underlying equations of motion. As a concrete example, we will report on reverse engineering of the euglenoid movement. The lessons learned in the context of swimming motility will be then applied to selected case studies of crawling motility.

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IP2
Wrinkle Patterns in Thin Sheets

When confined in space, solid sheets exhibit a variety of patterns, often described as folds, blisters, wrinkles, creases, and crumples. The most elementary deformation type emerges from the classical buckling-wrinkling instability of thin objects under compressive loads. Nevertheless, experiments on nano-metrically thin sheets have shown that standard post-buckling theory fails to predict basic features of wrinkle patterns. I will describe some recent developments in studies of wrinkling phenomena, emphasizing the "far-from-threshold theory, a singular perturbation approach to address wrinkles in very thin, highly-bendable sheets. Focusing on class of "simplest yet nontrivial (radial stretching) models that exhibits the morphological complexity of thin sheets, I will describe the principles of the FFT wrinkling theory, and a few mechanisms by which wrinkles give way to other patterns.

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IP3
Asymptotics-based Model Reduction in Electronic Structure: Old and New

It has long been recognized that asymptotic analysis of well chosen scaling limits is a useful alternative (or companion) to semi-empirical methods in the design of reduced electronic structure models. Due to the curse of dimensionality of the full N-electron Schr"odinger equation, reduced models are necessary to facilitate the computation of ab-initio energy levels or potential energy surfaces for large systems. Early examples which have retained importance to this day include Dirac's (1930) and Becke's (1988) exchange energy functionals. In the talk I will focus on 1) asymptotics-based wavefunction methods which capture the anomalous filling order of transition metal atoms, missed e.g. by density functional theory (DFT) even with the best known functionals such as B3LYP. (Theory: G.F., B.Goddard, SIAM J. Math. Anal. 41, 2009; application to transition metals: Ch.Mendl, G.F., J.Chem.Phys.133, 184101, 2010). 2) exchange-correlation functionals in DFT emerging from the semiclassical limit of the (exact but unwieldy) Hohenberg-Kohn functional. The study of this limit was initiated by Seidl, Perdew, Levy, Gori-Giorgi and Savin, and leads, perhaps unexpectedly, into optimal transportation theory (C.Cotar, G.F., C.Kl"uppelberg, Comm. Pure Appl. Math. 66, 548-599, 2013).

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IP4
Scaling in Kinetic Mean-field Models for Coarsening Phenomena

Coarsening, that is the increase of typical length scales in a microstructure, plays a crucial role in the large-time behavior of numerous processes in physics and materials science. An important aspect is the dynamical scaling hypothesis suggesting that after some transient regime the system evolves in a universal statistically self-similar fashion. Kinetic mean-field models are often used to try to capture this self-similar behavior. However, despite typically simple looking, their analysis turns out to be a challenge. In this talk I will review the progress of recent years in the analysis of such equations and will also discuss major open problems.

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IP5
Numerical Methods in Molecular Dynamics

Molecular dynamics is now a very widely used tool to study the matter at the molecular level. It is used in various fields, such as biology, chemistry or materials science. The aim is in particular to understand the relationships between the macroscopic properties of a molecular system and its atomistic features. For example, one would like to compute the constitutive relations for materials from molecular models, or predict the most likely conformations of a protein in a solvent from its amino acid sequence. One of the difficulty to reach this aim is related to timescales: the typical timescale of a molecular dynamics simulation is much smaller than the typical timescale at which the crucial events, from a macroscopic viewpoint, occur. This is related to the metastability of a molecular dynamics trajectory: the system stays for a very long time in some regions of the configuration space (called metastable state), before hopping to another one, and it is difficult to observe and simulate such rare events. An associated feature is the multimodality of the statistical ensemble (a probability measure) sampled by the molecular dynamics trajectories. Many methods have been proposed in the molecular dynamics community to deal with these difficulties, and we will focus on two prototypical ones for which a mathematical analysis gives useful insights. We will first present adaptive importance sampling techniques, which have been proposed to sample efficiently statistical ensembles. Then, we will propose a mathematical analysis of the parallel replica algorithm which has been introduced by A.F. Voter to generate efficiently metastable dynamics.

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IP6

Tracking Multiphase Physics: Geometry, Foams, and Thin Films

Many scientific and engineering problems involve interconnected moving interfaces separating different regions, including dry foams, crystal grain growth and multi-cellular structures in man-made and biological materials. Producing consistent and well-posed mathematical models that capture the motion of these interfaces, especially at degeneracies, such as triple points and triple lines where multiple interfaces meet, is challenging. Joint with Robert Saye of UC Berkeley, we introduce an efficient and robust mathematical approach to computing the solution to two and three-dimensional multi-interface problems involving complex junctions and topological changes in an evolving general multiphase system. We demonstrate the method on a collection of problems, including geometric coarsening flows under curvature, incompressible flow coupled to multi-fluid interface problems, and (joint with C. Rycroft), the interaction of growing biological clusters with elastic basement membranes. Finally, we compute the dynamics of unstable foams, such as soap bubbles, evolving under the combined effects of gas-fluid interactions, thin-film lamella drainage, and topological bursting.

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IP7

Toward the Principles of Self Assembly and Self Replication

In biological systems, there are striking examples where complicated structures (i.e., the bacterial ribosome) can spontaneously assemble, driven by specific interactions between the components. But how can systems be designed to have this property? Recent technological advances have created the opportunity for making technologically relevant systems that self assemble, by e.g. coating colloidal particles with DNA. We will discuss how self assembly works in this system, through theory, numerical simulation and experiment – and start to speculate as to whether resulting principles might be useful for unravelling the rules of biological self-assembly. We also outline theoretical constraints on designing this system for self replication.

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IP8

Organic Crystal Growth in Thin Films

We examine solidification in thin liquid films produced by annealing amorphous films in a solvent vapor. Micrographs captured during annealing reveal the nucleation and growth of single-crystal needles. The needle lengths scale like power laws in time where the growth exponent depends on the thickness of the deposited film. The evolution of the thin film is modeled by a lubrication equation, and an advection-diffusion equation captures the transport of material and solvent within the film. We define a dimensionless transport parameter which describes the relative effects of diffusion and coarsening-driven advection. For large values of this parameter, needle growth matches the theory of 1D, diffusion-driven solidification. For low values, the collapse of droplets – i.e. coarsening – drives flow and regulates the growth of needles. Within this regime, we identify and analyze two asymptotic limits: needles that are small compared to the typical drop size, and those that are large.

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IP9

Metamaterials: High Contrast Composites with Unusual Properties

Composite materials can have properties unlike any found in nature, and in this case they are known as metamaterials. Materials with negative Poisson's ratio or negative refractive index are now classic examples. The effective mass density, which governs the propogation of elastic waves in a metamaterial can be anisotropic, negative, or even complex. Even the eigenvectors of the effective mass density tensor can vary with frequency. One of the exciting applications of metamaterials is to cloaking, yet we show here that there are limitations to electromagnetic cloaking: one cannot get broadband passive cloaking if the surrounding material is air, at least in the quasistatic limit. Non-linear metamaterials are also interesting and a basic question is what non-linear behaviors can one get in periodic materials constructed from rigid bars and pivots? It turns out that the range is enormous. Materials for which the only easy mode of macroscopic deformation is an affine deformation, can be classed as unimode, bimode, trimode,...hexamode, acccording to the number of easy modes of deformation. We give a complete chacterization of possible behaviors of nonlinear unimode materials.

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IP10

The Dynamics of Liquid Crystals

Many of the beautiful results of solid state physics are predicated on the positional order of the constituents of solid crystals. Liquid crystals are soft materials, characterized by orientational order whose implications and consequences are less well understood. Emerging new materials bring diversity to the symmetry, composition, length- and time-scales and interactions of orientationally ordered soft matter systems. The salient feature of these systems is their symmetry-mandated responsivity to stimuli. In this talk, I will describe dynamic phenomena in a variety of liquid crystalline systems in response to different excitations, and discuss approaches and challenges to modeling the dynamic response.

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IP11

Multiscale Mathematics and Renewable Energy

It is well understood that access to cheap energy underpins modern societies and that there is a direct correlation between a nations energy consumption per capita and its GDP. Finding enough energy to fuel industrialized economies and pull developing countries out of poverty without overheating the climate is a central challenge of the 21st century. Meeting it will require new technologies for producing, storing, and using energy with performance levels far beyond what is currently possible. Such technologies spring from scientific breakthroughs in new materials and chemical processes that govern the transfer of energy between light, electricity and chemical fuels. In applications ranging from renewable fuels production to generating electricity from wind and solar through energy storage, advanced materials play a crucial role in accelerating the development of new energy solutions. In this talk we will discuss mathematical approaches to modeling required to address the complexities of renewable energy technologies, which include coupled physical, chemical and biological processes, broad spans of spatial and temporal scales, many sources of uncertainty, and, in some instances, only a primitive understanding of the fundamental processes and phenomena.

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IP12

How Do Crystals Melt?

I will discuss the mechanism by which crystals melt. I will address the classical controversy between Born's and Lindemann's criteria for melting.

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MS1

Limit Theorems for the Random Conductance Model

An interesting characteristic of random resistor networks comes with the notion of effective conductance and resistance. These are the minimum values of a Dirichlet energy optimized over potentials or currents subject to appropriate boundary conditions. Homogenization theory predicts the existence of an almost-surely constant leading-order asymptotic for these quantities; my goal will be to go beyond the leading order and discuss fluctuations. Specifically, I will review recent proofs of the central limit theorem for the effective conductance in resistor networks on an integer lattice where edges are assigned independent and identically distributed random conductances. Time permitting, I will put these in the context of a larger class of limit theorems for the random conductance model that have been made available thanks to the recent groundbreaking work of Gloria and Otto. Based on joint work with Michele Salvi and Tilman Wolff.

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MS1

Homogenization of Elliptic Pde in Random Environments with Long--range Correlations

This talk will be concerned with rates of convergence in homogenization of divergence form elliptic PDE in random environments. Rates of convergence are obtained for environments which consist of a simple convolution of a function with an environment satisfying a Poincaré inequality. These environments can have long range correlations, as in the first results on the subject by Yurinskii (1986), but without his restriction that dimension must be at least 3. Rates of convergence for environments satisfying a Poincaré inequality were first proved by Naddaf--Spencer(1998). The method has been much further developed in recent work of Gloria and Otto (2011). Correlations in environments which satisfy a Poincaré inequality are typically short--range.

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MS1

Quantitative Homogenization of the Heat Equation with Random Coefficients

We consider the heat equation with random coefficients on Z^d. The randomness of the coefficients models the inhomogeneous nature of the medium where heat propagates. We assume that the distribution of these coefficients is invariant under spatial translations, and has a finite range of dependence. If a solution to this equation is rescaled diffusively, then it converges to the solution of a heat equation with constant coefficients. In probabilistic terms, this convergence corresponds to the fact that the associated random walk satisfies a central limit theorem. I will present recent progress on the estimation of the speed of this convergence, based on the random walk representation.

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MS1

Normal Approximation for Random Elliptic Equations

I will discuss solutions to an elliptic PDE with conductivity coefficient that varies randomly with respect to the spatial variable. It has been known for some time that homogenization may occur when the coefficients are scaled suitably. Less is known about fluctuations of the solution around its mean behaviour. For example, imagine a conductor with an electric potential imposed at the boundary. Some current will flow through the material. What is the net flux? For a finite random sample of the material, this quantity is random. I will describe a recent result about normal approximation: the probability law of the net current is very close to that of a normal random variable having the same mean and variance. Closeness is quantified by an error estimate in total variation; the error vanishes as the size of the material sample goes to infinity.

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MS2

Time-averaging of ODE Systems with Highly Oscillatory Response

A progression of ideas leading to a practical computational technique for time-averaging nonlinear, fast oscillatory response of ODE systems under slow forcing is described. The key idea is to introduce running finite time-averages of phase functions that are provably robust 'slow' variables whose evolution can be approximated. The strategy induces a separation of time scales in an augmented dynamics, even when the original system does not come equipped with one.

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MS2

Statistical Mechanical Foundation of the Peridynamic Nonlocal Continuum Theory

My presentation derives the energy and momentum conservation laws of the peridynamic nonlocal continuum theory using the principles of classical statistical mechanics. The peridynamic laws allow the consideration of discontinuous motion, or deformation, by relying on integral operators. These operators sum forces and power expenditures separated by a finite distance and so represent nonlocal interaction. An important conclusion is that nonlocal interaction is intrinsic to continuum conservation laws when derived using the principles of statistical mechanics.

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MS2

Kinetic Equation for Spatial Averages of Particle Dynamics

We propose a kinetic equation for the moment-generating function that contains the dynamics of the continuum spatial averages of particle systems. The exact, but not closed, evolution equation for the generating function is obtained directly from the particle equations of motion. This equation is then closed using the recently developed deconvolution method. The result is an approximate kinetic equation suitable for liquids and to some extent, solids.

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MS2

Statistical Foundations of Liquid-Crystal Theory

I will outline how one can derive the continuum-level balances for liquid crystals using statistical mechanics. I will start by considering a discrete system of rigid rods, which motivates an appropriate state space. A probability function is then introduced that satisfies the Liouville equation. This equation serves as the starting point for the derivation of all of the continuum-level balances. The terms appearing in the derived balances, some being nonstandard, are interpreted as expected values.

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MS3

Fluctuation-Dissipation Based Integrators for Brownian Dynamics

This talk presents explicit methods for simulating Brownian Dynamics with Hydrodynamic Interactions that have the following features: ergodicity with respect to the limiting distribution of the governing equations; weak accuracy at finite noise; and, higher order accuracy in the small noise limit. The first property is our stability concept, and the second/third properties are our convergence concept. To design methods with these properties, ideas from probability theory and numerical analysis were used. The basic framework consists of combining a Metropolis Monte Carlo method to sample the limiting distribution of the SDE with an optimized Runge-Kutta type discretization. While Metropolis integrators are known to be ergodic and weakly accurate, there are important situations where existing schemes may reject all moves in the small noise limit. This issue is reminiscent of the scaling problem that occurs with Metropolis algorithms in high dimension. An asymptotic analysis of the rejection rate in this limit reveals the necessity of multiple stages per step. Among two and three stage methods, it turns out that the Ralston and Kutta methods are optimal. The Metropolis integrator is also designed to avoid computing the divergence of the mobility tensor. An 'infinitesimal fluctuation dissipation lemma' guided how to do this while maintaining dynamic accuracy. Numerical examples including application to Brownian dynamics with hydrodynamic interactions will be presented. For this example, it will be shown that the resulting integrator is able to accurately compute dynamics at time steps an order of magnitude (or more) larger than those permitted with explicit predictor-corrector schemes. The compatibility of the technique with fast multipole method or Ewald type computational methods for the hydrodynamic interactions will also be addressed.

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MS3

Coupling a Fluctuating Fluid to Immersed Particles

Bidirectional coupling of immersed structures, such as colloidal particles or polymer chains, to the surrounding fluid flow has been studied extensively; however, thermal fluctuations in the fluid equations are not usually considered even though they are responsible for Brownian motion. Achieving discrete fluctuation-dissipation balance in the coupled fluid-structure system is not trivial and requires special care in both the fluid solver and the fluid-structure coupling. I will describe an extension of the Inertial Cou-

pling Method developed for compressible flow by Usabiaga Balboa, Delgado Buscalioni and Pagonabarraga Mora to incompressible flow. The method allows for bidirectional coupling of inertial blob particles with a fluctuating fluid. Our algorithm is based on techniques used in the Immersed Boundary Method and recently-developed finite volume schemes for fluctuating hydrodynamics. We develop a temporal discretization that strictly conserves momentum and is limited in stability only by advection, and reproduces the correct spectrum and dynamics of the thermal fluctuations at both short and long times.

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MS3

Modeling of Thermal Fluctuations in Multicomponent Reacting Systems

We present a multicomponent version of the fluctuating Navier-Stokes equations that includes detailed transport and chemical reactions. The resulting system includes stochastic flux terms for momentum, energy and species transport and a Langevin-type model for fluctuations in the chemical reactions. We discuss isses in the numerical solution of the resulting systems and illustrate the impact of fluctuations on numerical solutions Turing patterns.

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MS3

Immersed Particle Dynamics in Flucuating Fluids with Memory

Multibead passive microrheology aims at characterizing fluid properties via statistically measurable quantities. To correctly model the correlations, it is necessary to include a thermally fluctuating force in the Stokes equations. We present a model for an immersed particle passively advected by a fluctuating Maxwellian fluid. We then highlight the stochastic spectral numerical method. Finally, we seek to find a signal due to the fluid's memory in the statistics of the particles velocity autocorrelation.

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MS4

Elastic Theory for Shape Selection of Self-Assembled Macromolecular Ribbons

We suggest a geometric-mechanical model for chemical systems that undergo self-assembly into chiral ribbon structures. The model predicts a morphological transition from twisted to helical configurations and to tubes, as seen in many such systems. Our simple model, based on incompatible elasticity, allows a quantitative description of a wide variety of systems, using only a few parameters. We identify the significant dimensionless parameters that determine the equilibrium configurations and accurately predict the above transition and other morphological phenomena.

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MS4

How Bilayer Shape Influences Bilayer Bending

A bilayer is two thin layers of different materials, bonded together. When actuated, the two layers have different equilibrium strains, and the total elastic energy of the bilayer is decreased by bending. Using computations and experiments, we consider how the bilayer shape (in the dimensions normal to the thickness) determines its bending direction, through the presence of edge layers. We consider rectangles with different aspect ratios, and more general shapes by developing a hexagonal-lattice discretization of bilayers.

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MS4

Blister Patterns and Energy Minimization in Compressed Thin Films on Compliant Substrates

Thin films on compliant substrates subject to compressive elastic misfit can display a variety of blistering patterns. We study the minimum energy achievable by blistering on a fixed area fraction; a variational problem involving three small parameters. In 1D we determine how the minimum

energy scales with respect to these parameters. In 2D we show that in a certain regime, the energy of a blister lattice is lower than a few, large blisters.

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MS4

Shape Transitions in Hyperbolic Non-Euclidean Plates

Swelling thin elastic sheets are ubiquitous in nature and industry and are capable of forming complex patterns of various geometries. The equilibrium shapes of such sheets is usually modeled as the minimum of an elastic energy that is the minimum of a (strong) stretching energy and a (weak) bending energy. In this talk I will present a study of such swelling sheets when stretching free deformations correspond to local isometric immersions of the hyperbolic plane. Motivated by recent experiments studying the morphology of swelling hydrogels, we focus on annuli with periodic profiles.

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MS5

Effective Dynamics of Phase Transitions in Nonlocal Fokker-Planck Equations

This talk concerns the asymptotic analysis of certain nonlocal and nonautonomous Fokker-Planck equations which model the hysteric behaviour of many-particle systems with dynamical control (e.g. charging and discharging of Lithium-ion batteries). The equations involve two small parameters and are hence capable of describing different types of phase transitions. We focus on the fast reaction regime, in which the dominant effect can be understood by adapting Kramers formula for large deviations, and characterize the small-parameter limit by rate-independent evolution equations.

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MS5

Unexpected Thermodynamic Properties of Some Exact Far-from-equilibrium Solutions in Molecular Dynamics

We describe a time-dependent invariant manifold of the equations of molecular dynamics (MD). The manifold is independent of the description of the atomic forces within a general framework: it is exactly the same manifold whether the atoms are those of steel, water or air. Some version of this manifold is inherited by all accepted models of continuum mechanics, as well as the Boltzmann equation. Some of the MD solutions correspond to certain far-from equilibrium, unsteady flows, while others are naturally associated with the dynamics of particular nanostructures. Both simulations and a study of the Boltzmann equation suggest the presence of certain thermodynamic relations that are completely unexpected in these far-from-equilibrium situations. We describe these relations. Joint work with Amin Aghaei, Kaushik Dayal, and Stefan Mueller.

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MS5

Multi-Time Scale Modeling of Dynamics of Phase Transition

We aim to construct coarse evolution equation for autonomous fine ODE systems. The coarse variables are defined as finite time averages of phase functions. The approach is based on the idea of Young measure theory. The time averaged coarse variables turn out to be 'slow' in a precise sense. This allows their evolution to be phrased in terms of averaging utilizing limit measures (probability distributions) of the fast flow.

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MS5

From Simple Particle Models to Thermodynamic Flows

The diffusion equation is the scaling limit of Brownian motion, and can be reformulated as gradient flow of the entropy in the Wasserstein metric. How can we directly obtain this entropic formulation from particle models? More generally, how can we obtain thermodynamic flows from simple particle models, that is, infer energy and entropy as well as their evolution laws from mesoscopic models? The talks will sketch some approaches and results based on large deviation principles.

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MS6

Solidification Fronts in Supercooled Liquids: How Rapid Fronts Can Lead to Disordered Glassy Solids

We determine the speed of a crystallisation (or more generally, a solidification) front as it advances into the uniform liquid phase after the system has been quenched into the crystalline region of the phase diagram. We calculate the front speed by assuming a dynamical density functional theory model for the system and applying a marginal sta-

bility criterion. Our results also apply to phase field crystal (PFC) models of solidification. As the solidification front advances into the unstable liquid phase, the density profile behind the advancing front develops density modulations and the wavelength of these modulations is a dynamically chosen quantity. For shallow quenches, the selected wavelength is precisely that of the crystalline phase and so well-ordered crystalline states are formed. However, when the system is deeply quenched, we find that this wavelength can be quite different from that of the crystal, so that the solidification front naturally generates disorder in the system. Significant rearrangement and ageing must subsequently occur for the system to form the regular well-ordered crystal that corresponds to the free energy minimum. Additional disorder is introduced whenever a front develops from random initial conditions. We illustrate these findings with results obtained from the PFC.

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MS6

Kinetic Density Functional Theory - Time Dependent Hydrodynamic Density Functional Theory for Freezing

Understanding solid liquid phase transition is of great importance in many applications starting from growth of nano-crystals in solutions for solar cells to making the perfect ice cream. Classical Density Functional Theory (CDFT) has been very successful in predicting the phase transition of pair potential fluids. However the CDFT only characterizes the equilibrium of the system and does not shed light on the time evolution of the system. This talk will present an approach starting with the Revised Enskog Kinetic Theory (RET) as a definition of time evolution to develop a hydrodynamic model for freezing of a hard sphere liquid. The relation between Kinetic Theory, CDFT and Phase Field Crystal (PFC) models will be outlined. Some numerical results characterizing the time evolution of the model and its applications will also be discussed.

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MS6

Scale Coupling in Phase-Field-Crystal Modeling of Materials Growth

Continuum field theories have been of continuous great interest in modeling and understanding complex properties during materials growth and processing. Traditionally such approaches are featured by the description of long wavelength or coarse-grained scale of a system, while typical material phenomena involve a variety of spatial and temporal scales that interact and couple. The recently developed phase-field-crystal (PFC) methods can overcome such limit of conventional approaches via incorporating microscopic crystalline details into mesoscopic continuum theory. In this talk I will discuss recent progress in the development of the PFC methodology that bridges different scales, in particular the coupling effects between mesoscopic and microscopic spatial scales identified in the amplitude representation of PFC.

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MS6

Density Functional Theory and Phase-Field-Crystal Modelling for Liquid Crystalline and Active Systems

Liquid crystal exhibit many fascinating meso-phases which are neither completely disordered nor completely crystalline examples of which include the nematic, smectic or plastic-crystalline state. In this talk, it is shown how concepts of density functional theory of freezing and associated phase-field-crystal modelling can be extended to treat anisotropic liquid crystalline phases. We further extent the theory to polar active particles which are self-propelled along an intrinsic orientation and show that a wealth of possible crystalline state exist in nonequilibrium.

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MS7

Vortices for a Two-Component Ginzburg-Landau Model

We study Ginzburg–Landau equations for a complex vector order parameter $\Psi = (\psi_+, \psi_-) \in \mathbf{C}^2$. We consider symmetric vortex solutions in the plane $\mathbf{R}^2$, $\psi(x) = f_\pm(r)e^{in_\pm\theta}$, with given degrees $n_\pm \in \mathbf{Z}$, and prove existence, uniqueness, and asymptotic behavior of solutions as $r \to \infty$. We also consider the monotonicity properties of solutions, and exhibit parameter ranges in which both vortex profiles f_+, f_- are monotone, as well as parameter regimes where one component is non-monotone. We also treat the stability of symmetric vortices for degrees $n_\pm = 1$, in the sense of whether the solutions are local minimizers of the energy. Our results partially generalize those of Alama-Bronsard-Mironescu to more general forms of Ginzburg-Landau systems.

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MS7

The Superheating Current for a Reduced Ginzburg-Landau Model

We consider the time-dependent Ginzburg-Landau model in the absence of a magnetic field but in the presence of an electric current. In the large domain limit, for a general 2D setting we show that for sufficiently small current densities (that may result in strong currents) there exists a linearly stable purely superconducting solution. For wire-like domains, for stronger current densities we also prove the existence of such a solution and discuss its stability.

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MS7

Thin Film Superconductors in Strong Magnetic Fields

We consider singular limits of the three-dimensional Ginzburg-Landau functional for a superconductor with thin-film geometry, in a constant external magnetic field. The superconducting domain has characteristic thickness on the scale $\epsilon > 0$, and we consider the simultaneous limit as the thickness $\epsilon \to 0$ and the Ginzburg-Landau parameter $\kappa \to \infty$. We assume that the applied field is strong (on the order of ϵ^{-1} in magnitude) in its components tangential to the film domain, and of order $\log \kappa$ in its dependence on κ. We prove that the Ginzburg-Landau energy Γ-converges to an energy associated with a two-obstacle problem, posed on the planar domain which supports the thin film. The same limit is obtained regardless of the relationship between ϵ and κ in the limit. Two illustrative examples are presented, each of which demonstrating how the curvature of the film can induce the presence of both (positively oriented) vortices and (negatively oriented) antivortices coexisting in a global minimizer of the energy.

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MS7

Kinematic Vortices in a Thin Film Driven by An Electric Current

Using a Ginzburg-Landau model, we study the vortex behavior of a rectangular thin film superconductor subjected to an applied current fed into a portion of the sides and an applied magnetic field directed orthogonal to the film. Through a center manifold reduction we develop a rigorous bifurcation theory for the appearance of periodic solutions in certain parameter regimes near the normal state. The leading order dynamics yield in particular a motion law for kinematic vortices moving up and down the center line of the sample. We also present computations that reveal the co-existence and periodic evolution of kinematic and magnetic vortices.

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MS8

Semiclassical Approximations to Electronic Structure via Density/Potential Functionals

Kohn-Sham DFT (KS-DFT) computations have become the most employed tool to obtain electronic structure properties of molecules and solids. Further application is thwarted by two main issues: a) KS-DFT requires solution of a set of effective Schrodinger equations for the generation of the noninteracting kinetic energy, and b) approximations for the exchange-correlation functional are generally severely limited in their scope. Semiclassical methods aided with asymptotic analysis provide guiding principles for the construction of density functionals which could improve on the two issues raised above. In this talk the semiclassical limits of electronic structure theory in the context of DFT will be discussed and the leading order corrections to semiclassical local approximations will be provided for 1D systems with box and general boundary conditions. In particular, accurate uniform approximations to the density, density matrix and kinetic energy density of a class of 1D systems will be provided and discussed.

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MS8

Numerical Analysis of Augmented Plane Wave Methods for Full-Potential Electronic Structure Calculations

This presentation talks about the augmented plane wave methods which are widely used in full-potential electronic structure calculations. We first construct a nonconforming method based on this idea and present an a priori error estimate for both linear eigenvalue problems and nonlinear Kohn-Sham equations. Then we analyze the augmented methods under the same framework and show some numerical experiments to support the theory. This presentation is based on the joint work with Reinhold Schneider.

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MS8

BerkeleyGW: A Massively Parallel Tool for Computing Quasiparticle and Optical-Properties of Materials

The GW-BSE approach has, in practice, been prohibitively expensive on systems with more than 50 atoms. We show that through a combination of methodological and algorithmic improvements, the standard GW-BSE approach can be applied to systems with hundreds of atoms. We

discuss improving the traditional GW-BSE methodology through accurate starting points and reductions in empty state requirements. We show that the GW-BSE methodology can scale to tens of thousands of CPUs on high performance supercomputers.

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MS8
Strong Correlation in Density Functional Theory

The exact strong-interaction limit of density functional theory provides a highly non-local functional of the density able to capture strong correlation in the self-consistent Kohn-Sham formalism. I will discuss the formal aspect of this approach and illustrate it with some examples. I will also show that this limit is equivalent to an optimal transport (or mass transportation theory) problem, highlighting the advantages of this connection.

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MS9
Minimal Interface Structures

Soap bubble clusters and material structures can be modeled mathematically by minimizing interface areas or energies subject to volume constraints. The presence of singularities makes the mathematics interesting and difficult, requiring geometric measure theory to make sense of the problem, prove that minimal structures exist and are reasonable, and describe and compute them. The presentation will include open questions and work by undergraduates.

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MS9
Polyhedral Geometries and Symmetry

Over the past 35 years, various classes of highly symmetric skeletal polyhedra have been described. While these structures exhibit the essential characteristics of ordinary polyhedra, the more general skeletal polygonal complexes can be viewed as hybrids of polyhedra and incidence geometries. A complete enumeration of regular polygonal complexes is presented.

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MS9
Capturing the Essence of Infinite Graphs in Quotient Graphs

Describing crystal structures by graphs has the advantage that not only the atoms are represented but also the bonds between them. Space group elements are transformed into graph automorphisms and the orbits under these automorphisms give rise to a quotient graph which still displays crucial information about the original structure. A highly interesting question is the reverse process: construct periodic graphs such that the orbits under their automorphisms result in a prescribed quotient graph.

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MS9
Nanostructures Arising from Crystallographic Tilings

In this talk, we present geometric models for structural analogues of single wall carbon nanotubes and nanotubes with non-hexagonal morphologies which arise from colorings of vertex transitive plane crystallographic tilings. The approach in determining the symmetry groups of these nanotubes will be discussed using concepts in color symmetry theory. The method is extended to study the symmetry properties of the carbon nanotori.

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MS10
Homogenization and Elastoplasticity

In this joint work with A. Giacomini, we propose to address the homogenization of the evolution of a periodic multiphase elasto-plastic composite. The obtained evolution is described in terms of the two-scale limits of the various kinematic fields. The dependence upon the fast variable cannot be integrated out, resulting in a model with an infinite number of internal variables, essentially the plastic strains at each point of the torus of periodicity.

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MS10
The Nonlinear Elastic Response of Suspensions of Rigid Inclusions in Rubber

In the first part of this talk, we present a solution for the fundamental problem of the overall elastic response of ideal (Neo-Hookean) rubber reinforced by a dilute isotropic distribution of rigid particles under arbitrarily large deformations. The derivation makes use of a novel iterative homogenization technique in finite elasticity that allows to construct exact solutions for the homogenization problem of two-phase nonlinear elastic composites with particulate microstructures. In the second part, we make use of the dilute solution as a fundamental building block to derive a simple explicit variational solution for the overall nonlinear elastic response of filled elastomers with finite concentration of particles under arbitrarily large deformations.

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MS10

An Energy-Based Variational Approach to Incremental Homogenization of Elasto-Visco-Plastic Composites

An original approach is proposed, based on an incremental variational principle according to which the local stress-strain relation derives from a single incremental potential constructed from free energy and dissipation functions. The key feature of the model is the explicit use of the elastic trial strain in order to define a Linear Comparison Composite, representative of the actual composite at a given time step. The proposed method competes well with previously proposed schemes in elasto-(visco)-plasticity.

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MS10

Homogenization and Plasticity: Variational Approximations

In this joint work with N. Lahellec, we discuss the effective response of composite materials made from constituents with a partially reversible and partially irreversible behavior. Attention is restricted to behaviors deriving from two potentials. A "Rate Variational Principle" is derived and used to propose approximate schemes to predict the overall response, as well as the field statistics in viscoelastic, elasto-viscoplastic or elasto-plastic composites or polycrystals. The model is applied to particle-reinforced composites and to polycrystalline ice.

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MS11

The Harvard Clean Energy Project: Finding Renewable Energy Materials One Screensaver at a Time

Abstract not available at time of publication.

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MS11

Data Mined Compound and Crystal Structure Prediction for High-Throughput Materials Discovery

Abstract not available at time of publication.

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MS11

Algorithms for Discovery of Nanoporous Materials for Energy Applications

We present a set of approaches for discovery of porous materials for clean energy. They are based on both enumeration and optimization based approaches. They also involve tools to analyze the structure and topology of the void space of porous materials. The latter tools map regions accessible to guest molecules, calculate accessible volume and surface areas as well as pore size distributions.

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MS11

First Principles View on Chemical Compound Space

Abstract not available at time of publication.

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MS12

Modeling and Simulation of Shear Banding in Polymer Solutions from a Monotonic Constitutive Curve

The current theoretical understanding is that shear banding requires a nonmonotonic constitutive relationship. However, recent experimental studies show that shear banding can occur in entangled polymer solutions although the constitutive equation is accepted to be monotonic. Additionally, multiple steady-states have been observed depending upon the wall ramp speed. Here we provide the theoretical framework for predicting these phenomena as well as new results revealing the possibility of > 2 bands, which is not possible through nonmonotonicity.

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MS12

Modeling and Simulation of Shear Banding Phenomena in Concentrated Solutions of Wormlike Mi-

celles

In this talk, we present a new model for concentrated solutions of wormlike micelles, a class of viscoelastic fluids [N. Germann, L.P. Cook, A.N. Beris, Nonequilibrium thermodynamic modeling of the structure and rheology of concentrated wormlike micellar solutions, J. Non-Newt. Fluid Mech. (in press)]. This model is completely based on nonequilibrium thermodynamic arguments and therefore serves as a viable alternative to the VCM model [P.A. Vasquez, G.H. McKinley, L.P. Cook, A network scission model for wormlike micellar solutions I. Model formulation and viscometric flow predictions, J. Non-Newt. Fluid Mech. 144 (2007) 122-139]. An adaptive collocation method was used to perform time-dependent simulations on the coupled nonlinear PDE system. The formation of localized bands with different shear rates, known as shear bands, will be analyzed.

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MS12

Mesoscale Modeling and Simulation of Transient Networks

Many soft gels with a polydisperse entangled mesoscale structure exhibit "slow" relaxation, compared with exponential decay. The slow relaxation behavior is due to the entanglements and the distribution of energetic interactions among the network components at the mesoscale. In order to capture the macroscale behavior, to explore the mesoscale interactions, and to avoid inaccurate closure relationships when constructing continuum-scale models, we perform mesoscale simulation and model the fluid dynamics of the transient network deformation.

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MS12

Diffusive Effects on the Transient and Steady State Shear Response of the Vcm Model

Wormlike micelles are known as living polymers. In this talk, transient and steady state responses of the VCM model under shear are discussed. The important roles that diffusion and elasticity play during the formation of shear bands, in the transient stress response, and in the shape of the steady-state flow curve are examined. A conformal mapping strategy is used to control the spatial discretization so that the shear-band kink remains well resolved for small diffusion.

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MS13

Wrinkling of a Stretched Annular Elastic Thin Sheet - Identification of the Optimal Scaling Law for the Energy of a Ground State

In [Bella & Kohn: Wrinkles as the result of compressive stresses in an annular thin film, to appear in CPAM] we identified the optimal scaling law of the minimum of the elastic energy of a stretched annular thin elastic sheet. In this talk I will describe the next step towards the understanding of this problem – I will identify the optimal prefactor in the scaling law. Moreover, this prefactor can be characterized as a minimum of a much simpler (scalar) variational problem.

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MS13

Instabilities in Axisymmetrically Constrained Sheets

We propose to review different situations where axisymmetric constraints applied to thin sheets induce the formation of radial wrinkles. I a first experiment a thin annulus floating at the surface of water is compressed by a contrast of surface tension resulting from the addition of surfactant molecules. In a second experiment a flat disc is squeezed in between a sphere and a hollow shell. We shall describe in both cases the different morphologies of the wrinkling patterns.

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MS13

Wrinkling Behavior of Highly Stretched Rectangular Elastic Films via Parametric Global Bifurcation

We consider the wrinkling of highly stretched thin rectangular films. We first propose a rational model that correctly accounts for the large mid-plane strain. We then carefully perform a numerical bifurcation, continuation and stability analysis. Our results are often at odds with those obtained using the classical Foppl-von Karman (FK) theory of plates, which has been a popular choice in the literature. E.g., for a given fine thickness, only a certain range of aspect ratios admit stable wrinkling, whereas the FK theory predicts wrinkling outside of that range as well. Also when stable wrinkling emerges as the applied macroscopic strain is steadily increased, the amplitude first increases, reaches a maximum, decreases, and then returns to zero again. In contrast, the FK model predicts an ever-increasing wrinkling amplitude as the macroscopic strain is increased.

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MS13

Stretch-induced Wrinkling of Thin Sheets: Experiments and Modeling

Experiments were conducted to measure stretch-induced wrinkling of rectangular polyethylene thin sheets with two opposite ends clamped and other two edges free. It was observed that the wrinkle amplitude first increased and then decreased with increasing nominal strain. Meanwhile the wrinkle profile remained nearly unchanged with the same number of wrinkles. Finite element analyses were performed to investigate the stretch-induced stress patterns, the critical condition for onset of buckling, and post-buckling evolution of the wrinkles. As a prerequisite for wrinkling, development of compressive stresses in the transverse direction is found to depend on both the length-to-width aspect ratio of the sheet and the applied tensile strain in the longitudinal direction. In addition, the critical condition for wrinkling and the post-buckling behavior both depend sensitively on the sheet thickness. Using a hyperelastic material model, the wrinkle amplitude first increases with the applied strain and then decreases, eventually flattened beyond a moderately large strain. In comparison with the experiments, a hyper-viscoelastic material model is proposed to better capture the rate-dependent behavior of polyethylene and the residual wrinkles observed at high strains. It is found that the wrinkle wavelength is less sensitive to the material model and is well predicted by a scaling analysis.

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MS14

A Mathematical Analysis of Temperature Accelerated Dynamics

Abstract not available at time of publication.

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MS14

A Scalable Method to Compute Transition Rate Prefactors

When describing kinetics in the solid state, the role of the energetic component of the activation free energy is usually emphasized, while vibrational entropic contributions are often assumed to behave in a standard way. While this rule of thumb is often adequate, it can sometimes fail dramatically. I will present a method to efficiently compute vibrational prefactors in the context of Harmonic Transition State Theory. This method is based on a Kernel Polynomial approximation to the vibrational density of states. The algorithm is scalable, enabling calculations on systems of very large size.

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MS14

A Posteriori Estimates for Accelerated Dynamics

An outstanding problem in the practical implementation of parallel replica dynamics is to identify good values of the decorrelation and dephasing time parameters. We propose to use stationarity testing diagnostics for dynamically determining when these stages of the algorithm have been run long enough. We examine various diagnostics for different problems and show that this may be an effective way of automatically determining the values of these parameters.

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MS14

Combining Hyperdynamics with the Quasicontinuum Method

I will decribe our recent progress in combining hyperdynamics, an accelerated molecular dynamics method for reaching long times in infrequent-event systems, with the finite-temperature version of the quasicontinuum (QC) method, a spatial multiscale method for treating large systems, in which atoms are fully resolved only in spatially important regions. The resulting "hyper-QC" method, which combines the strengths of the two methods, looks promising for reaching experimentally relevant time and length scales for intrinsically multiscale systems.

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MS15

Evaluating Microstructural Parameters of Three-dimensional Grains Generated by Phase-field Simulation or Other Voxel-based Techniques

The MacPherson-Srolovitz relation describes the volume change rate of a grain in a three-dimensional polycrystalline system using microstructural parameters — the mean grain width and the triple line length — as well as isotropic values for the grain boundary mobility and energy. We introduce methods to accurately determine these microstructural measures for grain structures described by a voxel-based microstructure representation (VBMR), such as those generated by phase-field simulations, Monte Carlo Potts models, or three-dimensional reconstructions of experimentally measured polycrystalline microstructures. We evaluate the mean rate of volume change of grains during a phase-field simulation of grain growth and discuss the results in terms of the MacPherson-Srolovitz relation.

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MS15

Grain Topologies in Three Dimensional Polycrystalline Microstructures

The prevailing method of characterizing grain topologies in three-dimensional polycrystalline microstructures considers only their number of faces. This information is interesting but it is clearly incomplete. For example, it cannot tell us what fraction of all twelve-faced grains are pentagonal dodecahedra, or what fraction of all fourteen-faced grains are truncated octahedra. I will describe an efficient, graph-theoretic technique that allows for the complete characterization of grain topologies, and show how this can be used to obtain meaningful descriptors of polycrystalline microstructures.

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MS15

Triple Junctions in Microstructure Design

Many materials properties are governed by the grain boundary (GB) network, and empirical studies that manipulate the GB network have demonstrated large improvements in properties. We propose that a rigorous materials design paradigm for GB networks can be centered on the so-called triple junction distribution function (TJDF). We demonstrate how the TJDF allows texture to be linked to GB network topology, which in turn permits network sensitive property predictions and identification of optimal GB networks.

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MS15

Statistical Analyses of Complex Microstructures and Its Application to Coarsening Phenomena

Coarsening is a fundamental subject in materials science, yet we have limited understanding of this phenomenon for complex microstructures. To develop insights, we have applied phase-field models to generate a self-similar, bicontinuous structures and quantified its evolution through statistical analyses of the interfacial morphologies. As an initial step toward developing a theory of coarsening in morphologically and topologically complex systems, we describe the evolution of interfacial shape distribution in the form of a continuity equation.

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MS16

Cryo-Tem Imaging of Thermotropic Bent-Core Liquid Crystals

Layered [N, SmCP (B2), SmAP, modulated smectic (B7) and helical nanofilament (B4)] phases of bent-core thermotropic liquid crystals have been studied by cryo-TEM technique. The technique is able to visualize a sub-

nanometer periodic structure with a wave vector normal to the electron beam and provides complimentary information to freeze fracture TEM measurements. The results will be compared with FFTEM observations, and will be discussed in terms of available theoretical models.

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MS16

Topological Defects and the Ground State Manifold

Do homotopy groups completely characterize topological defects? In this presentation, I will describe the pitfalls to this notion and describe some progress in working around the ambiguities and puzzles that arise in such descriptions.

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MS16

Orientation Waves: The Order Parameter for Some QuasiCrystals

In their text "Statistical Mechanics" Landau and Lifschitz assert that the Landau order parameter for crystals is a density wave. We present convincing evidence that hard tetrahedra, like blue phase liquid crystals, have as an order parameter an orientation wave rather than a density wave, with density waves as secondary order parameters. The consequences of this for understanding quasicrystals and phase transitions will be discussed.

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MS16

Analysis of An Active Liquid Crystal Suspension Model

Active liquid crystal systems is common in biological systems and artificial active materials with microscale force generating reactions. In this presentation, we present a director based model for solutions of active liquid crystal systems and study the model prediction in a systematical way to identify its prediction for the active liquid crystal in various materials and flow regimes. Numerical simulations in the cases where analysis is intractable will be given to illustrate the solution behavior.

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MS17

Evolution of Clean Foams

Clean, low liquid fraction, two-dimensional foams evolve by van der Waals rupture of lamillae between bubles causing their coalesence and the coarsening of the foam. A new network approach to model the evolution follows the creation of disordered states requires a knowledge of instability conditions for thin free films with thinning flows, non-planar shapes, and finite aspect ratio. This instability to rupture will be discussed in detail.

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MS17

Singularities in Electrified Liquid Drops and Jets

We discuss the presence of singularities at the surface of a drop electrically charged or subject to an external electric field. These singularities appear in the form of the so-called dynamic Taylor cones, whose structure we discuss in detail. We will also present regularization due to electrokinetic effects that take into account the finite electric conductivity of the liquid medium.

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MS17

Towards a Regularity Theory for Thin-film Equations

Thin-film equations are a class of fourth-order degenerate PDEs which model the evolution of droplets over solid substrates. We will discuss the regularity of their solutions in the regime of complete wetting, where a null slope is prescribed at the (free) contact line where solid, liquid, and gas meet. Our focus will be on the case of strong slippage, including the classical Navier slip condition.

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MS17

On the Moving Contact Line Singularity in Diffuse-Interface Approaches

We describe analytically the moving contact line singularity and its resolution for diffuse-interface approaches, models of increasing interest where a liquid-gas problem is rep-

resented by a single fluid with continuous density varying rapidly near the interface. We relate the models to the minisymposium thin-film setting and discuss advances in rigorous modelling of the contact line with density functional theory, from which the phenomenological diffuse-interface models are obtained under certain assumptions.

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MS18
Defects and Ripples in Graphene

Ripples in suspended graphene sheets are small randomly oriented ondulations with wavelengths below 25 nm. The equations of motion of a suspended membrane discretized on a hexagonal lattice yield stable defects as pentagon-heptagon and Stone-Wales defects, vacancies, divacancies, etc that are dislocations or dislocation pairs. When coupled to stochastically flipping spins, these equations produce ripples similar to observed ones. A soft spin version of this model can be calibrated using available data from graphene resonators.

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MS18
Force-extension Curves of Biomolecules

Force extension curves of molecular proteins, DNA, or RNA hairpins have a sawtooth shape when the overall length is fixed. Sweeping the same curves under force controlled conditions, sudden transitions at a critical force appear. We propose a model of coupled molecule modules undergoing overdamped Langevin dynamics in bistable potentials under the same external force. For fixed lengths, long-range interactions produce sawtooth curves. Fixing the force, interactions are short-range. Abrupt transitions encompassing force-extension branches appear.

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MS18
Compatibility Conditions and Damage Spread in Lattices

We consider lattice models of breakable and composite materials and metamaterials. Particularly, we study compatibility conditions in dense lattices and their continuous limits, damage propagation and and equilibrium of partially damaged lattices, lattice models of composites and optimal lattice microstructures. Some results were obtained in collaboration with Enrico Rogora and Seubpong Leelavanichkul.

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MS18
Grain Boundaries and Dislocations in the Swift-Hohenberg Equation

We study existence of defects in the Swift-Hohenberg equation using bifurcation methods. We show how to reduce the existence problem to universal coupled-amplitude equation using normal form theory. The reduces equations exhibit kink-type heteroclinic orbits which represent various types of defects. This is joint work with Mariana Haragus and Qiliang Wu.

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MS19
Random Fluctuations Beyond the Homogenization Limit

Abstract not available at time of publication.

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MS19
Effective Properties of Bacterial Suspensions

We introduced a stochastic PDE model for a dilute suspension of self-propelled bacteria with tumbling and obtained an explicit asymptotic formula for the effective viscosity (E.V.) that explains the mechanisms of the drastic reduction of E.V. We next introduce a deterministic ODE/PDE model for bacterial suspensions that includes pairwise interactions and excluded volume constraints. This model is analyzed analytically and numerically. Comparison with

dilute case leads to a phenomenon of stochasticity arising from deterministic system.

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MS19

Homogenization of Dislocation Dynamics

In this talk, we are interested in the collective behaviour of linear defects in crystal, called dislocations, when the number of dislocations goes to infinity. We will study a simple model for such a dynamics and we will present an homogenization result in its simplest form. The goal is to pass from the dynamics of several dislocation lines to the dynamics of dislocation density. We will also give some qualitative properties of the effective hamiltonian. Finally, we will explain how the method developed allows us to get homogenization results for particles system. This is joint works with Cyril Imbert and Rgis Monneau.

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MS19

Polyharmonic Homogenization, Rough Polyharmonic Splines and Sparse Super-localization

We introduce a new variational method for the numerical homogenization of divergence form elliptic, parabolic and hyperbolic equations with arbitrary rough (L^∞) coefficients. Our method does not rely on concepts of ergodicity or scale-separation but on compactness properties of the solution space and a generalization of polyharmonic splines to differential operators with arbitrary rough coefficients. This is a joint work with Lei Zhang (Jiaotong University) and Leonid Berlyand (PSU).

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MS20

Fast Algorithms for Mesoscale Evolution of Large Particle Systems

We design fast algorithms for simulating space-time averages of large systems of ODEs. Averaging produces exact mesoscale PDEs but they cannot be simulated without solving the underlying microscale ODEs. We use recently proposed regularized deconvolution closure method to approximate PDEs. The resulting equations depend only on mesoscale variables and thus can be simulated on much coarser meshes. We investigate effects of various parameters on accuracy of approximation and efficiency to optimize performance of closure method.

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MS20

Optimal Multicomponent Plane Elastic Composites

The paper establishes tight lower bound for the energy and effective elastic stress energy of two-dimensional three-material anisotropic composites. The materials are mixed with fixed volume fractions; one of the materials is void. The bound expands the Hashin-Shtrikman and translation bounds to multiphase structures. In the high-porosity regime, the obtained energy bound is exact and it is realized by special high-rank laminates. Optimal structures for low-porosity strongly anisotropic composites are conjuncted.

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MS20

Sea Ice, Climate, and Multiscale Composites

Sea ice is a leading indicator of climate change, and a key component of Earth's climate system. As a material, sea ice is a porous composite of pure ice with millimeter scale brine inclusions whose volume fraction and connectedness vary significantly with temperature. Fluid flow through the brine microstructure mediates a broad range of geophysi-

cal and biological processes. Sea ice also displays composite structures over much larger scales. For example, the sea ice pack itself is a fractal composite of ice floes and ocean, while surface ponds on melting Arctic sea ice exhibit complex dynamics and self-similar geometrical configurations. I will discuss how methods of homogenization and statistical physics are being used to study the effective properties of such systems. This work helps improve our understanding of the role of sea ice in the climate system, and the representation of sea ice in climate models.

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MS20

Identifying the Strongest Composites

In this talk we develop variational methods for identifying the strongest composite geometries for prescribed boundary loads. Here the "strongest' composite has a microgeometry for which the local stresses and strains are smallest in the L^∞ norm over all composites comprised of two materials in fixed proportion. The analysis is carried out for composites with and without thermal prestress.

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MS21

Compositional Interface Dynamics Within Symmetric and Asymmetric Planar Lipid Bilayer Membranes

Compositional domains within multicomponent lipid bilayer membranes are believed to facilitate many important cellular processes. Experimentally, it has been shown that synthetic membranes whose overall compositions mimic those of the extracellular leaflet of the cell membrane can phase separate into distinct liquid phases, while the ones whose compositions mimic those of the cytoplasmic leaflet do not display any compositional heterogeneities or domains. Interestingly, in asymmetric membranes, where the two leaflets have compositions mimicking those of the extracellular and cytoplasmic leaflets of the cell membrane, phase separation can either be induced or suppressed altogether. Furthermore, when both leaflets contain compositional lipid domains, they are often found in perfect registry. These observations indicate that a significant thermodynamic coupling exists between the lipids across the two leaflets. While the effects of the thermodynamic coupling between the leaflets has been theoretically investigated recently with regard to equilibrium behavior of asymmetric multicomponent lipid bilayer membranes, its effects on the compositional domain dynamics have received less attention. In this talk, I will first derive the general equations that describe the dynamics of compositional domains within planar membranes with asymmetry in leaflet properties and in the presence of a thermodynamic coupling between the leaflets. These equations are then employed to develop analytical solutions to the dynamics of the recurrence of registration for both laminar and circular domains in the case of weak coupling. It is shown that experimentally measuring these dynamics will enable one to determine the strength of the thermodynamic coupling between the leaflets. A closed-form expression for the decay rate of interface fluctuations in the case in which only one leaflet supports compositional domains, is also derived.

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MS21

Three Dimensional Vesicles in Fluid Flow and Electric Fields: Jump Conditions and a Numerical Method

The electrohydrodynamic response of vesicles is due to a complex interplay between the fluid, the shape of the vesicle membrane, and the surrounding electric field. In order to construct accurate numerical models of vesicle in electrohydrodynamic flows the physical jumps in the fluid and electric fields must be determined and accounted for. In this talk the jump conditions for the pressure, velocity, and electric field for a three-dimensional vesicle with discontinuous viscosities, an in-extensible interface, and with a surface voltage potential are presented. The jump conditions are used in a sharp interface immersed interface solver. Sample analytic solutions have been developed to verify the methods and will also be presented.

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MS21

Numerical Algorithms for Vesicle Flows

Direct numerical simulations of vesicles, bubbles, and other soft-particle suspensions in arbitrary confined geometries is extremely challenging owing to the near-singular interaction forces, nonlinear interfacial forces and nonlocal hydrodynamics. In this talk, we will present some recent advances in computational algorithms for simulating such systems. Integral equation formulations for confined flows and mixtures of soft and rigid particles will be discussed. A new fast algorithm for accelerating the singular integral evaluations on the interfaces will be presented. Integrating semi-implicit time stepping schemes with reparameterization and anti-aliasing techniques enables us to overcome numerical instabilities. We will review some of these computational components, which are essential for simulating large number of particles in dense flows.

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MS21

Nonlinear Dynamics of An Incompressible Elastic Membrane in An Electric Field

Cells are enveloped by a lipid membrane, which is imper-

meable to ions and acts as a capacitor when an electric field is applied. In this work we present a long-wave model for the nonlinear dynamics of a planar (unsupported) lipid membrane under a DC field. The lipid membrane is modeled as an interface with a constant area. The governing equations for the non-linear long-wave dynamics are derived under different conditions. Analysis on the equilibrium profile shows the existence of multiple equilibrium profiles. Numerical simulations of the nonlinear dynamics illustrate various novel behaviors, and elucidate the importance of charge distribution on the membrane. We will also examine the possible effects of tangential electric field on the membrane dynamics.

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MS22
Mechanics of a Folded Elastic Ribbon

When a thin, annular strip cut out in a sheet of paper is folded along its circular centerline, it buckles out-of-plane (Dias et al., PRL, 2012). We derive an equivalent rod model for the folded strip. A nonlinear effective constitutive law capturing the underlying geometrical constraints is obtained. A stability analysis is presented, which explains the buckled shapes reported in the literature, and predicts a new type of buckling patterns.

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MS22
Folding of a Fluid-Supported Sheet

A thin elastic sheet lying on a heavy fluid buckles under uniaxial compression via localized folds. This system is integrable, allowing us to analytically describe the entire progression from a weakly displaced sinusoidal buckling to a single large fold that contacts itself. Underlying the integrability is an unexpected symmetry, which leads to large ground-state degeneracy. We find a connection between this nontrivial symmetry and the obvious symmetries of the higher-dimensional sine-Gordon equation.

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MS22
Wrinkles and Folding on Curved Topographies

An intrinsically flat, elastic film forced to wrap a curved surface spontaneously develops wrinkles. We show how the relaxed membrane energy of the wrinkled film, and a separate equation for the wrinkled microstructure appear as the zeroth and first order equations in a multiscale perturbation expansion of a fully rotationally invariant plate-bending model. Applying these equations to curved surfaces, we show how geometry can both suppress wrinkles and enhance them into singular folds.

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MS22
First Steps Toward a Multipole Construction of Thin Sheets

An elastic sheet may contain pointlike conical singularities that carry a metrical 'charge' of Gaussian curvature. Adding such elementary defects to a sheet allows one to make many shapes, in a manner broadly analogous to the familiar multipole construction in electrostatics. However, here the underlying field theory is non-linear, and superposition of intrinsic defects is non-trivial as it must respect the immersion of the resulting surface in three dimensions. We consider the first terms of this construction: the monopole which corresponds to a conical singularity, and the "charge-neutral' dipole. Such a dipole is composed of two conical singularities of opposite sign. Unlike the relatively simple electrostatic case, here there are two distinct stable minima and an infinity of unstable equilibria. We determine the shapes of the minima and evaluate their energies in the thin-sheet regime where bending dominates over stretching. Our predictions are in surprisingly good agreement with experiments on paper sheets.

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MS23
Title Not Available at Time of Publication

Abstract not available at time of publication.

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Abstract not available at time of publication.

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TBD

MS24
Spatio-Temporal Self-Organization at the Nanoscale in Alloys Subjected to Sustained Irradiation

Recent atom probe experiments have shown that, in binary alloys, ion irradiation can stabilize self-organized structures comprised of nanoscale solute-rich precipitates that contain smaller solvent-rich precipitates. We investigate and elucidate by kinetic Monte-Carlo simulations the mechanisms leading to the formation of these precipitate-within-precipitate structures, which we term 'cherry-pit" structures. Asymmetries in thermodynamic and kinetic properties between solvent and solute atoms are shown to play a key role.

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MS24
Self-Assembled Nanoscale Patterns Produced by Ion Bombardment of Two-Component Materials

We have developed a theory that explains why astonishingly regular hexagonal arrays of nanoscale mounds can form on the surface of a binary solid when it is bombarded with a normally-incident, broad ion beam. The coupling between a surface layer of altered composition and the surface morphology is the key to understanding the phenomenon. Our theory also predicts that remarkably defect-free surface ripples can be produced by oblique-incidence bombardment of a binary material.

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MS24
Composition Patterning in Irradiation-driven Materials

Following a brief discussion of recent progress in phase field modeling of radiation effects in materials, this presentation will focus on the problem of composition patterning in irradiation driven systems. A coupled set of nonlinear stochastic PDEs of diffusion-reaction type is developed in which non-local forcing terms represent the irradiation field. Aspects of the spatial and temporal stiffness of these equations will be discussed as part of presenting the numerical solution and model predictions.

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MS24
Multi-Scale Modeling of Irradiated Alloys: Atomistically-Informed Continuum Models

We consider the estimation, by means of atomistic simulation, of parameters in theories of ion irradiation of binary materials. By extending the "crater function" formalism to the case of binary materials, we are able to estimate four important parameters in these theories. This seems to suggest that an important morphological instability mechanism may not be active; therefore, we generalize the existing model to admit the alternate mechanism of phase separation, and discuss its predictions.

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MS25
Mathematical Modeling of Colloids

This talk deals with mathematical modeling of colloids. We think of colloids as soft matter systems consisting of particles suspended in fluid. These particles may be electrically charged or may posses permanent electric or magnetic dipoles. Renewed interest in colloids occurs in several technological areas, including liquid crystal display, microfluidic apparatus and also in modeling particle clustering in biology. We will focus on ferromagnetic nano-particles in a liquid crystal matrix. These systems show two very distinctive features: formation of defects around the particles and the tendency to form clusters, with the subsequent failure of the device. We will construct effective energies of ferrofluids and explore how to harness defects to prevent clustering. The presence of a defect causes a buildup of elastic energy of the liquid crystal between two particles, hence favoring configurations with an optimal inter-particle

distance.

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MS25

Electromagnetic Wave Propagation Through a Liquid Crystal Layer

We study the propagation of electromagnetic waves through a liquid crystal layer paying particular attention to the problem of optimizing the transmitted intensity. For a homogeneous liquid crystal orientation field, we derive analytical formulas for the orientation that maximizes the transmission. The minimizing orientation is unique for a given wavelength and we define its value implicitly. For a heterogeneous liquid crystal orientation, we carry out numerical simulations to study the optimization problem.

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MS25

Defect Patterns in Liquid Crystal Films

We analyze stable textures in thin smectic C* films using the Ginzburg-Landau type model

$$\int_\Omega [k_s(\text{div } u)^2 + k_b(\text{curl}\, u)^2 + \frac{1}{2\varepsilon^2}(1-|u|^2)^2]\, dx$$

for $\varepsilon > 0$ and small. We prove that if the c director u has degree deg $(u, \partial\Omega) = d > 0$ then the pattern has d degree-one defects. Moreover if $0 < k_s < k_b$ the pattern near each defect is splay dominated while if $0 < k_b < k_s$ the pattern is locally dominated by bend.

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MS25

Efficient Numerical Schemes for Phase-Field Models of Multiphase Complex Fluids

We present an energetic phase-field model, which admits a dissipative energy law, for a mixture of two immiscible, incompressible fluids: one is a Newtonian fluid, and the other is the nematic liquid crystals. We shall construct efficient time discretization schemes which satisfy discrete dissipative energy laws, and present numerical results which demonstrate the versatility of the model and the effectiveness of our numerical schemes.

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MS26

Microstructure As a Result of Differential Growth of Thin Films

In this talk I will discuss wrinkling of a thin elastic sheet caused by a prescribed non-Euclidean metric. This is a model problem for the patterns seen, for example, in torn plastic sheets and the leaves of plants. Following the lead of other authors I adopt a variational viewpoint, according to which the wrinkling is driven by minimization of an elastic energy subject to appropriate constraints and boundary conditions. The main result is the identification of the scaling law (in terms of thickness) for the minimum of the elastic energy.

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MS26

Ambrosio-Tortorelli Approximation for Cavitation

An approximation of Ambrosio-Tortorelli type is presented for the variational model for cavitation and fracture introduced by Henao & Mora-Corral (2010). A proof is provided for the liminf inequality in the Γ-convergence, and some numerical examples of void coalescence using this model are shown, following the numerical study by Xu & Henao (2011).

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MS26

Continuum Limits of Discrete Dislocation Energies: The Case of the Idealised Pile-up

Dislocations are defects in the crystal lattice of metals, and their collective motion gives rise to macroscopic permanent deformations. The major obstacle to the motion of dislocations is the presence of grain and phase boundaries. When dislocations encounter such barriers, they pile up against them, causing the material to harden. Modelling and upscaling dislocation pile-ups is therefore a key step for predicting the mechanical behaviour of metals and for the design of better performing materials. Starting from a discrete model of an idealised pile-up we derive a continuum, mesoscopic dislocation model via Gamma-convergence. Moreover, we show that various existing mod-

els arise as special cases of our results.

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MS26

About a Γ-Convergence Approach to a Quasicontinuum Method in 1D

We analyze the validity of a quasicontinuum approximation of a one-dimensional atomistic model for fracture mechanics. To this end we derive a development by Γ-convergence and compare the limiting functional and its minimizers with those obtained for a fully atomistic system in [L. Scardia, A. Schlömerkemper, C. Zanini, *MMMAS* **21** (2011)]. Further we estimate the minimal size of the atomistic region needed in order to capture boundary layer effects and discuss the effect of the choice of the representative atoms.

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MS27

Unstable Multilayer Homoepitaxial Growth: From 2D Islands to 3D Mounds

Abstract not available at time of publication.

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MS27

Variational Methods for Crystal Surface Instability

Abstract not available at time of publication.

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MS27

Motion of Elastic Thin Films by Surface Diffusion with Curvature Regularization

Abstract not available at time of publication.

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MS28

Spectral Representation and Evolution of Microstructure

In rheological fluids, optimally designed composites, biological materials, structure self-organizes in response to external loads or applied fields. We relate microstructural transformation in such materials to evolution of the spectral measure in an integral representation of the effective properties of composite. Using nonlinear diffusion and viscoelasticity examples, we show that Pade approximants of the spectral measure link evolution of the microgeometry to the effective behavior of material and allow to uniquely recover some microstructural parameters.

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MS28

Models and Analysis for Cohesive Dynamic Fracture

We derive models for cohesive dynamic fracture using force balance, stationary action, and maximal dissipation, for a range of cohesive energy densities. For 1-D, we give some partial existence results, examples where homogenization is required, and some surprising examples of non-existence. This is joint with V. Slastikov.

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MS28

Double Negative Behavior in Metamaterials and Multi-Scale Analysis

Metamaterials are a new form of structured materials used to control electromagnetic waves through localized resonances. In this talk we introduce a rigorous mathematical framework for controlling localized resonances and predicting exotic behavior inside optical metamaterials. The theory is multiscale in nature and provides a rational basis for designing microstructure using multiphase nonmagnetic materials to create backward wave behavior across prescribed frequency ranges.

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MS28

Large Deviations, Metastability and Monte Carlo Methods for Multiscale Problems

We discuss large deviations and Monte Carlo methods for multiscale dynamical systems that are stochastically perturbed by small noise. The large deviations principle can then be used to study metastability for such problems, as well as asymptotic problems for related PDE's. Furthermore, we derive a change of measure that allows to design asymptotically efficient importance sampling schemes for the estimation of associated rare event probabilities and expectations of functionals of interest.

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MS29

Physical Bounds, Potentials and Fundamental Limitations of Metamaterial Cloaks

In this talk we establish fundamental physical bounds on bandwidth and cloaking performance for arbitrary passive cloaking schemes. We apply the Bode-Fano theory to derive general limitations relating the maximum achievable bandwidth and overall scattering reduction to the size and electromagnetic properties of the scatterer to be hidden. We derive a few general theorems limiting ideal cloaking performance, which represent a pivotal achievement to understand the applicability of cloaking devices to real-world problems.

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MS29

Towards Digital Metamaterials

Inspired by the Boolean algebra and the notion of digital electronics and the binary number theory, we have developed the concept of digital metamaterials, in which we explore how an arbitrary value of the permittivity function can be synthesized by judicious combinations of only two constituent materials with two different permittivity parameters. We have analyzed the conditions upon which one can achieve such synthesis, including the role of loss, shape and dimensions of constituent elements.

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MS29

Branch-cuts and Sharp Corners in Composite Inclusions

The calculation of effective transport properties such as dielectric permittivity or magnetic permeability for systems containing inclusions immersed in a continuous matrix can be challenging. This is particularly the case in the situation encountered in the study of metamaterials- when the inclusions and matrix have permittivities or permeabilities of opposing signs- and the problem is compounded when the inclusions have sharp corners. We explain the physical and mathematical properties of such systems.

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MS29

Radiationless Electromagnetic Modes in Open Plasmonic Nanostructures

In open systems the energy associated with a photonic mode may continuously leak away in the form of a radiated wave, and hence all the lifetimes are finite. This property is closely related to the problem of instability of the Rutherford atom in classical physics. Here, we will theoretically show that in the limit of no loss plasmonic materials may offer an opportunity to have light localization in open bounded systems with infinitely long lifetimes.

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MS30

The Micromechanics of Colloidal Dispersions

What do corn starch, swimming spermatozoa, DNA and self-assembling nanoparticles have in common? They are all (or can be modeled as) particles dispersed in a continuum suspending fluid where hydrodynamic interactions compete with thermal (Brownian) and interparticle forces to set structure and determine properties. These systems are soft as compared to molecular systems largely because their number density is much less and their time scales much longer than atomic or molecular systems (both scaling with the colloidal to atomic size cubed). In this talk I will describe the common framework for modeling these diverse systems and the essential features that any hydrodynamic modeling must incorporate in order to capture the correct behavior. Actually computing the hydrodynamics in an accurate and efficient manner is the real challenge, and I will illustrate past successes and current efforts with examples drawn from the diffusion and rheology of colloids to the swimming of catalytic nanomotors.

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MS30

Collective Dynamics in Suspensions of Motile Micro-particles

We describe a computational method for the dynamics of thousands of micro-swimmers interacting with each-other, the fluid, and surfaces. The method is illustrated with suspensions of pusher and puller motile particles. The model satisfactorily captures the macroscopic structures observed in bacterial baths. We discuss dense and confined swimmer suspensions where organization emerges as a result of steric effects. Last we show examples of swimmers inside a peristaltic pump where the dynamics and transport are affected.

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MS30

Statistical Analysis of Passive Particle Tracking in Microrheology

Passive particle tracking in microrheology has received much attention in the recent years, but the statistical methods for data analysis are still quite primitive. To this end, we develop new methods for analyzing stochastic differential equations (SDEs) driven by colored noise. Traditionally, most SDEs are modeled as driven by white noise, which implies a Markovian assumption. We present a method of driving SDEs with col- ored noise, which provides acces to a rich collection of time-dependent models. Our model has a natural discretization scheme, the key to a missing data inference framework for white noise SDEs. Many compu- tational methods from the white noise set up can easily be adapted to our framework. We present applications of our methodology for single particle tracking for passive microrheology.

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MS30

Biofilm Streamers in Porous Environments

Biofilms are ubiquitous and are generally associated with surfaces. Despite their importance, basic information about biofilm dynamics is common ecological environments is lacking. Using model flows in microfluidic channels, we demonstrate that in the presence of flow biofilms develop three-dimensional thread-like structures, or streamers, which in common pressure-driven flows can lead to sudden clogging of the channels. We document several aspects of the development in space and time, and use biological mutants to further understand the genes important to the streamer formation. Our results are interpreted in terms of a model that characterizes trapping of cells in a sieve-like network that exhibits exponentially fast growth of the typical streamer radius and is independent of the bacterial growth rate. Finally, we demonstrate similar effects in flow through soil-like porous materials, industrial filters, and medical stents to emphasize how these ideas can impact environmental, industrial and medical systems.

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MS31

Nonlinear Structure and Mechanics of Filament Bundles: Intrinsic Geometry of Twist and Defect-Riddled Ground States

Rope-like bundles of filamentous proteins provide a mechanical bridge from the molecular scale to the microscopic scales of in a broad range of cells and tissues. Motivated by the "almost crystalline" packing of biofilament bundles, we develop continuum approaches to the non-linear geometric coupling between inter-filament strain and backbone orientation in dense bundles. We exploit a correspondence between stresses induced in elastic sheets subjected to (positive) curvature and inter-filament stresses in the cross-section of twisted bundles to develop a quantitative theory of defect-riddled optimal packings of twisted (chiral) filament bundles.

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MS31

How to Derive Equilibrium Equations for Fully Nonlinear Bending Theories in Euclidean and Non-Euclidean Elasticity

A key feature of nonlinear bending theories for thin elastic films is an isometry constraint on the admissible deformations. It means that only 'pure bending' deformations are allowed, i.e., no stretching or shearing is permitted. Such a constraint is a serious obstacle when one wants to derive the equilibrium equations satisfied by deformations with minimal bending energy. In the talk I will explain how to overcome it.

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MS31

Riemannian Analysis of Pre-stressed Elastic Materials

Dimension reduction is a classical theme in elasticity, dating to centuries ago. Significant progress has been achieved in recent years in the rigorous derivation of dimensionally reduced theories from 3D elasticity. The recent renewed interest in pre-stressed (or incompatible) materials has raised a new challenge in deriving reduced models for materials that may have complex internal geometries. In this lecture I will present a single theorem that gives in one fell swoop reduced theories for "Euclidean" and "non-Euclidean" plates, shells, and rods. The relevance of these reduced models in several pattern forming systems will be demonstrated.

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MS31

A Riemannian Approach to Dimension Reduction in Non-Euclidean Elasticity

The renewed interest in non-Euclidean (or incompatible) elasticity has raised a new challenge in deriving dimensionally reduced models for such elastic bodies. In this talk I will present a Riemannian approach to this problem that enables us to treat Euclidean and non-Euclidean materials with arbitrary number of slender dimensions. I will present two theorems based on this approach one that gives reduced theories of plates, shells and rods, and the other a reduced membrane model.

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MS32

Critical Aspect Ratio in a Single Crystal Shear Experiment

Consideration is given to a non-convex variational model for a shear experiment in the framework of single-crystal linearised plasticity with cross-hardening. The rectangular shear sample is clamped at each end, and is subjected to a prescribed horizontal shear, modelled by a hard Dirichlet condition. We ask: how much energy is required to impose such a shear, and how does it depend on the aspect ratio? Assuming that just two slip systems are active, we show that there is a critical aspect ratio, above which the energy is strictly positive, and below which it is zero. The energy required to impose a shear depends on the presence of cross hardening and the energetic penalization of geometrically necessary dislocations. This result therefore provides a way to distinguish microscopic models by their macroscopic behavior.

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MS32

A Theory and Challenges for Coarsening in Microstructure

Cellular networks are ubiquitous in nature. Coarsening is governed primarily by the attempt of the system to decrease the energy of its interfaces. The Grain Boundary Character Distribution, GBCD, represents the distribution of interfacial energy and its evolution provides some understanding of the order in the system. This gives rise to interesting questions and some challenges.

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MS32

Multiscale Modeling of Ge Nano-Crystallization from Amorphous Phase

Complex nanostructures are observed in laser-driven crystallization of amorphous Ge films. In this talk, a multiscale model will be presented to study the kinetics of rapid phase-transformations and the interplay between nucleation and growth processes. The core of the model is based on the phase-field method and the parameters involved are obtained via molecular dynamics. The results from the simulations are compared to observations with dynamic transmission electron microscopy (DTEM)." 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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MS32

Mathematical Challenges in Interpretation of Hedm Data

High Energy Diffraction Microscopy (HEDM) is a non-destructive orientation and strain mapping technique that uses high energy (¿50KeV) monochromatic x-ray beam. Recent experimental developments enable the interrogation of polycrystalline materials under thermal and mechanical loading resulting in abundant information with resolution at the micron level. The technique provides three dimensional microstructure snapshots during the loading process. This is the first opportunity to examine theories regarding microstructure evolution in such materials using in a non-destructive technique. In this talk I will discuss mathematical formulations using optimization techniques that address several problems of engineering interest including: (i) the extraction of material properties such as energy and mobility form HEDM, and (ii) the validation of microstructural evolution theories for material behavior under thermal and mechanical loading. Techniques from optimal transport theory will be reviewed and explained in the context of these problems.

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MS33

Modeling Defect Structures and Associated Slow Processes in 3D Materials with Phase Field Crystal Methods

A wide variety of phenomena in crystalline solids are driven and/or limited by defect evolution processes. Examples include plasticity, structural phase transformations, and recrystallization. It is not currently possible to model complex, collective defect processes over the vast range of

length and time scales often involved, but the ability to access diffusive time scales with phase field crystal (PFC) models should open new avenues of research in this area. In this talk, applications of the PFC approach to defect statics and dynamics in FCC, BCC, and HCP materials will be discussed. The most prevalent dislocations in FCC and BCC crystals have been stabilized within the PFC formulation and shown to exhibit properties consistent with both continuum elasticity and molecular dynamics. Additional levels of structural and dynamic complexity naturally emerge when defected PFC crystals are subjected to slow mechanical, chemical, or thermodynamic driving forces. A few examples of such higher-level effects involving jogs, obstacles, and sources will be explored along with selected results concerning larger-scale collective defect behaviors.

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MS33

Particles at Fluid-fluid Interfaces: A New Navier-Stokes-Cahn-Hilliard Surface Phase-Field Crystal Model

Colloid particles that are partially wetted by two immiscible fluids can become con- fined to fluid-fluid interfaces. At sufficiently high volume fractions, the colloids may jam and the interface may crystallize. The fluids together with the interfacial col- loids form an emulsion with interesting material properties and offer an important route to new soft materials. We develop an improved Navier-Stokes-Cahn-Hilliard-Surface-Phase-Field-Crystal model based on the principles of mass conservation and thermodynamic consistency. To validate our approach, we derive a sharp interface model and show agreement with the improved diffuse interface model. Using simple flow configurations, we show that the new model has much better properties and does not lead to spurious velocities. Finally, we demonstrate the solid-like behaviour of the crystallized interface by simulating the fall of a solid ball through a colloid-laden multiphase fluid.

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MS33

Phase Field Crystal Modeling of Microstructure in Multi-Component Alloys

This talk will begin with a comparison of differences and similarities of recent PFC approaches in the context of 2D/3D structural stability and of 3D defect stability. A recent model for structural transformations (so-called XPFC) will be singled out and its extension to ternary and multi-component alloys will be discussed. Some examples of the types of phase transformations that are possible with this approach will be demonstrated, with particular emphasis on new results relating to interface kinetics and solute trapping, solid-state precipitation and magneto-crystalline interactions. We end with a new derivation of an amplitude model of structural transformations, discussing the advantages and drawbacks of such models, and illustrating their use in solidification and secondary phase formation.

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MS33

Phase Field Crystal Models of Grain Growth

Traditional Phase Field Crystal (PFC) models contain solid and liquid phases, however many important materials processing phenomena involve a vapor phase as well. In this work, we add a vapor phase to an existing PFC model and show realistic interfacial phenomena. For example, the PFC model exhibits density oscillations at liquid-vapor interfaces that compare favorably to data available for interfaces in metallic systems. Additionally, the strain field beneath a stepped interface is characterized and shown to qualitatively reproduce predictions from continuum models, simulations, and experimental data. Further examples will be given.

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MS34

Analysis of Two-Dimensional Phases in Bent-Core Liquid Crystals

We consider a Landau-de Gennes type model used in the physics literature to describe two-dimensional modulated structures in bent-core liquid crystals. We will discuss a simplified version of the model, and present some remarks about the full version.

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MS34

Equidistribution Results for the Renormalized En-

ergy and 2D Coulomb Gases

The renormalized energy is a Coulomb interaction energy for an infinite number of points in the plane. It has been introduced and derived by Sandier and Serfaty as the limit interaction energy for vortices in the 2D Ginzburg-Landau model of superconductivity. It can also be derived as a limit interaction for droplets in the Ohta-Kawasaki energy, as well as particles of a Coulomb gas at zero temperature. It is expected to be minimized when the points are arranged in an "Abrikosov" triangular lattice. In joint work with Simona Rota Nodari, we show that for minimizers of the renormalized energy in various suitable senses, as well as for minimizers of the Coulomb gas Hamiltonian, the energy and the points are uniformly distributed at any scale larger than the interpoint distance.

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MS34

Vortex Dynamics with Pinning and Strong Fields

We study a mixed heat and Schrödinger Ginzburg-Landau evolution equation that is meant to model a superconductor containing impurities and subjected to an applied electric current and electromagnetic field. Such a current is expected to set the vortices in motion, while the pinning term drives them toward minima of the pinning potential and pins them there. We derive the limiting dynamics of a finite number of vortices in the limit of a large Ginzburg-Landau parameter, or $\epsilon \to 0$, when the intensity of the electric current and applied magnetic field on the boundary scale like $|\log \epsilon|$. We show that the limiting velocity of the vortices is the sum of a Lorentz force, due to the current, and a pinning force. Comparing the two then allows us to identify the critical depinning current.

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MS34

On the Nature of Defects in the Q-Tensor Theory of Nematic Liquid Crystals

Nematic liquid crystals are modelled mathematically using either: unit-length vectors in the Oseen-Frank theory (2 degrees of freedom), scalars and unit-length vectors in Ericksen theory (3 degrees of freedom) or symmetric and traceless 3x3 matrices in Landau-de Gennes theory (5 degrees of freedom). We will look into specific features of nematics that require a tensorial description, with an emphasis on the interpretation of defects in various theories.

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MS35

Fast Numerical Methods for Electronic Structure Calculations

The standard diagonalization method for solving the Kohn Sham density functional theory (KSDFT) scales cubically with respect to system size. In the recently developed pole expansion plus selected inversion method (PEXSI), KSDFT is solved by evaluating the selected elements of the inverse of a series of sparse symmetric matrices. We show that the PEXSI method scales at most quadratically with respect to system size for all materials, and can scale to tens of thousands of processors on leadership class machines.

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MS35

Many-Body Propagators and the GW Approximation of the Self-Energy Operator

We discuss the Green's function formalism of many-body perturbation theory. In this approach, the excitation of the material is described in terms of quasi-particle energies of a single-particle Hamiltonian that contains a self-energy term. The self-energy operator should properly describe many-body excitation effects. It can be approximated properly by the so-called GW method. We will point out the advantage and computational challenges of this approach.

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MS35

Exciton Diffusion in Organic Solar Cells: First--Principles Investigations

Exciton diffusion length and time are among the most important factors that govern the performance of organic solar cells and light-emitting diodes. We have developed a first-principles approach based on time-dependent density functional linear response theory to describe the energy and many-body wave-functions of excitons. The non-adiabatic ab initio molecular dynamics is used to calculate phonon-assisted transition rates between localized exciton states with the spontaneous emission determined by the dipole approximation. With Mont Carlo simulations, we are able to calculate the exciton diffusion length, time, and diffusivity for a prototype polymer system P3HT, and have obtained excellent results comparing to experiments as well as physical insight into the microscopic nature of exciton diffusion. The work was partially supported by NSF-Solar grant DMR-1035480.

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MS35

Fixed-Point Optimization of Atoms and Density in Dft

DFT methods require solving a fixed-point problem for the density, and all practical codes use a multisecant variant of Broyden's second (bad) method. I will describe an extension including the atomic positions within the same fixed-point problem. The method involves an implicit trust-region for the unpredicted step and adapting the concept from optimization of a Broyden family to the fixed-point problem with a conventional stability constraint, plus fail-safe trust region controls.

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MS36

Recent Advances in Mathematical Diffraction Theory

The discovery of quasicrystals called for an extension of classical diffraction results to aperiodic systems. For cut and project sets, the diffraction is pure point, and the locations and intensities of Bragg peaks can be calculated explicitly. Recent rigorous and constructive approaches to the case of diffuse scattering provide a better understanding of systems with singular continuous and absolutely continuous diffraction. This talk reviews the development of mathematical diffraction theory following the discovery of quasicrystals.

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MS36

A Stroll Along Structural Paths: Symmetry, Pseudo-Symmetry and Their Exploitation to Understand and Design Structures

Structural relations between aristotypes ("basic structures") and hettotypes ("derivative structures") are of paramount importance to understand at the atomic level how a displacive phase transition occurs, what features different structures share, how a structural continuity is realized at the interface separating crystal associations. The approach and the method will be illustrated with the help of several examples.

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MS36

Periodicity, Aperiodicity and Prehistory

On February 28, 1918, the American Museum of Natural History in New York hosted a gala birthday party for the great French mineralogist René Just Haüy. (The honoree, having died 96 years before, missed out on the seven course banquet, including a Whale Steak named for him.) Curiously, from our vantage point 95 years later, the then-recent vindication by x-ray diffraction of his periodic model of crystal structure went uncelebrated in the great hall. Which of his achievements had mineralogists gathered to celebrate? And which should we celebrate in 1914, the International Year of Crystallography?

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MS36

Coincidence Site Lattices and Well-rounded Sublattices in the Plane

Given a lattice Γ a lattice of the form $\Gamma \cap R\Gamma$ is called a CSL if it is a sublattice of full rank. A lattice is called well-rounded, if its lattice vectors of minimal length span the underlying space. We use the connection between a certain class of CSLs and the well-rounded sublattices of a lattice to determine all its well-rounded sublattices, to count them, and to calculate the asymptotic growth rate via suitable generating functions.

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MS37

On the Coupling Between Transformation and Plasticity in Polycrystals

Abstract not available at time of publication.

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MS37

Nonlinear Asymptotic Homogenization of Thermoelectric Composites

We develop a nonlinear asymptotic homogenization theory to analyze the effective behavior of layered thermoelectric composites. The nonlinearly coupled thermoelectric transport equations are homogenized using asymptotic analysis, from which the macroscopic field distributions are derived with local fluctuation averaged out, and overall thermoelectric conversion efficiency is established using an idealized thermoelectric module. The analysis sheds considerable insight into the effective behavior of thermoelectric composites for their design and optimization.

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MS37

Constitutive Models for Magneto-Active Elastomers at Finite Strains

This paper deals with the application of a finite-strain homogenization framework to develop constitutive models for magneto-active elastomers consisting of initially aligned, rigid magnetic particles distributed randomly in an elas-

tomeric matrix. For this purpose, a novel strategy is proposed to partially decouple the mechanical and magnetostatic effects. The theory predicts the existence of certain extra stresses that can be directly linked to changes in the effective magnetic permittivity with the deformation. We show that particle rotations can be used to generate large magnetostriction.

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MS37

Continuum Electromechanical Theory for Nematic Continua with Applications to Freedericksz Instability

A general theory for nematic continua that accounts for electromechanical coupling is presented, based on a Lagrangian variational formulation. An application of this theory is presented next to the study of the stability of a nematic liquid crystal confined between two parallel plates and subjected to an electric field perpendicular to them. As the electric field reaches a critical value, the nematic directors, which are initially parallel to the bounding plates, change orientation (Freedericksz transition). It is shown that in this bifurcation problem, the lowest (critical) electric field corresponds to a global (long wavelength) instability and that the bifurcated equilibrium path is stable.

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MS38

Lagrangian Treatment of Systems Composed of High-Loss and Lossless Components

We study here Lagrangian dissipative properties of composite systems with two components one of which is highly lossy and the other is lossless. A principle result of our studies is that any general Lagrangian system, with losses accounted by a Rayleigh dissipative function, its dissipative properties can be studied within the general framework introduced in our previous work Dissipative properties of systems composed of high-loss and lossless components, J. Math. Phys. 53, 123508 (2012). The phenomenon of overdamping in such composite systems is studied and the eectiveness of this framework demonstrated.

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MS38

On the Sensitivity of the Annomallous Localized Ressonance Phenomenon to Small Variations in the Loss Level

Anomalous localized resonance (ANR) phenomena appears at the interface between negative index and and positive index materials when approached by a charge distribution. This phenomenon manifests itself in a very large "unnatural" accumulation of dissipated power in a small layer around the respective interface between the two materials. In this talk we will discus about the (two-dimensional) anomalous localized resonance phenomena appearing at BOTH interfaces between a slab (infinite in the y-direction) with permittivity having a real part equal to -1 and small dissipation d¡¡1 and two "natural" materials, one to the left with a permittivity $1 + i * (d + d^b)$ and the other to the right with permittivity 1, when one approaches the slab with a discrete or continuous localized charge distribution. We will briefly highlight several results already know in the literature and then present our recent findings which show a high dependence of the ANR phenomenon on b when $0 < b < 1$. We will show how the rate of accumulation of dissipated power and how the region where the charge distribution should be for the ANR phenomenon to be observed depend on b. The results presented are a joint work with Graeme Milton and Andrew Thaler from University of Utah and Taoufik Meklachi and Gregory Funchess from University of Houston.

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MS38

Optical Topological Insulators and Spin-cloaking Based on bi-anisotropic Metamaterials

Science thrives on analogies, and a considerable number of inventions and discoveries have been made through making an unexpected connection to a very different field of inquiry. Perhaps one of the best known examples is that of photonic crystals (PhCs) that have been referred to as semiconductors of light because of the far-reaching analogies between electron propagation in a crystal lattice (the domain of condensed matter physicists) and light propagation in a periodically modulated photonic environment (the domain of engineers and applied physicists). More recently, photonic crystals have been followed in their footsteps by their close cousins: electromagnetic metamaterials. Metamaterials dramatically expand the space of possible electromagnetic responses enabling such exotic phenomena as negative index propagation and invisibility cloaking of macroscopic objects. However, one aspect of electron behavior, its spin, so far escaped emulation by photonic systems. Emulation of the electron spin and spin-orbit coupling which is known to give rise to one-way states will be reported in this talk. Using suitably designed electromagnetic media (metamaterials) we theoretically demonstrate a photonic analogue of a topological insulator. We show that meta-crystalssuperlattices of metamaterials with judiciously designed propertiesprovide a platform for designing topologically non-trivial photonic states, similar to those that have been identified for condensed-matter topological insulators. The interfaces of the meta-crystals support helical edge states that exhibit spin-polarized one-way propagation of photons, robust against disorder. Our results (Khanikaev et. al., Nature Materials 12, 233 (2013)) demonstrate the possibility of attaining one-way photon transport without application of external magnetic fields or breaking of time-reversal symmetry. Such spin-polarized one-way transport enables exotic spin-cloaked photon sources that do not ob-

scure each other.

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MS38

Causality of the Inverse of Causal Constitutive Parameters for Natural Materials and Metamaterials

Given a causal function, $\chi(x) - \chi(\infty)$, that satisfies the Kramers-Kronig relations, we determine the sufficient conditions for the related inverse function

$$\xi(x) = \frac{1}{\chi(x) - \chi(\infty) + 1} - 1$$

to also be a causal function that satisfies the Kramers-Kronig relations. For $\chi(\infty) = 0$, the function $\xi(x)$ corresponds to the inverse of the traditional continuum relative permittivity or permeability minus 1 and, in this case, a similar result is obtained by N.N. Meiman (see sec. 123 of *Statistical Physics, 3rd Ed.* by Landau and Lifshitz).

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MS39

The Chemo-mechanics of Cytoskeletal Force Generation

In this talk we will present an extension of our recent work on focal adhesion dynamics [Olberding, JE, Thouless, MD, Arruda, EM and Garikipati, K. The non-equilibrium thermodynamics and kinetics of focal adhesion dynamcs, PLoS ONE, 5(8), e12043, 2010] to address sub-cellular contractile force generation. The problem is a chemo-mechanical one, which is at mechanical equilibrium. The chemistry, however, is far from equilibrium. The mathematical model, computations and experimental comparisons will be shown.

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MS39

Coarse-grained Molecular Dynamics Modeling of the Disordered Domain of Nuclear Pores

The molecular transport between the cytoplasm and nucleus in eukaryotic cells is solely controlled by the nuclear pore complex (NPC). To gain insight into the transport mechanism, the conformation of the disordered proteins (FG-Nups) that cover the interior of the NPC is investigated through super-coarse-grained molecular dynamics simulations. The results show that the FG-nups adopt a unique conformation inside the pore which is encoded in the sequence of the FG-nups and driven by hydrophobic and electrostatic interactions.

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MS39

A Sequence-dependent Rigid Base Model of DNA, and its Continuum Birod Limit

A recent rigid base model of DNA (http:lcvmwww.epfl.ch/cgDNA) will be described, and its continuum birod limit (a generalization of the Worm Like Chain model) will be computed. Then various predictions of the model pertaining to crystal structure data, persistence length, and looping probabilities will be discussed.

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MS39

Torsion of Fluctuating DNA

We will present a heterogeneous fluctuating rod model for studying the statistical mechanics of DNA. We will interpret DNA torsion experiments where base pair level variation in mechanical properties is measured. The two key applications we consider are: (a) determine whether a newly discovered left-handed DNA conformation called L-DNA is a mixture of two known DNA states, and (b) what is the mechanical behavior of DNA when drugs and small molecules bind to it.

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MS40

Elastic Concertina and Tearing of Sheets

We consider a thin elastic film, pushed laterally up to a distance d, at one point of a rim of length W. We show experimentally and numerically that the "constitutive relation" of this system is more complex than a power law $F \sim (d/W)^n$, as previously assumed. When the ends of the rim are allowed to propagate via cracks, their evolution is determined by the way in which the film stores and releases elastic energy.

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MS40

Disclination Induced Wrinkles in Free Standing Smectic Membranes

The ability to create any curved surface merely by imprinting its metric onto a flat sheet has great appeal for use in materials, manufacturing, and diagnostics applications. The effects of topological defects and anisotropic elasticity in a free standing monolayer of cylinder-forming diblock copolymers generate curved surfaces. Disclinations prove to be sources of Gaussian curvature, which when coupled with surface tension and elasticity, produce a long-ranged pattern of wrinkles perpendicular to the underlying smectic layers.

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MS40
Geometry of a Crumpled Sheet

I will report on experiments in which we investigate the 3-dimensional spatial structure of crushed elastic and plastic sheets. One of the objectives of the experiments is to understand the effect of the protocol and boundaries imposed on the crumpling process. We follow the development of stress-focused structures as well as the emergent organization of structural elements, such as the condensation of planar facets. I will discuss the evidence for an ordering transition underlying the complex geometry of the object.

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MS40
Computational Crumpling via Discrete Developable Surfaces

When thin developable shells such as a sheet of paper or an aluminum can are crushed, they deform nearly isometrically, with stretching concentrated near ridges and cone points. We exploit this observation by discretizing the shell as an isometric embedding of a discrete developable surface – an r- and h-adaptive meshing of the development of the surface by discrete ridges and rulings. This reduced representation of the surface does not require the very fine elements needed to resolve the stiff stretching force, and does not suffer from membrane locking. We demonstrate that our method produces the familiar Yoshimura diamond patterns seen when axially compressing a thin cylindrical shell.

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MS41
Rare Event Simulations for Systems Far from Equilibrium

This talk will introduce steered transition path sampling (STePS), which allows efficient study of transient relaxation properties of microscopically irreversible dynamics. The method works by decomposing a trajectory in time, estimating the probability of satisfying a progress constraint, modifying the dynamics based on that probability, and then reweighting to calculate averages. I will demonstrate that the method outperforms others for selected problems and show its use in simulating a living system.

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MS41
A Micro / Macro Parareal Algorithm for a Class of Multiscale-in-time Systems

We introduce and analyze a micro/macro parareal algorithm for the time-parallel integration of a class of multiscale-in-time systems. The systems we consider includes some fast and some slow variables, the limiting dynamics of which (in the limit of infinite time scale separation) is known. The algorithm first computes a cheap but inaccurate macroscopic solution using a coarse propagator (by only evolving the slow variables according to their limiting dynamics). This solution is iteratively corrected by using a fine-scale propagator (simulating the full microscopic dynamics on both slow and fast variables), in the parareal algorithm spirit. The efficiency of the approach is demonstrated on the basis of numerical analysis arguments and representative numerical experiments. Joint work with T. Lelievre and G. Samaey.

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MS41
Transition Path Sampling

We are investigating collections of atoms as their positions evolve under Brownian (over-damped Langevin) dynamics. In the cases where the collection changes conformation, an energy barrier often exists. Such transitions are rare events when the thermal energy is small compared to the energy barrier. The understanding of such rare events is the goal of our studies. I will display some results for transitions in small atomic clusters.

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MS41
Reaction Pathways of Metastable Markov Chains with Application to Lennard-Jones Clusters Reorganization

Abstract not available at time of publication.

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MS42
Analyzing Upper Tails of Grain Size Distributions Using Extreme Value Theory

Polycrystalline materials generally display grain size distributions thought to correspond to the log-normal distribu-

tion. While the grains size distribution near the mean is often lognormal, significant tail departure from log-normality is observed for extreme values. Due to the importance of large grains in applications such as fatigue, understanding the distribution of extreme values beyond the assumption of complete log-normality is necessary. We present a method to fit the upper tail of grain size distributions based on extreme value theory. The method fits the grains sizes above a chosen threshold value to the generalized Pareto distribution (GPD). The fitted GPD allows for the probability for particular extreme grain sizes to be calculated.

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MS42

Finding Order in Disorder: Shape Matching and Other Tricks

Abstract not available at time of publication.

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MS42

Modeling Heterogeneous Materials via Lower-order Spatial Correlation Functions Extracted from Limited Experimental Data

Heterogeneous materials abound in nature and synthetic situations. Examples include porous media, composites and alloys. It is well known that the effective properties of heterogeneous materials depend on their complex microstructures, which can be characterized via certain statistical descriptors (spatial correlation functions). Here, I will present an efficient computational procedure that enables one to generate virtual 3D material microstructure from a wide class of correlation functions, obtained either from 2D slices/surface images of the sample or from scattering experiments. The accuracy of the reconstruction is ascertained by quantitatively comparing it to the actual microstructure obtained via x-ray tomography. Our reconstruction procedure is employed to characterize an anisotropic multiphase Al-alloy, to model microstructure evolution in a Pb-Sn alloy during annealing, and to study microphase separation in a nano-porous material. These examples show that our procedure enables one to model a wide class of heterogeneous materials via the associated spatial correlation functions.

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MS42

Fast Automated Detection of Crystal Distortion and Crystal Defects in Polycrystal Images

Given an image of an atomic crystal, we propose a variational method which at each image location determines the local crystal state and which localizes and characterizes crystal defects. In particular, the local crystal orientation and elastic distortion are detected, as well as dislocations, and grain and twin boundaries. To this end an energy functional is devised whose minimization yields a tensor field G describing the local crystal strain at each point. The desired information about the local crystal state can then be read off from this tensor field; in particular, its curl provides information about grain boundaries and dislocations. As is typical for variational image processing, the energy functional is composed of a fidelity and a regularization term. It has a simple L^2-L^1 type structure so that its minimization can be performed via a split Bregman iteration. GPU parallelization results in short computing times.

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MS43

Analysis of Liquid Crystal Phase Transitions in Biological Networks

Cytoskeletal networks consist of rigid, rod-like actin protein units jointed by ?exible crosslinks, presenting coupled orientational and deformation effects analogous to liquid crystal elastomers. The alignment properties of the rigid rods influence the mechanical response of the network to applied stress and deformation, affecting functionality of the systems. Parameters that characterize these networks include the aspect ratio of the rods and the average length of the crosslinks, with a large span of parameter values found across in-vivo networks. For instance, cytoskeletal networks of red blood cells have very large linkers and small rod aspect ratio, whereas those of cells of the outer hair of the ear have large aspect ratio and short linkers favoring well aligned nematic, in order to achieve optimal sound propagation. We propose a class of free energy densities consisting of the sum of polyconvex functions of the anisotropic deformation tensor and the Landau-de Gennes energy of lyotropic liquid crystals. The growth conditions of the latter, with respect to the rod density and the nematic order tensor at the limit of the minimum eigenvalue -1/3 are essential to recover the limiting deformation map from the minimizing sequences of the anisotropic deformation gradient. We consider a bulk free energy density encoding properties of the rod and the network based on the Lopatina-Selinger construction for the Maier-Saupe theory. We then analyze the phase transition behavior under uniform expansion, biaxial extension and shear deformation, showing that the nematic-isotropic transition may be accompanied by a change of volume, which manifests itself in the nonconvexity of the stress-strain relation. We also account for the fact that in-vivo networks are found in the gel state. We conclude with some remarks on the roles of active elements in the model.

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MS43

Liquid Crystals: Revisiting Kinetic Equations and

Picking the Best Order Parameters

I will review the general problem of deriving mean-field and kinetic equations from microscopic dynamics in the context of nematic liquid crystals. Analytical results will then be compared to numerical studies of the defect core structure.

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MS43

Chevron-Like Defects in Smectic Liquid Crystals

We investigate the structure of a smectic C liquid crystal body trapped between two parallel plates. This is modeled using the Chen-Lubensky energy that couples a second order energy that accounts for smectic layer formation and the first order nematic Frank energy. In the smectic C phase the smectic layers meet the plates at an acute angle. In order for this to happen the layers' profiles should form a zig-zag or chevron pattern. We prove that these patterns occur in minimizers for this model, for the case that the layer bending constant is small. This is carried out by using gamma convergence.

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MS43

Efficient Energy Stable Numerical Schemes and Simulations of Two Phase Complex Fluids on Phase Field Method

Our goal here is to expand the hydrodynamic toolkit to two-phase fluids consisting of an immiscible homogeneous LCP phase (initialized as droplets) immersed in a viscous or polymeric phase. To do so, we first put the two-phase kinetic model through the same preliminary benchmarks that were applied to the Doi-Hess theory for LCPs. We project onto the scalar zeroth moment and tensorial second-moment of the rod number density function to achieve a generalized Landau-deGennes model for equilibria and imposed shear of LCP droplets in a viscous fluid. A numerical algorithm in two space dimensions is developed to study global droplet defect structure versus interfacial anchoring energy. The simulations reveal topological defects (surface boojums for tangential anchoring and interior degree 1/2 or radial defects for normal anchoring), as well as new predictions about the structure of the various defect cores in equilibrium and in simple shear.

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MS44

Capillary Fracture of Soft Gels

A droplet of surfactant spreading on a gel substrate can fracture the gel surface and create a starburst pattern of fracture arms. We develop an elastic model to predict the number of fractures, consistent with experimental results. In experiments, the arm length grows with universal power law $L = t^{3/4}$, which we understand via a model for the transport of an inviscid fluid into the fracture tip of an incompressible Neo-Hookean material.

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MS44

Thin Film Models of Liquid Displacement on Chemically Patterned Surfaces for Lithographic Printing Processes

We examine in this work a model problem relevant to the liquid displacement that occurs in lithographic printing processes. The model problem consists of two stratified thin liquid films confined between parallel plates, one of which is chemically heterogeneous. The results provide physical insights into and numerical estimates of the smallest and largest feature sizes that can be printed, as well as the minimum spacing between feature sizes that can be tolerated.

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MS44

Boundary Conditions for the Moving Contact Line Problem and the Spreading of Thin Films

In this talk, I will discuss a contact line model derived based on principles of non-equilibrium thermodynamics and molecular dynamics simulations. Macroscopic thermodynamic is used to place constraints on the form of the boundary conditions; the detailed constitutive relations are then computed from molecular dynamics. The contact line model consists of the Navier-Stokes equation, a boundary condition for the slip velocity, and a relation between the dynamic contact angle and the contact line velocity. A thin film model is formulated based on lubrication approximation, and different spreading regimes are identified.

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MS44

Electrostatically Induced Singular Dynamics in Long-Wave Annular Film Flows

We investigate the evolution and stability of a viscous, leaky dielectric fluid layer wetting the surface of a cylindrical electrode, surrounded by a leaky dielectric gas and a concentric electrode. Electrostatic forces are induced at the interface in competition with surface tension and viscous stresses. Asymptotic methods are used to derive a one dimensional long-wave system of evolution equations that exhibit a wide variety of dynamics including the formation

of finite time touchdown singularities.

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MS45
On the Nonlinear Dynamics of Granular Lattices

We investigate on the highly nonlinear propagation of solitary waves in one and two dimensional granular lattices, with particular focus on the control of stress propagation for the development of shock protecting devices. The analysis included discrete particle approaches and the corresponding continuum limits. The study discloses composite granular structures that enable forced energy confinement and transverse pulse-trapping within the granular matter. The granular medium converts transverse impacts into shifted superficial pulses with weak amplitude, thus acting as a pulse-trapping device and energy container.

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MS45
The p-Schrdinger Equation and Granular Crystals

We consider a Hamiltonian lattice consisting of a chain of particles in a local potential, coupled by fully-nonlinear nearest-neighbors interactions of order $\alpha > 1$. This system describes in particular a Newton's cradle, i.e. a chain of beads attached to pendula and coupled by Hertzian contact. We show that the evolution of small initial data is governed by the discrete p-Schrödinger equation (involving a p-Laplacian with $p = \alpha + 1$), which yields the existence of breathers.

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MS45
Inertia-Induced Criticality in Martensites

Intermittency and power law statistics of avalanches have been recorded in several martensitic materials subjected to cyclic loading. It implies long spatial and temporal correlations whose origin is still unclear. It has been proposed previously that behind such self organization towards criticality is a limited dislocational activity. In this talk we discuss an alternative explanation based on an idea that inertia may play an important role in marginally stable systems. We consider a prototypical quasi-statically driven lattice system with double well energy and show that the power law correlations with realistic exponents can appear in this model if it is moderately under-damped. Joint work with U. Salman.

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MS46
Effective Behavior of Interfaces in a Random Elastic Medium

We consider a model for the propagation of an interface in a random elastic medium. From a physical point of view, we answer the question whether a microscopically viscous (force=velocity) dynamics transitions into a macroscopically rate independent hysteresis through the interaction with the obstacles. mathematically, the problem consists of finding a stationary supersolution to a fractional diffusion equation which is coupled nonlinearly to a random field.

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MS46
From Polymer Physics to Rubber Elasticity: a Stochastic Homogenization Approach

Rubber materials are prototypical examples of hyperelastic materials, best described at the continuum by the integral of a frame-invariant and isotropic energy density of the strain gradient. On a microscopic scale, rubber materials are constituted by a network of interacting polymer-chains, best described by their Boltzmann free energy. The aim of this talk is to give the first steps towards a rigorous derivation of rubber elasticity from polymer-chain physics using a qualitative and quantitative discrete homogenization theory of random graphs. I shall focus both on the theoretical and computational aspects. high-level commands.

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MS46
Macro and Micro-Based Solutions for Random Heterogeneous Microstructures

At small scale, material properties fluctuate randomly in space and are usually described by random functions. At the scale of the representative volume element, material properties are deterministic and independent of boundary conditions under some assumptions. Quantities of interest, $U_{micro}(x)$ and $U_{macro}(x)$, based on material properties at micro- and macro-scales are random fields and deterministic functions, respectively. We view $U_{macro}(x)$ as an approximation for $U_{micro}(x)$ and examine the quality of this approximation.

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MS46
On a Class of weakly Stochastic Problems

Amenable to Rapid Computational Approaches in Stochastic Homogenization

We define and describe a class of problems in stochastic homogenization that, in a sense made precise, are only "weakly" stochastic. Dedicated approaches can then be applied, that significantly reduce the computational workload. We also mention how the approach can be useful to reduce variance in actually fully (that is, non "weakly) stochastic problems. All the equations and examples are issued from materials science.

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MS47

Model Reduction and Recovery of Structural Information in Heterogeneous Materials

The talk discusses reconstruction of the spectral measure in the Stieltjes integral representation of the effective properties of composite materials using Pade approximation. We consider a case of matrix valued measure corresponding to anisotropic composites. Matrix Pade approximants are derived using matrix polynomials orthogonal with respect to the spectral function. We discuss applications to inverse homogenization theory and to numerical simulation of propagation of waves in composites.

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MS47

Approximation of DtN Map in a High Contrast Conductivity Problem

A model of a composite material consisting of a matrix of finite conductivity with ideally conducting almost touching particles is considered, and a discrete network approximation for the Dirichlet-to-Neumann map is constructed and justified.

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MS47

Scattering and Resonances of Electromagnetic Waves by Thin High Contrast Dielectric Structures

We study the scattered electric field from a thin, high-contrast dielectric volume. The space occupied by the scatterer is the Cartesian product of a bounded two-dimensional region with a finite interval; that is, the scatterer is cylindrical, and of finite volume. The electric field is a solution of the time-harmonic Maxwell equations. We will discuss four theorems. In the first, we establish an integral representation for the electric field which accounts for the jumps in the index of refraction which occur at the object boundary. This integral representation includes a surface integral over the boundary of the object. In our second theorem, we find an explicit formula for the limit as the thickness of the scatterer vanishes for the operator associated to this surface integral. In our third and fourth theorems, we demonstrate that under some uniform regularity assumptions, the normal trace of the electric field on the object boundary goes to zero as the thickness of the object goes to zero simultaneously as the contrast goes to infinity. This is joint work with David Ambrose.

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MS47

The Underlying Analytical Links Between Various Effective Coefficients of a Poroelastic Medium: a Dehomogenization Approach

Poroelastic materials are finely-structured composites of pore fluid and elastic solid, which are encountered very often in geophysics and biophysics. This talk is based on our preliminary results on how to use the analytic properties of effective properties of poroelastic composites to quantify the effect of microstructure on the dynamics of wave propagation in poroelastic materials described by the Biot-JKD model.

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MS48

A General Constitutive Framework for Modeling Elasto-Visco-Plastic Behavior, Yielding and Thixotropy in Waxy Crude-Oils, Microgels and Other Soft Solid Materials

Abstract not available at time of publication.

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MS48

Mathematical Modeling of the Mucus Barrier in Human Lungs

The first line of defense of human lungs against inhaled pathogens is mucus. Foreign particles are cleared if flow of the mucus layer toward the larynx dominates particle diffusion through the layer. Yet the flow and diffusive transport properties of mucus is poorly understood. Here we focus on progress understanding nonlinear phenomena in the oscillatory flow of viscoelastic fluids, and explaining why dynamic and spatial microstructural characterization is essential in the understanding of mucus transport.

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MS48

Modeling and Simulation of Complex Biological Fluids Biofilms

Biofilms are complex biological organisms ubiquitous almost everywhere in our daily life. Modeling and understanding the intricate biological, fluid mechanical, chemical-mechanical transduction of chemical signal and mechanical forces is a daunting task across multiple disciplines. In this presentation, we will present a systematic approach tooted in kinetic theory for complex fluids and expanded to include various biological and chemical mechanistic models to investigate how the biofilm flows in various geometry and boundary conditions. Hopefully, this will shed light on how to treat biofilm infections in medical settings or take advantage of the biofilm's barrier properties in their beneficial applications. Models and 3-D numerical simulations will be discussed in a few selected applications.

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MS49

Wrinkles on Curved Surfaces for Aerodynamic Drag Control

We present the results of an experimental investigation on the wrinkling of positively curved surfaces and explore their use towards drag reduction applications. In our precision model experiments we make use of rapid prototyping techniques to cast samples with custom geometry and material properties out of silicone-based rubbers. Our structures consist of a thin stiff shell that is chemically bonded to a thicker soft substrate. The substrate contains a spherical cavity that can be depressurized, under controlled volume conditions, to compress the ensemble structure. Under this compressive loading, the initially smooth outer-shell develops complex wrinkling patterns. We systematically characterize and quantify the morphology of the various patterns and study the phase diagram of the system. We consider both geometric and material quantities in the parameter space. Moreover, since the wrinkling patterns can be actuated dynamically using a pressure signal, we systematically characterize the aerodynamic behavior of our structures in the context of fluid drag reduction. An added advantage of our novel mechanism is that it allows for both dynamic switching and tuning of the surface morphology, thereby opening paths for drag control.

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MS49

The Wrinkle Patterns Caused by a Drop on a Sheet

Recent interest in the behavior of thin sheets far beyond the buckling threshold was inspired by experiments wherein a liquid drop was placed on a thin elastic sheet. Compressive forces due to surface tension effects created a wrinkle pattern near the contact line. We provide the first completely "far-from-threshold" analysis of this configuration, and predict the measured extent of the wrinkles. We also show that the liquid-solid contact angle is different from the Young-Lapace angle.

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MS49

Plate and Shell Models in Elasticity Obtained by Simultaneous Momogenization and Dimensional Reduction

We will give an overview of the models of plates and shells obtained by simultaneous homogenization and dimensional reduction from 3D nonlinear elasticity, by means of Gamma convergence. We will give the special emphasis on the homogenized bending plate model. This is collaboration with P. Hornung and S. Neukamm.

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MS49

Poking and Wrinkling of Thin Sheets and Shells

Poking an object is a useful way of testing its properties in a range of everyday applications from cooking meat to inflating a bicycle tyre. It is also used quantitatively in science to achieve the same thing. In this talk I will discuss what we can learn from poking pressurized elastic shells and floating elastic sheets. Of particular interest is the wrinkling pattern that forms in these scenarios. I will discuss these patterns from both the 'Near Threshold' and 'Far From Threshold' points of view.

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MS50

A Boundary Integral Method for Computing the Dynamics of An Epitaxial Island

At the early stages of epitaxial growth, adatoms on the substrate often form small isolated islands. The morphological evolution (e.g. growth or shrink) of these islands is determined by many physical processes such as atom adsorption and desorption, adatom diffusion, adatom attachment to island boundaries or detachment from the boundaries. Mathematical formulation of the problem leads to a moving boundary/interface problem. In this talk, we present a boundary integral method for computing the quasisteady evolution of an epitaxial island. The problem consists of an adatom diffusion equation (with desorption) on terrace and a kinetic boundary condition at the step (island boundary). The normal velocity for step motion is determined by a

two-sided flux. Numerical tests on a growing/shrinking island are in excellent agreement with the analytical solution and demonstrate that the method is stable, efficient and spectrally accurate in space.?Nonlinear simulations for the growth of perturbed circular islands show that sharp tips and facet-like edge will form during growth instead of the usual tip-splitting events for isotropic Laplacian growth. The numerical techniques presented here can be applied generally to a class of free/moving boundary problems in physical and biological science.

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MS50

Multiscale Modeling and Computation of Nano Optical Responses

We introduce a new framework for the multiphysical modeling and multiscale computation of nano-optical responses. The semi-classical theory treats the evolution of the electromagnetic field and the motion of the charged particles self-consistently by coupling Maxwell equations with Quantum Mechanics. To overcome the numerical challenge of solving high dimensional many body Schr odinger equations involved, we adopt the Time Dependent Current Density Functional Theory (TD-CDFT). In the regime of linear responses, this leads to a linear system of equations determining the electromagnetic eld as well as the current and electron densities simultaneously. A self-consistent multiscale method is proposed to deal with the well separated space scales. Numerical examples arepresented to illustrate the resonant condition.

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MS50

Dislocation Dynamics in Thin Films Using Fast Multipole Accelerated Boundary Integral Equation Method

We develop an efficient numericalmethod based on the boundary integral equation formulation and new version of fast multipole method to solve the boundary value problem for the stress field associated with dislocations in a finite medium. Numerical examples are presented to examine the influence from material boundaries on dislocations. Applications to dislocation dynamics in thin films will also be presented.

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MS50

Simulation on Liquid Crystal Elastomers Using Spectral Methods with a New Preconditioner

Liquid crystal elastomers (LCEs) are soft complex materials of enormous technological importance because of their remarkable responsiveness to excitations. In our previous work, we proposed a non-local continuum model to study the dynamical behaviors of LCEs. The preliminary simulation demonstrated that the model can successfully capture the shape changing phenomena observed in real experiments and other features of LCEs. However, due to the complexity of governing equations, the simulation is very time-consuming. In this talk, we introduce a novel preconditioner for solving the velocity equation using Chebyshev spectral collocation method and present new simulations to show its efficiency.

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MS51

Phase Field Crystal Models with Fast Dynamics

Abstract not available at time of publication.

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MS51

Nonlocal Phase Field Models

Abstract not available at time of publication.

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MS51

Some Equations with a Logarithmic Nonlinear Term

Abstract not available at time of publication.

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MS51

Phase Field Models of Vacancy Mediated Deformation

Abstract not available at time of publication.

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MS52

Magnetic Ratchet for 3-dimensional Memory and Logic

One of the major challenges for future electronic memory and logic devices is finding viable ways of moving from todays 2-dimensional structures which hold data in an XY mesh of cells to 3-dimensional structures in which data are stored in an XYZ lattice of cells. This could allow a many-fold increase in performance. A suggested solution is the shift register - a digital building block that passes data from cell to cell along a chain. In digital microelectronics, 2-dimensional shift registers are routinely constructed from a number of connected transistors. However, for 3-D devices the added process complexity and space needed

for such transistors would largely cancel out the benefits of moving into the third dimension. Physical shift registers, in which a low-level physical phenomenon is used to move data near-atomic distances, without requiring conventional transistors, are therefore much preferred. We have discovered a way of implementing a 3-dimensional spintronic unidirectional vertical shift register between sub-nanometer thickness perpendicularly magnetized CoFeB layers similar to those used in MRAM. By carefully controlling the thickness of each magnetic layer and the RKKY exchange coupling between layers we form a ratchet which allows information in the form of a sharp magnetic kink soliton to be pumped unidirectionally from one magnetic layer to another. In this talk I show experimental results from a 44-layer sample in which digital bits are injected into the bottom layer and then progressively shifted from layer to layer before emerging from the top. This simple and efficient shift-register demonstrates a route for spintronics to be used to create 3-dimensional microchips for memory and logic applications.

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MS52
The Spin-Cherenkov Effect

We report on the Cherenkov-type excitation of spin waves in soft-magnet magnetic thin film elements. Our simulations show that a point-like magnetic field source moving with sufficiently high velocity above the film surface generates a spin wave "boom", propagating along a Mach-type conical wave front. This Spin Cherenkov Effect enables the excitation of well-defined spin waves with velocity-dependent frequency by means of a linearly moving perturbation, thereby providing a simple route towards tunable spin-wave generation.

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MS52
Rotating Vortex-Antivortex Pairs in Ferromagnets under Spin-Polarized Current

A rotating *vortex-antivortex dipole* may be generated due to spin-polarized current flowing through a magnetic element. We study its dynamics within the Landau-Lifshitz-Gilbert-Slonczewski equation. The rotation is due to *two forces:* the interaction between the two vortices and an external in-plane magnetic field. The nonzero *skyrmion number* of the dipole is responsible for both forces giving rise to rotational dynamics. The spin-torque acts to stabilize the steady state.

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MS52
Analysis of Complex Domain Patterns in Bulk Ferromagnets

The rich world of magnetic domains, extending from visible dimensions down to the nano-scale, forms the mesoscopic link between the fundamental physical properties of a magnetic material and its macroscopic properties typically measured in a hysteresis loop. Most challenging is the analysis of hidden (internal) domains in bulk material, which requires surface imaging in combination with domain modeling. In this presentation a review of (experimental) bulk domain analysis is given, based on surface domain observation by Kerr microscopy, metallographic domain analysis and neutron imaging.

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MS53
Variational Analysis of Some Atomistic Systems Exhibiting Spatially-modulated Phases

I will present some results concerning the continuum Gamma-limit of a family of atomistic systems exhibiting spatially-modulated phases

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MS53
Microstructures in Nematic Elastomers

Abstract not available at time of publication.

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MS53
Continuum Limit of Microscopic Models of Solids

Abstract not available at time of publication.

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MS53

Lattice Equivalent Models

We investigate the macrocospic behavior of hexagonal lattices. We obtain a non explicit formula for the equivalent energy density. Numerical computation tends to prove that this homogenized formula cannot be replaced by a simpler expression. Additionnaly, numerical simulations show that in most cases Cauchy-Born rule fails to give the proper behavior.

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MS54

Equilibrium vs. Kinetic Steady States in Epitaxial Growth

Abstract not available at time of publication.

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MS54

Phase Field Modeling of Epitaxial Graphene Growth

Abstract not available at time of publication.

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MS54

Lattice and Off-lattice KMC Models for Strained Epitaxial Growth

We present weakly off-lattice and off-lattice kinetic Monte Carlo formulations for strained epitaxial growth. We have implemented the weakly off-lattice method in 2+1 dimensions and it is capable of realizing many experimentally observed features. The off-lattice method has been implemented in 1+1 dimensions with a Lenard-Jones potential. This method is able to simulate Stranski-Krastanov growth, and capture the formation of edge dislocations, interstitials, and vacancies.

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MS54

Analytical Study of Morphology of Strained Films: Role of Misfit and Volume

Abstract not available at time of publication.

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MS55

A Multiscale Atomistic-to-Continuum Method for Atomic Monolayers Undergoing Bending

The framework of Objective Structures introduced by Richard James provides a method to systematically examine the behavior of various geometrically complex nanostructures. These nanostructures include rod-like objects as well as flat sheets. In this talk, we describe an extension of this framework to sheets that undergo bending in complex ways. We then apply the extended framework to develop a computational atomic multiscale method to understand the atomic structure of defects in these systems.

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MS55

Estimates for Two-phase Nonlinear Conductors via Iterated Homogenization

Estimates for the overall response of two-phase nonlinear conductors are derived via an iterated homogenization approach. The approach consists in the construction of sequentially laminated microgeometries for which the overall response can be determined exactly. The estimate depends on the one- and two-point microstructural correlations through the volume fractions of each constituent phase and the H-measures of the microstructure. Sample results for power-law random conductors are provided and compared with earlier predictions. We conclude with a discussion on the possible extremal character of sequential laminates in the nonlinear context.

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MS55

Sharp Inequalities which Generalize the Divergence Theorem

Subject to suitable boundary conditions being imposed, sharp inequalities are obtained on integrals over a region Ω of certain special quadratic functions $f(E)$ where $E(x)$ derives from a potential $U(x)$. This has application to bounding the response of bodies containing an inclusion, and inversely to estimating the volume of the inclusion. With $E = \nabla U$ it is known that such sharp inequalities can be obtained when $f(E)$ is a quasiconvex function and when

U satisfies affine boundary conditions (i.e., for some matrix D, $U = Dx$ on $\partial\Omega$). Here we allow for other boundary conditions and for fields E that involve derivatives of a variety orders of U. We also treat integrals over Ω of special quadratic functions $g(J)$ where $J(x)$ satisfies a differential constraint involving derivatives with, possibly, a variety of orders. The results generalize an example of Kang and the author in three spatial dimensions where $J(x)$ is a 3×3 matrix valued field satisfying $\nabla \cdot J = 0$. We also present an algorithm for generating extremal quasiconvex quadratic functions.

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MS55

Homogenization of Generalized Micro-Resonances and Coupled Properties

Abstract not available at time of publication.

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MS56

Energy Barriers for Interior Nucleation of Martensite

The phase transformation between martensite and austenite is typically accompanied by the creation and growth of small inclusions of the new phase. We consider geometrically linear elasticity with sharp interface penalization of phase boundaries. Following earlier work, we present matching upper and lower bounds for the elastic energy of these inclusions in terms of the volume. The methods are based both on real and Fourier space representation of the energy.

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MS56

Hysteresis in Thermodynamically-Consistent Mesoscopic Model of the Ferro/paramagnetic Transition

A continuum model for micromagnetics is presented that, beside the standard magnetic balance laws, includes thermo-magnetic coupling. Inspired by relaxation method of static minimization problems, our model is mesoscopic in the sense that possible fine spatial oscillations of the magnetization are modeled by means of Young measures. Existence of weak solutions is proved by backward Euler time discretization. It is a joint work with B. Benesova and T. Roubicek.

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MS56

Mathematical Analysis of Microstructures in Low-Hysteresis Shape Memory Alloys: Onset of Complex Patterns

Experimental findings suggest that the compatibility of the highly symmetric austenite phase and the martensitic variants is an important parameter controlling the width of the thermal hysteresis in certain martensitic transformations. This observation forms the basis of a theory of hysteresis that assigns an important role to the energy of the transition layer (Zhang, James, Mueller, Acta mat. 57(15):4332-4352, 2009). Following this ansatz, we study analytically the energy barriers leading to hysteresis and analyze the onset of complex microstructures in the transition layers for low-hysteresis alloys.

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MS57

Hybrid Continuum-Particle Thermostats based on Fluctuating Hydrodynamics : Dynamic Implicit-Solvent Coarse-Grained Simulations of Planar Lipid Bilayers and Vesicles

Many coarse-grained models have been developed for efficient equilibrium studies of lipid bilayer membranes by treating implicitly interactions mediated by the solvent. However, for problems involving dynamics, such CG studies require accounting for the momentum transfer through the missing solvent degrees of freedom. We introduce new thermostats for such CG models and computational methods based on fluctuating hydrodynamics. We show our momentum conserving approach yields results significantly different than conventional Langevin dynamics. We then present a number of simulation results both for self-assembled planar-bilayer sheets and vesicles.

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MS57

Regularization Method for the Numerical Solution of Periodic Stokes Flow With Application to Ciliary Beating

In this talk, I will introduce a regularization method that gives a smooth formulation for the fundamental solution to Stokes flow driven by an infinite, triply-periodic array of point forces. With this formulation, the velocity at any spatial location may be calculated, including at and very near the point forces; these locations typically lead to numerical difficulties due to the singularity within the Stokeslet when using other methods. For computational efficiency, the current method is built upon previous methods in which the periodic Stokeslet is split into two rapidly decaying sums, one in physical space and one in reciprocal, or Fourier, space. I will show a few validation studies and then discuss a recent extension of the method to doubly-periodic flow. Finally, using the extended method, simulations of doubly-periodic arrays of beating cilia will be presented.

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MS57

Modeling Neutralization Kinetics of HIV by Broadly Neutralizing Monoclonal Antibodies

Eliciting broadly neutralizing antibodies (bnAb) in cervicovaginal mucus (CVM) is potentially a critical aspect of an HIV vaccine that blocks initial vaginal HIV infections. To neutralize HIV in the vaginal lumen, bnAb must accumulate on virions at sufficient stoichiometry to inhibit viral entry before virions penetrate CVM and infect target cells in the submucosa. Nevertheless, the relative rates of these competing processes remain poorly understood. In this talk I will highlight our existing work to model these dynamics with an eye toward some of the unsolved problems that would benefit from an improved description of the basic particle-fluid coupling.

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MS57

A Computational Model of Microtubule-Based Motion in the Single-Celled C. Elegans Embryo

We present a model of microtubule-based pronuclear motion in the Caenorhabditis elegans embryo. Microtubules stochastically grow/shrink, encountering motor proteins in the viscous cytoplasm that attach and exert pulling forces. Our computational method is based on an immersed boundary formulation that allows for the simultaneous treatment of fluid flow and the dynamics of structures immersed within. Our simulations demonstrate nuclear centration and rotation, while generating minus-end directed flows along MTs similar to those observed in vivo.

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MS58

Metric Description of Discontinuities in Amorphous Elastic Materials

We suggest a description for dislocations using a torsion-free Riemannian manifold equipped with a reference metric. This metric expresses the local equilibrium geometry within the material. In this description, dislocations are singularities in the intrinsic curvature structure. The model is not based on a crystalline structure; therefore it can describe dislocations even in amorphous materials. We provide explicit expression for edge dislocation, which is a dipole of curvature. The model is supported with experimental results.

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MS58

Monge-Ampère Constraints in Thin Film Elastic Models

We will review a few results and some open problems regarding the variational model of thin films consisting in minimizing the bending energy $\int_\Omega |\nabla^2 u|^2$ of an out-of-plane displacement $u : \Omega \to R$ under the Monge-Ampère constraint $\det \nabla^2 u = f$, where f is a prescribed curvature function and $\Omega \subset R^2$ represents a thin plate.

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MS58

Growth-Induced Folding, Conformal Maps, and Optimal Design

I will discuss the growth-induced buckling of sheets with zero Gaussian curvature except at discrete points. This simplified problem already shows the hallmarks of more complicated swelling patterns, yet appears to be tractable. This sheds some light on the problem of finding "optimal" swelling patterns for complex shapes that can be implemented experimentally.

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MS58

Emergence of Spontaneous Twist and Curvature in Non-Euclidean Rods: Application to Erodium Plant Cells

We present a limiting model for thin non-Euclidean elastic rods. Originating from the three-dimensional (3D) reference metric of the rod, which is determined by its internal material structure, we derive a 1D reduced rod theory. Specifically, we show how spontaneous twist and curvature of a rod are emerged from the reference metric derivatives. Thus, the model allows calculating the unconstrained equilibrium configuration of a thin rod directly from its internal structure. The model is applied to the study of stork's bill and cranesbill cells and their configurational response to dehydration. We show how the geometrical arrangement of cellulose fibrils on the cell walls determines the helical

shapes of isolated cells.

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MS59

Nonequilibrium Processes for Current Reservoirs

Stationary non equilibrium states are characterized by the presence of steady currents flowing through the system. Currents are produced by external forces and we are interested in forces acting on the boundary trying to establish a given current. We model this process considering the simple exclusion process in one space dimension with appropriate boundary mechanisms which create particles on the one side (right) and kill particles on the other (left). The system is then "unbalanced" and in the stationary measure there is a non-zero steady current of particles flowing from right to left. The system is designed to model Fick's law which relates the current to the density gradient. In statistical mechanics non-equilibrium is not as well understood as equilibrium, hence the interest from a physical viewpoint to look at systems which are stationary yet in non-equilibrium: in our case the stationary process is in fact non-reversible and the stationary measure not Gibbsian. In this presentation we give an overview of the results we obtained in collaboration with Anna De Masi, Errico Presutti and Maria Eulalia Vares. We prove that the hydrodynamic limit is given by the linear heat equation with Dirichlet boundary conditions obtained by solving a non-linear equation which essentially fixes the values of the density at the boundary. Then we show that the rescaled limiting density profile of the (unique) invariant measure of the process coincides with the unique stationary solution of the hydrodynamic equation. Last, we obtain a spectral gap estimate in the (non equilibrium) stationary process uniformly on the system size.

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MS59

Covariant Statistical Theory of Phase-Ordering Kinetics via Emergent Symmetries

The emergent symmetry group of a non-equilibrium phase-ordering system is shown to naturally provide a covariant action on the associated universal coarsening statistics. Our *Covariant Universality Theory* ($\mathcal{CUT}$) naturally subsumes the classical *Dynamic Scaling Hypothesis*. To exhibit $\mathcal{CUT}$'s utility, a certain non-equilibrium, nano-faceting crystal growth model is considered. Combining the discovery of exact thermo-kinetic translating solitons, which violate the Wulff construction, with a novel, generally applicable, asymptotic geometric methodology, we identify an emergent Super-symmetric Lorentzian-Parabolic symmetry group G. The resulting G-covariant universal, 1-point length statistics are then completely characterized up to a unique supra-universal, empirically determined distribution.

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MS60

Exponential Convergence to Equilibrium for Subcritical Solutions of the Becker-Dring Equations

The Becker-Dring equations are a well-known model for nucleation and growth. We show that solutions with mass under the critical one converge exponentially to equilibrium. Our main tool is a study of the linearization of the equation close to equilibrium, for which we are able to show a spectral gap. We use several techniques that have been developed in the context of kinetic equations, and find strong parallels with the study of the homogeneous Boltzmann equation.

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MS60

Coarsening for the Diffusive Carr-Penrose Model

The Carr-Penrose (CP) model is a linear model of coarsening which has many similar features to the non-linear and physically important LSW model. In their original 1998 paper Carr and Penrose showed that their model has a family of self similar solutions and that self-similar solutions are globally asymptotically stable in some sense. In a 2008 paper Smereka considered solutions to a discrete approximation of the CP model with initial data of finite support. He proved that these solutions converge at large time to a particular self-similar solution of the CP model. The result confirms the intuition that diffusion provides a selection principle for the physically relevant self-similar solutions of this class of coarsening models. In the case studied by Smereka effective diffusion is provided by the discretization. This talk is concerned with the model obtained by adding a second order diffusion term to the first order PDE of the CP model. The speaker will discuss some recent progress in understanding coarsening behavior for this model. The work is joint with Jingchen Wu.

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MS60

Motion of Interfaces Under the Cahn-Hilliard Equation with One or Two Sided Degenerate Diffusion Mobility

We use the asymptotic matching method to study the motion of interfaces in two phase systems governed by Cahn-Hilliard type equations with one or two-sided degenerate diffusion mobilities. We find that there is a nonlinear diffusion process that solves a quasi-stationary porous medium equation in the phase(s) where the mobility degenerates, which is the mechanism for such systems to coarsen. When the mobility is disparate, scaling arguments suggests a crossover in the coarsening rate from $t^{1/3}$ to $t^{1/4}$.

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MS60

Self-similar Solutions to Coagulation Equations

In this talk I will describe some methods which allow to obtain qualitative information about self-similar solutions of the coagulation equations. For some specific kernels it is possible to derive very detailed asymptotics. General estimates concerning the behaviour of the solutions for a large class of kernels for small and large values of the argument of the solutions will be also discussed.

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MS61

Navigating Energy Landscapes in Ginzburg-Landau Problems with Long-Range Interactions

Energy-driven pattern formation induced by competing short and long-range interactions is common in many physical systems. A nonlocal perturbation (of Coulombic-type) to the well-known Ginzburg-Landau/Cahn-Hilliard free energy gives rise to a mathematical paradigm with a rich and complex energy landscape. I will discuss some recent work on developing methods for (i) assessing whether or not a particular state is a global minimizer and (ii) navigating from metastable states to states of lower energy.

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MS61

Projection Valued Functions on Perforated Domains in the Plane

We study the minimizers of the Dirichlet integral among (rank 1, orthogonal) projection valued maps in a perforated domain in the plane, subject to a Dirichlet condition on the outer boundary. We assume that the boundary condition represents a non-contractible curve on the set of such projections. When the size of the perforation (which is a disk) goes to zero, we obtain an expression for the limits of the minimizers, which depends only on the location of the perforation, and the boundary data.

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MS61

Front Propagation in Stratified Media: A Variational Approach

We prove, under generic assumptions, that the special variational traveling wave that minimizes the exponentially weighted Ginzburg-Landau functional associated with scalar reaction-diffusion equations in infinite cylinders is the long-time attractor for the solutions of the initial value problems with front-like initial data. The convergence to this traveling wave is exponentially fast. The obtained result is mainly a consequence of the gradient flow structure of the considered equation in the exponentially weighted spaces and does not depend on the precise details of the problem. It strengthens our earlier generic propagation and selection result for "pushed" fronts.

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MS62

Efficient Algorithms for (Di-)Atomic Basis Sets

We present a fast algorithm to calculate Coulomb/exchange integrals of prolate spheroidal electronic orbitals, which are the exact solutions of the single-electron, two-center Schrödinger equation for diatomic molecules. Our approach employs Neumann's expansion of the Coulomb repulsion $1/|x-y|$, solves the resulting integrals symbolically in closed form and subsequently performs a numeric Taylor expansion for efficiency. Thanks to the general form of the integrals, the obtained coefficients are independent of the particular wavefunctions and can thus be reused later. Key features of our algorithm include complete avoidance of numeric integration, drafting of the individual steps as fast matrix operations and high accuracy due to the exponential convergence of the expansions. Application to the diatomic molecules O_2 and CO exemplifies the developed methods, which can be relevant for a quantitative understanding of

chemical bonds in general.

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MS62

Higher-order Adaptive Finite-element Methods for Large-scale Electronic Structure Calculations using Kohn-Sham Density Functional Theory

Electronic structure calculations using Kohn-Sham density functional theory (DFT) have played a significant role in predicting wide range of material properties, yet simulations of large-scale material systems with DFT are still computationally very demanding. In this work, we present an efficient computational approach to perform real-space electronic structure calculations using an adaptive higher-order finite-element discretization of DFT and show how the approach can be extended to develop a linear scaling method for metals and insulators on the same footing.

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MS62

Finite Elements for Large-Scale Electronic Structure Calculations: From Classical to Enriched to Discontinuous

Over the past few decades, the planewave (PW) pseudopotential method has established itself as the method of choice 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. Here, we discuss recent enriched and discontinuous finite element (FE) based methods for the solution of the Kohn-Sham equations which have made possible order-of-magnitude reductions in basis size relative to PW and full, self-consistent calculations of 4000 atoms or more.

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MS62

Entanglement Based Algortihms for Electronic Structure Computation of Strongly Correlated Systems

Based on an excitation number encoding for the Slater determinant basis functions, the full CI space could be easily embedded into a (discrete) Fock space isomorphic to $F := \bigotimes_{i=1}^{d} C^2$. These tensors can be represented and approximated in a hierarchical tensor (HT) format, known as tree tensor network states (TTNS). An important example are tensor trains (TT) which are nothing but matrix product states (MPS). The ranks are measures for the entanglement between corresponding parts. For given ranks these tensors form an analytic manifold and dynamics could be approximation by the Dirac-Frenkel variational principle. The resulting variational wave function method permeates the full CI space, but scales only polynomially w.r.t. the size of the basis set. Beside the alternating direction algorithms, namely DMRG (density matrix renormalization group), the dynamical treatment allow to apply first and second order optimization methods. We try apply this approach to the compuation of transiton metal complexes, often considered as strongly correlated and hard problems.

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MS63

Macroscopic Interface Dynamics in Forward-backward Lattice Diffusion

We consider a diffusive lattice equation with a non-monotone non-linearity. The formal continuum limit of such a problem is an ill-posed PDE, thus measure-valued solutions and hysteresis effects are to be expected. We discuss the phenomena that occur for different types of initial data, paying particular attention to the case when interfaces with non-trivial dynamics appear and persist in the macroscopic limit.

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MS63

Mesoscopic Peridynamics Derived from Microstructure

We describe a method for deriving peridynamic constitutive equations from the underlying molecular dynamics. First, we obtain convolution integral representations for the average density and momentum. This establishes a connection between mesoscopic averages and certain recoverable fine scale functionals. Then we use regularization to approximately invert convolutions, and thus represent the recoverable functionals by operators acting on the averages. Next, the peridynamical force state is rewritten as a non-linear operator acting on the recoverable functionals. The constitutive equations are obtained from this representation by replacing the exact recoverable functionals with their deconvoluted approximations.

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MS63

Travelling Waves in the Discrete FitzHugh-Nagumo Model

While the theory of nonlinear waves in partial differential equations is very well developed, understanding travelling waves in systems posed on lattices is challenging, and many basic questions remain open. Indeed, travelling waves on lattices can be found only by solving functional differential equations of mixed mode, which are ill-posed as initial-value problems. In addition, propagation failure or pinning occurs frequently for waves with small speeds, which makes

it hard to find such waves using perturbation arguments. In this talk, I will outline work on the existence and stability of travelling waves for the discrete FitzHugh-Nagumo system using geometric singular perturbation theory.

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MS63

Solitary Waves in the FPU Chain: A New Exact Solution

We consider solitary wave solutions in the Fermi-Pasta-Ulam problem with piecewise linear nearest-neighbor interactions. We show that in this case the problem reduces to a Fredholm integral equation of the second kind, which can be solved explicitly using Wiener-Hopf method. Taking advantage of the availability of an exact solution, we test the limits of applicability of the simplest quasicontinuum approximations of the discrete problem. We show that in agreement with the results of Friesecke and Matthies (2002), atomic-scale localization occurs in the high-energy limit. Numerical simulations suggest stability of the obtained solutions above a certain velocity threshold.

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MS64

Intersonic Crack Propagation in Fiber-Reinforced Composites: a Peridynamic Approach

We present a homogenization-based anisotropic peridynamic model for unidirectional fiber-reinforced composites and we use it to model an experiment by Coker and Rosakis (2001) in which intersonic crack growth is observed in asymmetrically loaded composites. We show that under sufficiently high amplitude loading, a splitting-type crack propagates intersonically, creating its own shock wave cone with an angle of about 18 degrees, very close to that seen from experiments. Under symmetric loading, mode I cracks grow subsonically.

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MS64

Peridynamic Balance Laws

My talk introduces the peridynamic balance laws of momentum and energy. The nonlocal force and energy densities are given by integral operators that are the nonlocal analogues for the classical force and energy densities. The resulting balance laws extend the classical theory of continuum mechanics to allow for discontinuities

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MS64

Peridynamic Instability and Damage

In this talk we explore connections between classic damage models and their relation to bond based peridynamics.

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MS64

Calibration and Ranking of Stochastic Peridynamics Models for Ring Fragmentation Phenomena

Using Bayes' formula and available uncertain experimental data D related to the rapid expansion and fragmentation of metal rings, we quantitatively compare two stochastic peridynamics modeling hypotheses proposed for simulating D. The methodology we discuss can be applied to any number of candidate hypotheses for simulating the same data D, and it consists of (i) statistically calibrating the random parameters in each modeling hypothesis, and (ii) calculating the hypotheses' plausibilities conditioned upon D.

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MS65

Austenite As a Local Minimizer in a Model of Material Microstructure with a Surface Energy Term

In this talk we present a simplified model of a single elastic crystal where the development of microstructure is influenced by both potential and surface energies. In particular, we will show that (i) $u = 0$ (corresponding to austenite) is a strict local minimizer of the energy in a suitable sense, and (ii) provided the potential well-depths are sufficiently large, there is an energy barrier between the austenite state and the global minimizer of the total energy.

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MS65

Swell Induced Wrinkling and Creasing on the Surface of Hydrogel Bilayers

Upon swelling in a solvent, a thin hydrogel layer on a rigid substrate may become unstable, developing various surface patterns. Recent experimental studies have explored the possibilities to generate controllable surface patterns by chemically modifying the molecular structures of the

hydrogel near the surface. In this paper, we present a theoretical stability analysis for swelling of hydrogel layers with material properties varying in the thickness direction. As a specialization of the general procedure, hydrogel bilayers with different combinations of the material properties are examined in details. For a soft-on-hard bilayer, the onset of surface instability is determined by the short-wave limit, similar to a homogeneous layer. In contrast, for a hard-on-soft bilayer, a long-wave mode with a finite wavelength emerges as the critical mode at the onset of surface instability, similar to wrinkling of an elastic thin film on a compliant substrate, and the critical swelling ratio is much lower than that for a homogeneous hydrogel layer. A smooth transition of the critical mode is predicted as the volume fraction of the top layer changes, linking surface instability of a homogeneous layer to thin film wrinkling as two limiting cases. Numerical simulations by a nonlinear finite element method show that, while surface creases form spontaneously in a soft-on-hard bilayer, surface wrinkles grow significantly before creases form in a hard-on-soft bilayer.

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MS65

Stability Conditions for Constrained and Unconstrained Multi-Phase Elastic Solids

Inclusion of a non-positive-definite phase in an elastic composite has the potential to give rise to greatly enhanced overall composite stiffness. While independent investigations have highlighted stability and effective properties of such composites, no clear connection has been established between the two. Therefore, we here compare stability and effective performance of elastic composites having non-positive-definite phases, and we conclude that only the effective dynamic response can be positively affected by inclusion of a negative-stiffness phase.

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MS65

Thermal Shock Crack Initiation: a Non Local Damage Model Stability Analysis

This paper studies the initiation of cracks in the thermal shock problem through the variational analysis of the quasi-static evolution of a gradient damage model. We consider a two-dimensional semi-infinite slab with an imposed temperature drop on its free surface. The damage model is formulated in the framework of the variational theory of rate-independent processes based on the principles of irreversibility, stability and energy balance. In the case of a sufficiently severe shock, we show that damage immediately occurs and that its evolution follows first a fundamental branch without localization. After a finite time, it bifurcates into another branch in which damage localization will take place to finally generate cracks. This bifurcation is studied through a partial Fourier decomposition which leads to the study of a Rayleigh ratio. The determination of the time and mode of that bifurcation allows us to explain the periodic distribution of the so-initiated cracks and to calculate the crack spacing in terms of the material and loading parameters. We then discuss the stability of the fundamental and bifurcated solution.

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MS66

Cytoskeletal Mechanics and Cell Motility

Abstract not available at time of publication.

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MS66

Lamellipodia Dynamics in Motile Cells

We develop a simple physical model that captures the large-scale lamellipodia dynamics in crawling cells and explains the observed spectrum of fish keratocytes behavior. We deviate from existing theoretical works and consider the lamellipodium leading edge as a propagating front. The agreement of our model with experimental works suggests that the large-scale migration features exhibited by keratocyte cells are a direct consequence of the closed feedback loop between the leading edge geometry and actin network density

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MS66

Swimming Micro-organisms in Complex Fluids

Swimming microorganisms commonly encounter non-Newtonian fluids such as mucus. In this talk I describe our work on swimming helices in polymeric liquids, in which we use theory, computation, and scale-model experiments to determine how the swimming speed of a rotating helical filament depends on frequency, polymer relaxation time, filament radius, and helical geometry. I also report on our more recent work on swimming in anisotropic fluids and near flexible boundaries.

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MS66

Cellular Pressure and Volume Regulation and Implications for Cell Mechanics and Cell Motility

In eukaryotic cells, small changes in cell volume can serve as important signals for cell proliferation, death and migration. Volume and shape regulation also directly impacts mechanics of cells and tissues. Here we develop a quantitative mechanism of cellular volume and pressure regulation, incorporating essential elements such as water permeation, mechanosensitive channels, active ion pumps and active motor-driven stresses in the cell cortex. The model can predict the cellular volume and pressure for several models of cell cortical mechanics. Furthermore, we show that when cells are subjected to an externally applied load, such as in an AFM indentation experiment, active regulation of volume and pressure leads to complex cellular response. Instead of the passive mechanics of the cortex, the observed cell stiffness depends on several factors working together. Finally, we examine the implications of volume regulation in cell motility, where polarized distribution of membrane channels and pumps can lead to directed cell migration in an actin-independent manner. Quantitative results from experiments and modeling will be discussed.

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MS67

Strain and Rotation Fields of Dislocations in Graphene

Recent experiments have revealed that the strain and rotation fields about dislocations in suspended graphene sheets are qualitatively different from those provided by conventional elasticity. The observed fields are explained by adding a term quadratic in the local rotation to the 2D isotropic elastic strain energy density and regularizing the singularity at the dislocation point in different ways.

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MS67

Pattern Formation in Indentation Tests

Nanoindentation is currently used to explore the mechanical properties of solid surfaces. Controlled generation of surface defects using indenters might render metallic surfaces stronger. Around each indentation mark, dislocation networks are formed. Patterns such as loops, terraces or hillocks are commonly identified. The formation of terraces and hillocks involves glide and cross-slip mechanisms that we justify solving anisotropic Hertz contact problems. We characterize dislocation nucleation below the indenter in terms of bifurcations in atomic models.

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MS67

Plastic Strain Recovery in Nanocrystalline Nickel

Grain refinement in crystalline materials leads to an enhancement of several materials properties including yield and fracture strength and superior wear resistance. These improved material responses benefit the reliability of micro and nano devices, including MEMS and NEMS with components made of nanocrystalline materials. On the other hand, this reduction in grain size is also responsible for new mechanisms that are not present in their coarse grained counterparts. One of these mechanisms is plastic strain recovery.
Even though, plastic deformation is not recoverable in coarse grained crystalline materials, recent experiments in nanocrystalline aluminum, nickel and gold thin films and bulk nanocrystalline aluminum recovered more than 50% of plastic strain after unloading.
We will present dislocation dynamics coupled to kinetic Monte Carlo simulations that show plastic strain recovery in nanocrystalline metals with large scatter in the grain size distribution. Our results show that this phenomenon is driven by the inhomogeneous distribution of residual stress in the sample when the applied load is removed. We analyze the effects of temperature, loading history, and grain size distribution on the time dependent plastic strain recovery.

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MS67

Kinematic Analysis of Finite Plasticity as the Limit of Dislocation Activity

This talk will present a plasticity model in the finite kinematic framework that is directly obtained as the limit of the dislocation activity. The project intends to provide a physically-based definition of the elastic and plastic deformation gradient at the microscale that leads to the standard multiplicative decomposition of the deformation gradient in the continuum limit. Additionally, an expression for the dislocation density tensor is provided at both the discrete and continuum scale. The work is 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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MS68

Long-Time Simulation of Steady Nonequilibrium Flow

Nonequilibrium molecular dynamics (NEMD) are widely employed in the study of molecular fluids under steady, homogeneous flow, such as in the computation of stress-strain constitutive relation using a microscopic stress formulation. We will discuss the use of the Nonequilibrium Langevin Dynamics, a stochastic dynamics for sampling a molecular system with a homogeneous flow field $\nabla \mathbf{u} = \mathbf{A}$. In such a simulation the unit cell moves with the flow, and we describe particular boundary conditions that allow for long-time simulation by avoiding extreme deformation of the unit cell.

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MS68

Markov Model Reduction with Perturbed Test Functions

Abstract not available at time of publication.

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MS68

Local Hyperdynamics

In hyperdynamics, a method for reaching long time scales in infrequent-event systems, the bias potential must be zero everywhere on the dividing surface bounding the state, with the consequence that for large systems the boost factor decays to unity, regardless of the form of the bias potential. I will describe a new, local form of hyperdynamics that circumvents this problem, giving a constant boost factor for arbitrarily large systems.

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MS68

Using Coarse Grained Models to Speed Convergence to the Minimum Energy Pathway

The minimum energy pathway (MEP) is the most likely transition pathway between reactant and product states in a chemical reaction at low temperature and provides a convenient, one dimensional, description of the reaction. For large complex systems interrogation of the reaction mechanism by straightforward simulation is often impossible due to the presence of a vast range of time scales. For this reason, efficient techniques that focus on discovery of the MEP are important. Unfortunately in large complex systems discovery of the MEP can itself be prohibitively expensive. In this work we develop a technique for discovery of the MEP (and other pathwise descriptions of reactions) that uses inexpensive, coarse grained models to accelerate convergence. In most practical settings the reaction pathway corresponding to the coarse grained model does not accurately describe the reaction of interest. Nevertheless, by carefully arranging the calculation, the coarse grained system can be used to accelerate convergence to the MEP of a more expensive, more accurate, model. We demonstrate the effectiveness of this approach on several test problems.

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MS69

Modeling Multiferroic Polycrystalline Materials

Multiferroics are materials that involve the coupling of elasticity, magnetization and polarization. In systems that contain all three properties the elastic coupling can be used to control polarization with magnetic fields or magnetization with electric fields. The latter is particularly advantageous for memory applications. In this talk I would like to discuss how these systems can be modeled efficiently by coupling the magnetization and polarization fields with a standard phase field crystal model.

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MS69

Phase Field Crystals - Modeling Structural Transformations at Diffusive Time Scales and Atomic Length Scales

Many different models have emerged in the past few decades to simulate phase transformations and the physical mechanisms which govern them. Correspondingly, with the increase in complexity, the demand on computational power has grown. Each transformation is broken down by its contributing physical components and an appropriate model is accordingly developed to simulate these components. The phase field crystal methodology is a relatively new model that attempts to incorporate many bulk and interface properties through an evolution of density fields which simultaneously represents both the bulk phases, elastic stresses and topological lattice defects. This method of simulation promises to provide atomic type simulations at diffusive time scales allowing the investigation of slow moving transformations and defect interactions. I will discuss some potential uses for the model and concepts behind it.

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MS69

Fluctuating Nonlinear Hydrodynamics formalism of the Density Functional Theory of solidification.

Recent developments in PFC modeling of crystalline pat-

tern formation in 2D and 3D are reviewed. This includes various aspects of dendritic solidification and growth on crystalline surfaces. Along these lines, we present results for the anisotropy of the solid-liquid interface free energy and kinetic anisotropy, including the respective Wulff shapes. Next, we compare dendritic patterns from atomistic theory in 2D and 3D with those predicted by a quantitative phase-field model under similar conditions (driving force and anisotropies), and discuss the validity range of the latter approach.

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MS69

Two-Dimensional Crystals - the Interplay of Geometry and Materials Defects

Using a phase field crystal model on a curved surfaces allows to investigate geometrical frustration on crystalline structures and the formation of defects. This will be studies in detail for various geometries demonstrating the occurance of new defect structures, such as grain boundary scars and pleats. Possible applications for pliable substrates will be discussed.

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MS70

Chiral Liquid Crystals in Poiseuille Flow

Chiral liquid crystal (CLC) ordering occurs in solid biocomposites such as insect cuticle, muscle, collagen and silk fibers. In this talk, we present a kinetic model for flowing CLCs. The underlying microstructures and linear viscoelasticity of CLCs in Poiseuille oscillatory permeation flows are presented and discussed, taking into account dynamic couplings between orientation and velocity fields.

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MS70

Modeling and Simulation of Organic Superconductors

In this talk, I report our recent study on the magnetic and pairing properties of newly discovered polycyclic aromatic hydrocarbon (PAH) superconductors including alkali-metal-doped picene, coronene, phenanthrene, and dibenzopentacene. Systematic computer simulations were carried out so to gain understandings on magnetism and electron correlation in PAH. We model the p-electrons on the carbon atoms of a single molecule by a one-orbital Hubbard model, in which the energy difference ? between carbon atoms with and without hydrogen bonds is taking into account. Our results demonstrate that the spin polarized ground state is realized for charged molecules in the physical parameter regions, which provides a reasonable explanation of local spins observed experimentally. In alkali-metal-doped dibenzopentacene, our results show that electron correlation may produce an effective attraction between electrons for the charged molecule with one or three added electrons, a necessary condition for superconductivity. We further propose a different doping pattern which may lead to higher transition temperature. Some results on the possible structure of PAH as functions of pressure and doing will also be discussed.

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MS70

Application of Active Liquid Crystal Models to Complex Biological Systems

In order to model complex biological systems, we have to treat the motility of their micro-constituents, cells in cellular systems, F-actins inside a cell, etc.. In this talk, I will discuss how active liquid crystal models can be used to study the chemical-mechanical coupling in live cellular systems. Numerical simulations will be presented to simulate a few selected cases.

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MS70

Kinetic Theory and Simulations of Active Nematic Polymers

A kinetic model is proposed for active nematic polymers in a viscous solvent, by coupling particle-activation physics to the Doi-Hess theory for passive nematic polymers. Numerical results are presented for the dilute regime where the stable passive isotropic phase is driven from equilibrium by activation physics, the nano-rod analog of non-Brownian, non-polar, active pusher suspensions. Unsteady (periodic and modulated periodic) and steady, 1D and 2D attractors are selected by varying active parameters, revealing rich diversity reminiscent of mesoscopic simulations of active semi-dilute nematics.

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MS71

Nonexistence Results for Energy Functionals with

Competing Attracting and Repelling Interactions

Abstract not available at time of publication.

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MS71

Existence and Qualitative Properties of Grounds States to the Non-Local Choquard-Type Equations

The Choquard equation, also known as the Hartree equation or nonlinear Schrodinger-Newton equation is a stationary nonlinear Schrodinger type equation where the nonlinearity is coupled with a nonlocal convolution term given by an attractive gravitational potential. We present sharp Liouville-type theorems on nonexistence of positive supersolutions of such equations in exterior domains. We also discuss existence, positivity, symmetry and optimal decay properties of ground state solutions under various assumptions on the decay of the external potential and the shape of the nonlinearity. In particular, we obtain a sharp decay estimate for the ground state solution which was discovered by E.Lieb in 1977.

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MS71

Verifying Global Minimizers for Ginzburg-Landau-type Problems: a Simple Approach via Convex Approximation

Energy functionals of Ginzburg-Landau-type are prominent in modeling material phenomena. These functionals are non-convex and contain many local minima and metastable states. As a result, through standard methods such as a gradient flow, it is easy to produce local minimizers or metastable states, however difficult to verify whether a given state is also a global minimizer. In our talk we present a new strategy for verifying candidate global minimizers. The approach relies on finding a good lower bound quadratic functional through a convex optimization procedure. Using a numerical method, we then solve the convex problem to obtain a bound on the order-disorder (ODT) transition curve. We apply this method to the Ohta- Kawasaki functional. We conclude with a discussion of the verification for non-constant states.

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MS71

Minimization of a Short-range Attractive and Long-range Repulsive Energy Related to a Nonlocal Aggregation Model

In this talk I will consider an energy consisting of a short-range attractive and a long-range repulsive term. This energy is related to aggregation models given by the equation $\rho_t + \nabla \cdot (\rho(-\nabla K * \rho))$ where ρ is the density of the aggregation and K is the interaction potential. Looking at the energy $E(\rho) = \int_{R^3} \int_{R^3} K(x-y)\rho(x)\rho(y)dxdy$ we will establish the existence of minimizers among the class of uniformly bounded, radially symmetric nonnegative functions of fixed mass. Moreover we will show that in the case of a quadratic attraction the sharp interface version of this minimization problem admits a unique global minimizer, namely the ball. This is a joint work with R. Choksi and R. Fetecau.

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MS72

Analyzing Capture Zone Distributions (CVDs) in Growth: Theory and Applications

We
describe CZDs using the generalized-Wigner-distribution (GWD): $P(s) = as^{\beta}\exp(-bs^2)$, with s the normalized CZ area. Near the experimentally-accessible central region, the GWD fits data well; β reveals physical information about nucleation. Careful simulations by Amar's and Evans's groups showed inadequacies in our mean-field Fokker-Planck argument and for behavior in the tails. Discussing underlying reasons, we propose improved, more-complicated descriptions of CZDs. We summarize applications to various pure and impurity-encumbered growth (also to societal) systems.

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MS72

Nanocluster Self-assembly: Far-from-equilibrium Shapes and Composition Profiles

Self-assembly of nanoclusters often occurs far-from-equilibrium in metallic systems. Consequently, shapes and composition profiles for multi-component clusters can be exquisitely sensitive to the formation kinetics. First, we discuss general features for both diffusion-limited and attachment- or reaction-limited growth. Then, we present a detailed analysis for diffusion-limited growth of 2D epitaxial clusters by metal deposition on crystalline surfaces. We present examples for one- and two-component clusters on simple fcc surfaces and on alloy surfaces.

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MS72

Kinetics in GaAs Thin-Film Growth with First-Principles Local Superbasin Kinetic Monte Carlo

A significant challenge in rare-event simulations is dealing with superbasins, or groups of recurrent free-energy minima separated from the full phase space of the system by high barriers that can considerably reduce the efficiency. We present a local superbasin kinetic Monte Carlo (LSKMC) method for identifying local superbasins in KMC simulations containing both superbasins and non-superbasin events. We demonstrate aspects of LSKMC in several examples, which highlight the computational efficiency of this algorithm.

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MS72

Directed Assembly of Nanoclusters on a Templated Surface: Rumpled Graphene

Deposition on templated surfaces can guide assembly of periodic arrays of nanoclusters. This process involves nucleation and growth in the presence of a periodically modulated adsorption energy and diffusion barrier. Suitable atomistic models are developed and analyzed by KMC simulation, and by coarse-graining. The model describes arrays of mono- and bi-metallic nanoclusters formed by deposition of Ru and Pt on a graphene sheet which exhibits a periodic moire structure when supported on Ru(0001) .

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MS73

Conditioning in Fractional Sobolev Spaces

We investigate the condition number of the stiffness matrix arising from piecewise linear and constant finite element discretization of nonlocal integral operator with singular kernels. Depending on the singularity, we study the condition number in respective fractional Sobolev spaces. We explicitly quantify mesh size and horizon dependence of extremal eigenvalues. We provide supplementary numerical results.

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MS73

Mathematical and Numerical Analysis of Nonlocal Models

We discuss mathematical and computational issues related to some nonlocal balance laws in this talk. We use peridynamic materials models and nonlocal diffusion as examples to provide physical motivations and to illustrate mathematical challenges. We present a nonlocal vector calculus as an attempt to study related nonlocal variational problems in more systematic and axiomatic ways. We also explore connections and differences between nonlocal and local models and address questions concerning efficient and reliable numerical approximations.

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MS73

Variational Analysis of Linearized Peridynamics for Heterogeneous Materials

We analyze the linearized state-based peridynamic model of continuum mechanics. The focus of the analysis is on models of isotropic heterogeneous elastic materials. Using standard variational techniques we prove the well posedness of the system of equilibrium equations as well as the equations of motion, given as nonlocal equations with a prescribed volumetric constraint. In the event of vanishing nonlocality solutions of the nonlocal system are shown to converge to the Navier-Lamé system of classical elasticity. Our analysis is based on some nonlocal Poincar´e-type inequalities and compactness of the corresponding nonlocal operators. This is a joint work with Qiang Du.

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MS73

Sparse Dynamics of Non-Local Evolution Equations

We investigate the approximate dynamics of several differential equations when the solutions are restricted to a sparse subset of a given basis. The restriction is enforced at every time step by simply applying soft thresholding to the coefficients of the basis approximation. By compressing the information needed to represent the solution at every step, only the essential dynamics are represented. In many cases, there are natural bases derived from the differential equations which promote sparsity.

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MS74

Rational Design of Molecular Materials: Piezoelectrics and Organic Solar Cells Via Genetic Lgorithms

Abstract not available at time of publication.

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MS74

Data Mining Big Materials Data

Abstract not available at time of publication.

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MS74

Taking Advantage of the Convexity of Chemical Compund Space

Efficient exploration of enormous chemical spaces requires new optimization schemes that search directly for the property optimum, and in the process discover new molecular architectures. We present an unbiased optimization paradigm that is free from preselected substitution frameworks. We propose directly optimizing on the space of possible compositions and structures subject to property constraints such as visual clarity. We exemplify this algorithm with non-linear optical chromophores with a transparency constraint in the visible spectroscopic region.

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MS74

Numerical Algorithms for Identification of Optimal Parameters in Material Models for Industrial Forming Processes

Combining classical quasi-static forming with electromagnetic pulse forming can increase formability in a sheet metal forming process. The numerical simulation of the combined forming process strongly depends on suitable material models. Recently proposed models take into account nonlinear kinematic and isotropic hardening. Fitting to experimental data identifies the model parameters. We present a second order optimization framework based on inner points to identify the model parameters by simulating uniaxial tensile tests.

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MS75

Excitability and Chaos in Active Nematic Suspensions

In this talk I will describe a model of mutually propelled filaments suspended in a two-dimensional solvent. The system undergoes a mean-field isotropic-nematic transition for large enough filament concentrations, and the nematic order parameter is allowed to vary in space and time. The interplay between nonuniform nematic order, activity, and flow results in spatially modulated relaxation oscillations, similar to those seen in excitable media. In this regime the dynamics consists of nearly stationary periods separated by bursts of activity in which the system is elastically distorted and solvent is pumped throughout. At even higher activity, the dynamics becomes chaotic.

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MS75

The Metaphase Spindle As An Active Liquid Crystal

Abstract not available at time of publication.

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MS75

Spontaneous Flow in Active Gels

Abstract not available at time of publication.

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MS75

Dynamical Structures in Active Nematics and Their Novel Behaviors

Abstract not available at time of publication.

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MS76

Reformulation of Continuum Mechanics for Multiscale Simulation

Abstract not available at time of publication.

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MS76

From Atomistic to Continuum Boundary Value Problems in Nonlinear Elasticity

We study the passage from atomistic systems to an effective continuum theory for boundary value problems in (moderately) nonlinear elasticity: Under suitable assumptions we will show that discrete solutions of the Euler-Lagrange equations converge to solutions of the continuum equations of nonlinear elasticity.

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MS76

Continuum Models for Dislocation Dynamics and Crystal Plasticity

We present continuum models for dislocation dynamics and crystal plasticity. The continuum models are derived from discrete dislocation dynamics models and incorporate the long-range interaction of dislocations, local line tension effect of dislocations, and dislocation multiplication by Frank-Read source. We use the disregistry across the slip plane to represent the continuous distribution of dislocations, which has the advantage of including the orientation dependence of dislocations in a very simple way. Applications of two dimensional grain size effect and creep of metals are presented.

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MS76

Continuum Limit of Discrete Motion of Interfaces

We will discuss some results on the motion of interfaces in a discrete environment. The model takes into account nearest and next nearest neighbor interactions leading to interfaces between patterns. Intricate stick-slip phenomena also arises through different spatial and temporal discretization.

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MS77

Wang-Landau Multiple State Transition Interface Sampling

The Multiple State Transition Interface Sampling (MSTIS) technique is a form of path sampling that can compute rare event kinetics in complex systems exhibiting multiple metastable states. I present a novel scheme combining MSTIS with a single replica exchange method based on Wang-Landau sampling, that, in principle, can explore the entire trajectory space starting from a single stable minimum. The method is illustrated on simple models as well as more realistic biomolecular transitions.

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MS77

Recent Developments in Adaptive Kinetic Monte Carlo

Adaptive kinetic Monte Carlo (AKMC) is a technique used to study the long timescale dynamics of rare event systems. AKMC is a type of kinetic Monte Carlo simulation where the events and their rates are calculated on-the-fly. The reactive events are represented by saddle points on the potential energy surface and their rates are calculated using harmonic transition state theory. Typically, saddles are found in AKMC with single-ended min-mode following saddle point searches. Here, I use high temperature molecular dynamics trajectories, as is done in temperature accelerated dynamics, to discover the reactive events in AKMC. In this approach, the error in the simulation can be estimated and controlled, little prior knowledge of the system is required, and in favorable cases, the efficiency of AKMC simulations are substantially increased.

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MS77

Multiscale Modeling of Macromolecular Dynamics

Abstract not available at time of publication.

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MS77

An Infinite Swapping Approach to the Rare-Event Sampling Problem

Infinite swapping (INS) is a recently developed method to overcome the rare-event sampling problem, Plattner et al., 2011. The method is based on a mathematical analysis of parallel tempering (PT) by large deviation theory, Dupuis et al., 2012. An expanded computational ensemble composed of a number of replicas at different temperatures is used for PT and for INS, but while the basic concept of PT is to sample various replicas of a system at different temperatures and exchange information between the replicas occasionally, INS uses the symmetrized distribution of con-

figurations in temperature space, which corresponds to the infinite swapping limit of PT. INS is a general method and therefore potentially useful for various application areas. So far it has been tested for Lennard-Jones clusters and different biological systems. In biological systems, rare-event sampling problems arise due to the different timescales on which biological processes occur and a number of challenges needs to be addressed due to the specific properties of functional free energy landscapes characterizing biological macromolecules.

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MS78

A Hierarchy of Coarse-Grained Molecular Dynamics Models for Material Defects

I will present a systematic approach to coarse-grain molecular dynamics models for solids. The coarse-grained models are derived by Galerkin projection to a sequence of Krylov subspaces. On the coarsest space, the model corresponds to a finite element discretization of the continuum elasto-dynamics model. On the other hand, the projection to the finest space yields the full molecular dynamics description. The models in between serve as a smooth transition between the two scales. I will also discuss some error estimation and numerical experiments.

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MS78

Fast Nanowire Simulations Using a Hash Table-Based Cache

We present an implementation of a rate cache designed to eliminate redundant calculations in Kinetic Monte Carlo (KMC) simulations as well as applications of the implementation to simulating nanowire growth. We present numerical evidence suggesting that the utilization of such a cache is computationally advantageous. We further describe a simulated annealing technique to search for effective, system-specific hash functions. Equipped with an efficient implementation, we are able to simulate nanowire growth by the vapor-liquid-solid method as an example. An energy parameter study is presented. We show that the KMC model captures a wide range of observed phenomena, including faceting at the liquid-solid interface and nanowire kinking.

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MS78

Kinetic Monte Carlo Simulations of Multicellular Aggregate Self-Assembly in Biofabrication

We present a three-dimensional lattice model to study self-assembly and fusion of multicellular aggregate systems by using kinetic Monte Carlo (KMC) simulations. This model is developed to describe and predict the time evolution of postprinting morphological structure formation during tissue or organ maturation in a novel biofabrication process (or technology) known as bioprinting. In this new technology, live multicellular aggregates as bio-ink are used to make tissue or organ constructs via the layer-by-layer deposition technique in biocompatible hydrogels; the printed bio-constructs embedded in the hydrogels are then placed in bioreactors to undergo the self-assembly process to form the desired functional tissue or organ products. Here we implement our model with an efficient KMC algorithm to simulate the making of a set of tissues/organs in several designer's geometries like a ring, a sheet and a tube, which can involve a large number of cells and various other support materials like agarose constructs etc. We also study the process of cell sorting/migration within the cellular aggregates formed by multiple types of cells with different adhesivities.

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MS78

Localized Bases for Numerical Homogenization of Heterogeneous Materials

Homogenization Theory deals with mathematical models of strongly inhomogeneous media with vastly different properties. Traditionally, it is described by PDEs with rapidly oscillating coefficients of the form $A(x/\epsilon)$, $\epsilon \to 0$. The homogenization of PDEs with periodic or ergodic coefficients and well separated scales is now well understood. We consider the most general case of arbitrary measurable coefficients. Specifically, we study divergence-form scalar elliptic equations and vectorial equations with such coefficients. For these problems we establish finite-dimensional approximations of solutions, which we refer to as finite-dimensional homogenization approximations. We introduce different constructions for the approximations and establish the error estimate with an explicit and *optimal* error constant *independent of the contrast* and regularity of the coefficients. A proper generalization of the notion of cell problem is the key technical issue in our consideration. In the language of numerical analysis, we are answering the following question: can we recover the typical $O(h)$ error estimate for Laplace equation for PDEs with rough (L^∞) coefficients? and what is the optimal cost (localization) to achieve this error estimate?

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MS79

The Cross-over from Symmetric to Asymmetric Domain Walls in Soft Ferromagnetic Films

We study the Landau-Lifshitz energy of domain walls in soft ferromagnetic films. At the cross-over from symmetric Néel to asymmetric Néel and Bloch wall, we derive a reduced model that confirms an optimal splitting of the minimal energy into a numerically accessible contribution from a stray-field free wall-core, and an explicit contribution from the logarithmic tails of a symmetric Néel wall that complete the rotation.

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MS79

Boundary Vortices in Micromagnetics

We study the asymptotic behavior of boundary vortices and their interaction energy in a certain regime of thin-film micromagnetics. The key tool relies on the notion of "boundary Jacobian" which detects the topological defects at the boundary. The concentration of the energy around boundary vortices is proven via a Gamma-convergence result and we determine the renormalized energy that represents the interaction between the boundary vortices leading to their optimal position. The major difficulty consists in estimating the nonlocal part of the micromagnetic energy generated by the static Maxwell equation in order to detect the exact terms corresponding to the topological defects

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MS79

Ferromagnetism Modeling: from Micro-Scale to Meso-Scale

In this presentation we will focus on the link between the micro-scale and the meso-scale for ferromagnetic models. The micro-scale designates a model where atom kernels are assimilated to point-wise magnetic charges and the meso-scale is the model of micromagnetism. Starting from the micro-scale description, we will give a stochastic description of heat effects. In the following, we will expose the link between the micro and meso-scale.

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MS79

Domain Wall Motion in Ferromagnetic Nanowires

We study the dynamics of magnetic domain walls in ferromagnetic nanowires under the influence of external magnetic fields and currents. We investigate properties of the traveling wave and oscillating solutions of the Landau-Lifshitz-Gilbert equation.

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MS80

Numerical Simulation of Dewetting of Nanodroplets

Abstract not available at time of publication.

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MS80

Theoretical Modeling of Droplet Breakup and Generation in Microfluidic Devices

Abstract not available at time of publication.

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MS80

Assembly of Anisotropic Particles at Interfaces

Abstract not available at time of publication.

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MS80

Self-Similar Rupture in Marangoni-Driven Thin Fluid Sheets

We derive a system of equations that govern the dynamics of a symmetrically heated thin incompressible viscous fluid sheet. We take surface tension to be temperature dependent and so the streamwise momentum equation includes thermocapillarity, inertia, viscous stresses and capillarity. This system reduces to two of our previous models in the limit of large and small Reynolds number respectively. In both limiting cases, we find conditions under which sufficiently large-amplitude initial temperature profiles induce film rupture in finite time, notably without the inclusion of disjoining pressures from van der Waals effects. In the case of large Reynolds number, the similarity solution is governed by a balance of inertia and capillarity near the rupture location, analogous to the isothermal case. In the case of small Reynolds number, the thermocapillary transients induce the same similarity solution over intermediate times that is found for the drainage of lamellas in foams. For O(1) Reynolds numbers, the dynamics are governed initially by the large Reynolds number evolution, and then a transition over several orders of magnitude in the sheet thickness needs to take place before the small Reynolds number similarity solution is observed.

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MS81

Local and Non-Local Continuum Limits of Energies for Spin Systems

I will present some recent result about the asymptotic behavior, as the lattice size tends to 0, of a general class of energies of spin systems defined by mixing ferromagnetic and antiferromagnetic type potentials accounting also for long-range interactions. Under very general assumptions on the potentials, the macroscopic limit is described by interfacial energies of perimeter type. I will also provide some examples in which the macroscopic limit is a non local type functional.

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MS81

Atomistic Energy Minimization and Wulff Shapes

In many situations, atoms self-assemble into specific shapes, governed by preferred solid-vapour interface orientations. I will explain the recent rigorous results (joint with Au Yeung and Schmidt, Calc.Var.PDE 44, 81-100, 2012) that (i) atomistic ground states of 2D short-range pair potentials form clusters of constant density whose indicator function belongs to the space BV of functions of bounded variation (ii) ground states of the 2D Heitmann-Radin model form regular hexagons which are the optimizers of a Wulff-Herring surface energy which emerges as the Gamma limit of the atomistic model. I will then discuss difficulties, as well as some progress, regarding generalizing these results to 3D.

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MS81

A Discrete-to-Continuum Model for Thin Rods Made from a Biphase Material

We discuss an atomistic model for heterogeneous nanowires, allowing for dislocations at the interface. We study the limit as the atomic distance converges to zero, considering simultaneously a dimensional reduction and the passage from the discrete to the continuum. Employing the notion of Gamma-convergence, we establish the minimal energies associated respectively to an elastic (defect-free) configuration and a configuration with dislocations at the interface. This shows under which conditions the dislocations are favoured.

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MS81

Asymptotic Analysis of Prestrained Materials

Abstract not available at time of publication.

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MS82

Global Estimation of the Critical Time Step for Peridynamic Models

Stability in explicit transient dynamic simulations is contingent on a sufficiently small time step. While numerous approaches have been explored for problems in classical solid mechanics, calculation of the critical time step for many peridynamic models remains unexplored. We present a global time step estimate for peridynamic models based on the Lanczos method. Because the Lanczos-based value of the critical time step is derived from an eigenvalue analysis of the stiffness matrix, its application to simulations involving arbitrary peridynamic constitutive models is straightforward. In the case of a bond-based elastic material model, this allows for direct comparison against the critical time step derived by Silling and Askari [2005]. In addition to bond-based elastic models, we present an evaluation of the Lanczos estimate for state-based and non-ordinary state-based material models. Analyses include a benchmark simulation of wave propagation in a bar, as well as a more complex simulation involving pervasive material failure. The Lanczos global time step estimate is shown to be a viable means for computing the critical time step in peridynamic simulations.

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MS82

Peridigm: A New Paradigm in Computational Peridynamics

Peridynamics is a nonlocal extension of classical solid mechanics suitable for modeling the failure and fracture of engineering materials. The classical theory of continuum mechanics is based on partial differential equations. These equations do not hold on crack surfaces and other singularities, as partial derivatives are not defined at discontinuities. In the classical theory, cracks are regarded as a pathological solution requiring special treatment. In contrast, the peridynamic theory is based on integral equations, for which discontinuous functions present no difficulty. By utilizing integral equations, the peridynamic theory avoids the need for the special techniques of fracture mechanics. In peridynamics, cracks are just another kind of solution and require no special treatment. We provide an overview and introduction to Peridigm, a new open-source massively parallel

code for computational peridynamics. We survey the capabilities of Peridigm, showing demonstration computations and highlighting several applications. We then discuss the numerical techniques used in Peridigm to solve the integro-differential equations of peridynamics, and end by presenting our current and future development directions.

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MS82

A Comparison of Concurrent Multiscale Methods in Peridynamics

The peridynamic theory of solid mechanics is a generalization of classical continuum mechanics. The governing equation in peridynamics is an integro-differential equation without spatial derivatives of displacement fields, in contrast to classical models based on partial differential equations. Discontinuous displacement fields do not represent a challenge in peridynamics; as a consequence, peridynamics has been applied to the description of material failure and damage. As a nonlocal model, peridynamics is computationally more expensive than classical models; this motivates the development of concurrent multiscale methods, for which peridynamics is applied on regions where discontinuities appear or may be generated, whereas classical models are used elsewhere. A main challenge in concurrent multiscale modeling is how to couple different models without introducing spurious effects. We present different concurrent coupling methods for peridynamics and classical elasticity and compare these methods with respect to different quantities of interest.

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MS82

Variable Length Scale in a Peridynamic Body

In applications of peridynamics, it is sometimes desirable to have a different value of the horizon in different subregions of a body. However, unintended effects can appear in solutions with a position-dependent horizon. This talk will describe recent work on scaling the material model as a function of horizon to minimize these effects. It will also discuss a means for modifying the peridynamic nonlocal operator to minimize artifacts in regions where the horizon is changing.

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MS83

On the Computation of Optical Force and Stress in Metamaterials

We will talk about the theory of the light induced force and stress. We show that some non-diffracting beams can attract particles with simultaneous electric and magnetic responses. We will then address the question of light induced stress inside a metamaterial. We find that the effective permittivity and permeability do not give sufficient information to determine the force density inside a metamaterial and we show that how the required additional parameters can be calculated semi-analytically.

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MS83

Amplitude Activated Acoustic Metamaterial

The acoustic metamaterial structure contains an assemblage of bistable elastic links that loose stability when the amplitude of the acoustic signal reaches a threshold and the excited inner high-frequency oscillations dissipate the acoustic energy. The material transmits signals with low magnitude but stops highamplitude signals: One can hear a whisper but not a roar.

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MS83

Wave Propagation in Multiple Scattering Media Near Resonances: Scaling and Universality

The propagation of electromagnetic waves in a medium made of parallel dielectric rods is studied in the vicinity of the Mie resonances of the rods. It is shown that in the low frequency domain the Maxwell equations can be homogenized, which leads to an equivalent permittivity and more surprisingly to an effective permeability. It is demonstrated that the magnetic resonance is a switch for the existence of a high density of states.The effect of spatial dispersion and the properties of universality and scaling are also investigated

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MS83

From Asymptotic Models of Structured Plates to Control of Seismic Waves

Abstract not available at time of publication.

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MS84

Undulatory Swimming in Complex and Heterogeneous Media

Many fluids in which microorganisms move, feed, and reproduce are complex and possess an internal structure. Examples include wet soil, mucus, gels, and tissues. In this talk, we experimentally investigate the effects of polymer concentration, spanning the dilute to the concentrated regimes, on the swimming behavior of the nematode Caenorhabditis elegans. Results show a 40% increase in the nematodes swimming speed once immersed in a concentrated solution; that is, the propulsion speed is enhanced by fluid viscosity. This enhancement seems to be related to the dynamics of rod-like polymer networks formed in concentrated solutions.

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MS84

Reverse Engineering the Euglenoid Movement

Euglenids exhibit an unconventional motility strategy amongst unicellular eukaryotes, consisting of large amplitude highly concerted deformations of the entire body (euglenoid movement or metaboly), poorly understood as compared to cilliary or flagelar locomotion. We investigate the kinematics and hydrodynamics of such motions with statistical learning and continuum mechanics. We examine the shape morphing mechanism of euglenids, which could be extended to engineering systems.

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MS84

Phase Separation and Jamming of Active Particles

Experiments on confluent layers of epithelial cells and self-propelled colloids have motivated interest in the behavior of active matter at high density, where the interplay of steric repulsion and activity can yield active glassy and solid states. In this talk I will discuss the behavior of dense collections of self-propelled particles in two dimensions. I will show that the suppression of self-propulsion due to steric repulsion yields phase separation of a dense active fluid in solid-like and gas phases in the absence of any aligning or attractive interaction and discuss the relevance of this phenomenon to recent experiments.

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MS85

Theory-Based Benchmarking of Blended Quasicontinuum Methods

Multiscale computational methods for materials need to be validated by benchmark numerical experiments designed and evaluated on the basis of theoretical error analysis. We have shown that optimized blended quasicontinuum methods can be formulated and practically implemented for general many-body interactions with a controllable error and with the same (or nearly the same) order of complexity as consistent methods.

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MS85

The Failure of the Continuum Theory to Evaluate the Elastic Energy of a Strained Alloy

It is established by an exact solution of a ball and spring model of a binary alloy that continuum theory fails to predict its elastic energy. This result also shows that finely mixed alloys tend to have more elastic energy than segregated systems, which is the opposite of predictions made by continuum theories. Results using density-functional theory are in qualitative agreement. This work demonstrates that it is critical to include the microscopic arrangements in any elastic model to achieve even qualitatively correct behavior.

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MS85

Atomistic and Continuum Simulation of Size Effects in Polycrystalline Metal Deformation

Polycrystalline nanowires are interesting for exploring size effects in deformation. The three important length scales are grain size d, sample diameter D, and sample length L. I present very large scale molecular dynamics simulations of these materials and use these to develop an analytical model for sample length effects, determine the role of these scales on deformation mechanism and failure and use these to propose a new dislocation dynamics model for polycyrstalline materials.

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MS85

A Continuum Model for Dynamics of Dislocation Arrays and Applications to Low Angle Grain Boundaries

We present a continuum model for dynamics of dislocation arrays. The continuum model is derived rigorously from the discrete dislocation dynamics model using asymptotic analysis. The obtained continuum model contains an integral over the dislocation array surface representing the long-range interaction of dislocations, and a local term that comes from the line tension effect of dislocations. We also present numerical simulations using this continuum model including applications to dislocation structures of low angle grain boundaries.

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MS87

Simulations of Polycrystalline Grain Growth with Unequal Surface Energies

An extension of the distance function-based diffusion-generated motion algorithm for the simulation of polycrystalline grain growth is presented. Well-resolved simulations beginning with over 600,000 grains in two dimensions are performed. The effect of the initial texture and the form of the surface energy on the long-time evolution of the misorientation distribution is studied, and comparisons to experimental data are presented.

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MS87

Collision Rates for the Dynamics of Interacting Slipping Droplets

Reduced ODE models describing collision dynamics of droplets in nanometric polymer film interacting on solid substrate in the presence of large slippage at the liquid/solid interface are derived from one-dimensional lubrication equations. In the limiting case of the infinite slip length a collision/absorption model then arises and is solved explicitly. The exact collision law is derived. Existence of a threshold at which the collision rates switch from algebraic to exponential ones is shown.

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MS87

On the Coarsening Rates for Attachment-limited Kinetics

We study the coarsening rates for attachment-limited kinetics during solidification processes which is mathematically modeled by volume-preserving mean-curvature flow. Experiments, numerical simulations, and heuristics suggest that the typical domain size ℓ of solid islands in an undercooled liquid phase grow according to the power law $\ell \sim t^{1/2}$, when t denotes time. We focus on the two-dimensional case. Using the Kohn–Otto method, we prove a one-sided, time-averaged version of this coarsening rate, which is relevant and new for relatively sparse configurations. The bound is uniform in the sense that we do not impose any explicit assumptions on the initial data. However, during the evolution, we have to assume that collisions of different islands are rare events. This is joint work with Luca Mugnai.

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MS87

Coarsening in Grain-boundary Networks and in a Gradient Flow of Voronoi Diagrams

Many materials have polycrystalline structure – they consists of many small crystallites (grains) of different shapes and orientations. Under appropriate conditions the grain boundaries move to reduce the interfacial energy. This curvature driven evolution, causes some grains to grow, while others get smaller and disappear. The typical grain size grows, while the number of grains is decreasing. One of the immediate questions is to say what us the rate at which the grain-boundary network coarsenes. While there are heuristic arguments that predict the rate of coarsening, obtaining rigorous results that hold for arbitrary initial network has turned out to be difficult. Here we present rigorous upper bound on the rate of coarsening that holds under some mild geometric assumptions on the network. We also introduce and study the coarsening of a gradient flow of Voronoi diagrams. For such systems we show a universal upper bound

on the rate of coarsening. Furthermore we carry out numerical simulations that confirm that the upper bound is sharp in terms of scaling.

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MS88

Phase Separation of Multiple Ginzburg-Landau Vortices Pinned by Small Holes

We consider a homogenization problem for magnetic GL functional in domains with a large number of small holes. For sufficiently strong magnetic field, a large number of vortices are pinned by the holes. We establish a scaling relation between sizes of holes and the magnitude of the external magnetic field when pinned vortices form a hierarchy of nested subdomains with different multiplicity that manifests a physical phenomenon of vortex phase separation.

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MS88

Layer Undulations in 2D and 3D Smectic Liquid Crystals

We study the Landau-de Gennes free energy to describe the undulations instability in smectic A liquid crystals subjected to magnetic fields. If a magnetic field is applied in the direction parallel to the smectic layers, an instability occurs above a threshold magnetic field. When the magnetic field reaches this critical threshold, periodic layer undulations are observed. We prove the existence and stability of the solution to the nonlinear system of Landau-de Gennes model using bifurcation theory. We also perform numerical simulations to illustrate the results of our analysis. An efficient numerical scheme for some free energy containing the second order gradient will be presented. Undulation instabilities on three dimensional systems will be also discussed.

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MS88

Analysis of Ferroelectric Liquid Crystals

In this talk, we discuss some mathematical problems of Ferroelectric Liquid Crystals when the induced electric field appears to be in the system. we begin with a brief introduction and discuss existence theorem and partial regularity.

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MS89

Highly Accurate Numerical Solutions of Dirac Equations

Abstract not available at time of publication.

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MS89

Coarse-Graining Density Functional Theory

We present a real-space formulation for coarse-graining Density Functional Theory that significantly speeds up the analysis of material defects without appreciable loss of accuracy. The proposed technique consists of two steps. First, we develop a linear-scaling method in terms of quantities amenable to coarse-graining. Next, we introduce a spatial approximation scheme which is adapted so as to furnish fine resolution where necessary and to coarsen elsewhere. We validate the formulation through selected examples.

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MS89

Adaptive Regularized Self-Consistent Field Iteration with Exact Hessian for Electronic Structure Calculation

We regularize the self-consistent field (SCF) iteration for minimizing the Kohn-Sham total energy functional subject to orthogonality constraints and establish rigorous global convergence to first-order optimal solutions. The Hessian of the total energy functional is further exploited. By adding the part of the Hessian which is not considered in SCF, our methods can obtain highly accurate solutions on problems for which SCF fails and achieve a better convergence rate than SCF in the KSSOLV toolbox.

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MS90
Imprimitivity in Non-Crystallographic Nets

Periodic nets are commonly used to represent the topology of crystal structures. Some properties of non-crystallographic nets with non-trivial finite blocks of imprimitivity for bounded automorphisms will be briefly discussed as well as the consequences for the respective labelled quotient graphs. The concepts of *equivoltage* partitions and *correlation groups* will be thoroughly worked out using the net associated to a newly reported sphere packing as an example.

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MS90
Tangled Nets

Self-tangled nets have been reported in molecular frameworks. Knot theory allows us to explore the entanglement of loops. A corresponding toolkit for entangled nets is more subtle and far less developed. We define the "untangled" ground state of nets via their barycentric embedding ion 3-space. These may contain knots. In contrast, knot-free net embeddings may be untangled. These ideas can be explored via simpler graphs, such as polyhedral graphs, whose simpler tangled versions can be enumerated from reticulations of the torus. Infinite three-periodic nets can also be entangled. These can also be generated from reticulations of hyperbolic surfaces.

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MS90
Self Assembly and the Structure of Matter

We describe recent work on a strategy for designing molecules that leads to efficient self-assembly of nanostructures. The method is based on the use of discrete groups of isometries. The method has the potential to design molecules that assemble into structures of preassigned dimensions and functionality. The method is aided by a different classification of discrete groups of isometries than the conventional one underlying the International Tables of Crystallography, that better reveals the dependence on parameters of the isometries. We present some preliminary results of a study of the kinetics of self-assembly based on this method using Langevin dynamics.

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MS90
Why Topology Matters to Crystal Engineers

The structure and properties of metal-organic materials (MOMs) have made them an attractive class of materials for various applications including carbon capture and methane storage. MOMs are amenable to design using the "node and linker' approach and they are typically classified according to their connectivity or topology. This paper will highlight why certain topologies are particularly salient because they represent blueprints for families of porous MOMs, i.e. they enable materials scientists to think as architects.

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MS92
Hysteresis in a Constrained Model for Magnetic Shape Memory Alloys

In a constrained model for magnetic shape memory alloys we show loading paths where hysteresis cycles can be observed. The occurrence of these cycles can be related to the microstructures formed by the magneto-elastic phases.

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MS92
Geometric Compatibility, Quasiconvexity and Nucleation

Remarkable experimental observations of Hanus Seiner, in which austenite is nucleated in martensite by localized heating in a rectangular specimen of a CuAlNi single crystal, clearly demonstrate the important role of geometric compatibility between phases in the nucleation process. This talk proposes an explanation for the experimental observations in terms of quasiconvexity conditions in the interior and the boundary of a bar-shaped domain. This is joint work with John Ball.

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MS92

Emergence of Rate Independence in Gradient Flows with Wiggly Energies

We show that continuum models for plasticity can be derived as rigorous limit starting from a discrete microscopic model describing a visco-elastic chain with quenched disorder. The constitutive structure changes as a result of two concurrent limiting procedures: the vanishing-viscosity limit and the discrete to continuum limit. References: Mielke, Truskinovsky, From discrete visco-elasticity to continuum rate-independent plasticity. Archive for Rational Mechanics and Analysis 203, 2012; Mielke, Emergence of rate-independent dissipation from viscous systems with wiggly energies. Continuum Mechanics and Thermodynamics 24, 2012.

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MS93

Hydrodynamic Suppression of Phase Separation in Active Suspensions

We simulate a suspension of active squirming disks over the full range of volume fractions from dilute to close packed, with full hydrodynamics in two spatial dimensions. By doing so we show that "motility induced phase separation" (MIPS), recently proposed to arise generically in active matter, is strongly suppressed by hydrodynamic interactions. We give an argument for why this should be the case, supported by counterpart simulations of active Brownian disks in a parameter regime more closely akin to hydrodynamic suspensions than in previous studies.

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MS93

Out-of-Equilibriumness of Light Activated Colloids

Self-propelled micro-particles are intrinsically out-of-equilibrium. This renders their physics far richer than that of passive colloids while relaxing some thermodynamical constraints and give rise to the emergence of complex phenomena e.g. collective behavior, swarming We will present a new form of self-assembly originating from non-equilibrium driving forces. When activated by light, a set of new self-propelled particles spontaneously assemble into living crystals which behaves as " self-propelled colloidal carpets" steerable with an external magnetic field. We will show that this phenomenon is intrinsically out-of-equilibrium and originates in the competition between self-propulsion, particles collisions and attractive interactions.The applications and the use of this system for colloidal cargo transportation in microfluidic will also be discussed.

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MS93

Analysis and Simulation of Model for Active Nematic Suspensions

In this presentation, I will give a brief report on the analysis of a model for active nematic suspensions in various material regimes. Numerical results on model predictions in more complicated regimes where analysis is not available will be discussed. 2-D numerical simulation of interfacial instability in active nematic suspension fluids will be studied using a high order numerical method. Different mode of activities can significantly alter the classical capillary instability in droplet and filament of the active nematic suspension material.

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MS93

Dynamics of Polyelectrolyte Gels

Abstract not available at time of publication.

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MS94

Quasiatomistic Method for Molecular Mechanics Model

Quasiatomistic method (finite element approximation) is used for studying the molecular mechanics model. Two efficiency issues are investigated. One is the optimal computational complexity in multigird with mesh refinement. The other one is the good approximation accuracy by enriching bases from Krylov subspace.

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MS94

Crack Initiation and Propagation: A Bifurcation Study

Crack propagation and kinking are two important mechanisms for crack growth. In this talk I will present some results of bifurcation analysis based on a two-dimensional lattice model. In particular, I will show how the loading modes affects such mechanisms.

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MS94

The Climbing String Method for Saddle Point Search

The string method was originally designed for computing minimum energy paths between two minima of a potential energy. It evolves a continuous curve in the path space by the steepest descent dynamics. In this talk, we discuss how the string method can be modified to find saddle points on the boundary of the basin of a given minimum. Compared to the existing algorithms, this new method has the advantage that the computed saddle points are guaranteed to be directly connected to the minimum. We will also discuss how the convergence can be accelerated using an inexact Newton method in the late stage of the computation.

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MS95

Non-Associated Plastic Flow in Crystalline Solids

Experimental evidence that non-associated flow appropriately characterizes dislocation glide has existed for some time, but not until atomistic simulations became sufficiently refined have we been in a position to build rigorous continuum theories for single and polycrystals. At all levels, non-associated flow is shown to persist and significantly affect strain localization. Under certain deformation histories, intermittent bursts of strain are predicted, which is somewhat surprising. Key features of the theory are in accord with experiments.

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MS95

The Supercell Method in Atomic Scale Simulation of Materials

The supercell method is the standard approach in atomic scale simulation of bulk properties of materials in the condensed phase. It consists in simulating a microscopic sample of the materials contained in a (typically) cubic box, called the supercell, with periodic boundary conditions in order to get rid of surface effects. In some respects, it is similar to the representative volume element (RVE) commonly used in mechanics. In this talk, I will present some mathematical and numerical results, and review some open questions, concerning the use of the supercell method to simulate perfect crystals, crystals with local defects, and disordered materials.

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MS95

A New Framework for the Interpretation of Modulated Martensites in Shape Memory Alloys

Shape memory alloys (SMAs) are a class of materials with unusual properties that have been attributed to the material undergoing a Martensitic Phase Transformation (MPT). An MPT consists of the material's crystal structure evolving in a coordinated fashion from a high symmetry austenite phase to a low symmetry martensite phase. Often in SMAs, the austenite is a B2 cubic configuration that transforms a Modulated Martensite (MM) phase. MMs are long-period stacking order structures consisting of $[110]_{\text{cubic}}$ basal planes. First-principles computational results have shown that the minimum energy phase for these materials is not a MM, but a short-period structure called the Ground State Martensite. It is commonly argued that energy contributions associated with kinematic compatibility constraints at the austenite-martensite interface explain the experimental observation of meta-stable MMs, as opposed to the expected Ground State Martensite phase. To date, a general approach for predicting the properties of the MM structure that will be observed for a particular material has not been available. In this work, we develop a new framework for the interpretation of MMs as natural features of the material's energy landscape (expressed as a function of the lattice parameters and individual atomic positions within a perfect infinite crystal). From this energy-based framework, a new understanding of MMs as a mixture of two short-period Base Martensite phases is developed. Using only a small set of input data associated with the two Base Martensites, this MM Mixture Model (M^4) is capable of accurately predicting the energy, lattice constants, and structural details of an arbitrary Modulated Martensite phase. This is demonstrated by comparing the M^4 predictions to computational results from a particular empirical atomistic model.

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MS95

Modeling Plastic Flow at Interfaces and in Glassy Polymers

The talk will first discuss contact of fractal surfaces with roughness on a wide range of scales. The amount of plastic deformation at the surface is strongly dependent on the detailed atomistic structure and the degree of adhesion. A multiscale approach is applied with a fully atomistic treatment at the interface. Long range deformations in the bulk are captured using a Greens function based on the quasiharmonic approximation that provides seamless boundary conditions for the atomistic region. The second part of the talk will discuss coarse-grained models of glassy polymers. Potentials derived from equilibrium simulations provide a poor description of the plastic flow stress. The origins of this discrepancy and methods to correct for it by alternating between coarse and fine grained simulations will be described. Supported by NSF Grant No. DMR-1006805 and

ARL/JHU Cooperative Agreement W911NS-12-2-0022.

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MS96

Threshold Dynamics for Networks with Arbitrary Surface Tensions

We present a new algorithm for simulating the mean curvature motion of multiple phases subject to arbitrary surface tensions. The departure point is the threshold dynamics algorithm of Merriman, Bence, and Osher (MBO) in two phases. Our algorithm is based on a new energetic interpretation of the original MBO scheme.

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MS96

On An Interfacial Motion by Surface Diffusion

The surface diffusion equation is one of the mathematical models which describe the thermal grooving in material science. It is a geometric evolution law and represented as a fourth order parabolic PDE. Also, it has the variational structure that the perimeter of an enclosed domain decreases whereas the volume is conserved. In this talk, the stability analysis of equilibrium states on this geometric equation will be studied.

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MS96

Stability and Bifurcation of Equilibria to Geometric Evolution Laws in the Axisymmetric Setting

We study the nonlinear qualitative structure of solutions near equilibria for the surface diffusion flow and averaged mean curvature flow. Working in the particular setting of axisymmetric surfaces, satisfying periodic boundary conditions, we characterize the equilibria of these flows. We further discuss how volume conservation and surface area reduction, together with a maximal regularity setting, can be utilized to prove nonlinear stability, instability and bifurcation of equilibria.

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MS96

Stability of a Bunch of Spirals Evolving with An Eikonal-Curvature Flow Equation

We consider on stability of a bunch of spirals evolving by an eikonal-curvature flow equation. In this talk we give a simple level set formulation for spirals and the covering space so that spirals divide the covering space into two regions called interior and exterior. From this formulation and the comparison of interior and exterior sets between sub- and super-solution we obtain the stability of a bunch of spirals in the sense of Lyapunov.

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MS97

Asymptotic Analysis of Minimizers for the Lawrence-Doniach Energy

We consider the behavior of minimizers for the Lawrence-Doniach energy describing layered superconductors in perpendicular megnetic fields of modulus h_{ex}. Assuming that $|\ln\epsilon| \ll h_{ex} \ll \epsilon^{-2}$ as $\epsilon \to 0$, where $1/\epsilon$ is the Ginzburg-Landau parameter, we prove an asyptotic formula for the energy of a minimizer in terms of the measure of the domain, h_{ex}, and ϵ as ϵ and the interlayer distance s tend to zero. We also prove asymptotic estimates on the behavior of minimizers. Our work relies on Ginzburg-Landau theory, pde estimates, and results on single layer potentials.

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MS97

The Hydrodynamic Limit of the Parabolic Ginzburg-Landau Equation

We study the parabolic Ginzburg-Landau equation for a complex-valued u, (PGL)

$$\frac{1}{|\log\varepsilon|}\partial_t u = \Delta u + \frac{1}{\varepsilon^2}u(1-|u|^2)$$

for initial data corresponding to n vortices. For a bounded number of vortices, (PGL) induces a motion of vortices by the gradient flow of a renormalized energy. In the limit $n \to \infty$, one obtains a hydrodynamic limit equation, formally obtained by E in 1994. In this talk I will explain how one can use explicit estimates for (PGL) valid at fixed ε to rigorously connect (PGL) to E's limit equation.

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MS97

Hydrodynamic limit of Gross-Pitaevksy vortices on the plane

We consider detailed properties of Gross-Pitaevsky vortices on the plane. By renormalizing both the Ginzburg-Landau energy and the winding number at infinity, we establish the vortex motion law for asymptotically large numbers of vortices. It is then shown that the vorticity measure converges to a weak solution to the Euler equations with vortex sheet initial data. This is joint work with Robert

Jerrard.

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MS98

Modeling and Simulation of Nematic Liquid Crystal Films

Abstract not available at time of publication.

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MS98

Stability of Liquid Rings

Abstract not available at time of publication.

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MS98

Directed, Liquid Phase Assembly of Patterned Metallic Films by Pulsed Laser Dewetting

Abstract not available at time of publication.

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MS98

Fingering Instability Down the Outside of a Vertical Cylinder

Abstract not available at time of publication.

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MS99

Effect of Melt Flow on Morphological Evolution of Nanocrystal Nucleates

Self assembly of nano-scale structures are of great importance in modern day materials. This talk aims to address the effect of flow on crystallization kinetics of nano-crystals nucleated in a fluid. A Classical Density Functional Theory (CDFT) based hydrodynamic model for systems of interacting particles will be discussed. A numerical study of the effect of flow on growth and morphological evolution of nano-crystal nucleates will be presented.

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MS99

Aspects of Faceting in Epitaxial Relaxation

Below the roughening transition, crystal surfaces develop macroscopic facets. At the microscale, surface evolution is driven by the motion of steps. In this talk, I focus on surface relaxation and present recent progress in analytically connecting step flow models in the presence of facets to continuum-scale variational principles and Partial Differential Equations. I address the evaporation-condensation and surface diffusion cases for radial structures. This is joint work with Kanna Nakamura and Joshua Schneider.

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MS99

Kinetic Monte Carlo Models for Nanoclusters and Dendrites

Abstract not available at time of publication.

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MS99

Symmetry-Breaking in Shape Transitions of Epitaxially-Strained Islands

During heteroepitaxy, strained islands undergo a series of shape transitions with increasing size. We examine the transition pathway using a model free-boundary problem and energy minimization, constructing the bifurcation diagram of possible shapes including saddle-point barrier states. We find that island shape transitions occur via sequential nucleation of facets and involve highly asymmetric transition states (eg half-dome) which can be metastable. In addition, we determine the effect of substrate miscut in promoting stable asymmetric shapes.

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MS100

Quasistatic Nonlinear Viscoelasticity and Gradient Flows

We study one-dimensional quasistatic viscoelasticity of rate type under hard (Dirichlet) boundary conditions, which

can be expressed as a gradient flow. There are continua of equilibria and we prove convergence as time $t \to \infty$ to one of these under a genericity assumption on the stress, which we establish in some interesting cases.

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MS100

Gradient Structures and Geodesic Convexity for Reaction-Diffusion System

In this talk I consider systems of reaction-diffusion equations that can be written as gradient systems with respect to an entropy functional and a dissipation metric. The latter is given in terms of a so-called Onsager operator, which is a sum of a diffusion part of Wasserstein type and a reaction part. I discuss methods for establishing geodesic λ-convexity of the entropy functional by purely differential methods, thus circumventing arguments from mass transportation.

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MS100

Existence Results for Generalized Gradient Systems with Applications to Finite-Strain Elasticity

In this talk, we focus on a class of abstract doubly nonlinear evolution equations in Banach spaces, with a gradient structure. The driving energies are nonsmooth and nonconvex. We enucleate some general sufficient conditions on the dissipation potential and on the energy functional, for existence of solutions to the related Cauchy problem. The main existence result is obtained by passing to the limit in a time-discretization scheme with variational techniques, inspired by the theory of Minimizing Movements by E. De Giorgi. Finally, we discuss an application to a material model in finite-strain elasticity. Based on joint work with Alexander Mielke and Giuseppe Savaré.

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MS100

An Approach to Nonlinear Viscoelasticity Via Metric Gradient Flows

We formulate quasistatic nonlinear viscoelasticity as a gradient system. Our focus is a new class of dissipation distances which are defined using weak diffeomorphisms keeping the boundary fixed and ensure frame-indifference of the viscoelastic stress. In order to pass from the time-discretized problem to the time-continuous limit, we need strong convergence for which we use evolutionary variational inequalities for abstract gradient systems in a one-dimensional setting.

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MS101

Bloch Waves Expansion for High Contrast Homogenization

Arrays of infinitely long dielectric rods can produce effective media with permeability and permittivity which are both negative. This has been evidenced in the case of s-polarized light (electric field parallel to the axis of the rods) by numerical experiments and nicely explained by the appearance of magnetic and electric dipole resonances (Didier Felbacq, Physic review Letters 2009). However it seems difficult to deduce this phenomenum in a mathematical framework by performing the asymptotic analyis of a suitably scaled diffraction problem. The classical two-scale method which uses periodic test functions fails and, passing to the limit, we lose some important resonances of the system. In this talk I will present an attempt to substitute the two-scale approach with a developement in Bloch waves well adapted to the high contrast case. Let us notice that, in the case of classical homogenization without contrast, the link between this approach and the two-scale technique has been peformed by Allaire, Conca and Vanninathan, but in their case, only the projection on the first Bloch mode is useful in order to characterize the homogenized limit.

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MS101

Controlling the Phase and Power Flow of Electromagnetic Fields with Metamaterials

A method for arbitrarily controlling the phase progression and power flow of electromagnetic fields within a region of space is introduced. Specifically, it is shown how a 2D

inhomogeneous, anisotropic medium can be designed that supports desired spatial distributions of the wave vector and Poynting vector direction. Plane-wave relations in anisotropic media are used in conjunction with an optimization process to find the required material parameters.

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MS101

Cloud Computing for Nanophotonics: Multiphysics and Ultra-Fast Solvers

Abstract not available at time of publication.

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MS101

Plasmonic Waves Allow Perfect Transmission of Light Through Sub-Wavelength Holes

Optically active meta-materials can nowadays be constructed as physical objects. They can have astonishing properties and can lead to striking effects, the key-words are negative refraction, perfect imaging, and cloaking. This talk is concerned with a mathematical analysis that demonstrates how the effect of a negative magnetic permeability of the effective material can occur, and how perfect light transmission through sub-wavelength holes in a metallic structure is possible. Mathematically, we analyze the time-harmonic Maxwell equations in heterogeneous media, the coefficients of the equation can oscillate on a small spatial scale and the contrast can be very large. The heterogeneity of the optical medium is prescribed by the permittivity coefficient $\varepsilon_\eta(x)$, where $\eta > 0$ is a small parameter that stands for the typical dimension of spatial oscillations in the medium, and $x \in R3$ stands for the position in space. The electric and the magnetic field E_η and H_η are given as solutions of the Maxwell system

$$\begin{aligned} \nabla \times E_\eta &= i\omega\mu_0 H_\eta, \\ \nabla \times H_\eta &= -i\omega\varepsilon_\eta\varepsilon_0 E_\eta, \end{aligned}$$

where $\omega \in R$ is a prescribed frequency and μ_0 and ε_0 are given physical parameters. We analyze the weak limits E and H of E_η and H_η and derive an equation for E and H, the so-called effective equation. The coefficients in the effective equation describe the behavior of the complex material. We present joint works with G. Bouchitté and with A. Lamacz.

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MS102

Cavitation in Rubber: An Elastic Instability of a Fracture Phenomenon?

In this presentation, we will confront the cavitation theory of Lopez-Pamies et al. [Cavitation in elastomeric solids: I — A defect-growth theory. *Journal of the Mechanics and Physics of Solids* 59 (2011), 1464–1487.] with a variety of cavitation experiments with the objective of establishing whether the phenomenon of cavitation is an elastic instability (and hence depends only on the elastic properties of the rubber), or, on the other hand, a fracture process (and hence depends on the fracture properties of the rubber).

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MS102

Quasistatic Evolution of Cavities in Nonlinear Elasticity

Starting with a variational static model for cavitation in nonlinear elasticity, we propose a quasistatic model for the evolution of the system also based on global minimization. We prove the existence of a quasistatic evolution, which takes into account the non-interpenetration of matter, the irreversibility of the process of cavity formation, and the growth of cavities. In the energy balance equation, a new term appears involving the mean curvature of the cavity surface.

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MS102

A Regularized Penalty-multiplier Method for the Computation of Fracture Surfaces in Strain Space

If a body occupies the region $\Omega \in R^n$, $\mathbf{Ax}$ for $\mathbf{x} \in \partial\mathbf{\Omega}$ represents an affine boundary displacement for such a body, and $E(\cdot)$ represents an energy functional (defined on some appropriate admissible set of deformations of Ω), then the *volume derivative* is given by:

$$G(\mathbf{A}) = \lim_{\mathbf{V}\searrow\mathbf{0}} \frac{\mathbf{E}(\mathbf{u_V}) - \mathbf{E}(\mathbf{Ax})}{\mathbf{V}},$$

where $\mathbf{u_V}$ is a minimizer of $E(\cdot)$ constrained to form a hole of volume V in Ω. For a large class of materials, the onset of cavitation–type instabilities can be characterized as the zero level set of G. In this talk we describe a regularized penalty–multiplier method and its convergence properties for the computation of $E(\mathbf{u_V})$ above. This method together with a *continuation method* form the basis for a procedure for approximating the zero level set of G. We present some numerical results that show the effectiveness of this procedure versus the more direct approach of using a contour finding routine.

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MS102

On the Global Stability of Elastic Cylinders under Tension

We consider the uniaxial extension of a three-dimensional, homogeneous, isotropic, hyperelastic cylindrical solid in which the length of cylinder is prescribed, the ends are assumed to be free of shear, and the sides are left completely free. We show that standard constitutive hypotheses on the stored-energy function imply that a homogeneous axisymmetric deformation is the unique absolute minimizer of the elastic energy. Therefore, such constitutive hypotheses are incompatible with necks and shear bands.

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MS103

Peierls Stress in Continuum Dislocation Mechanics

From the time of Peierls' (1940) classic paper and Nabarro's (1947) extension of that work, it is generally believed that a prediction of a threshold stress for dislocation motion is not possible within any 'continuum' pde model, without inducing the notion of lattice discreteness. We explore this conjecture within a pde model for dislocation dynamics.

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MS103

Asymptotic Analysis and Dynamics of a System of Straight Dislocations

We consider a discrete variational model for screw dislocations and exploit the relation with an XY model for spins systems. In the passage from discrete to continuum, in terms of Gamma-convergence, we get a leading term that behaves logarithmically in the lattice spacing, while the next order is given by a function of the positions of the dislocations. This function is used to study the dynamics of a system of screw dislocations.

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MS103

Continuum Dislocation Theory for Modeling Size Effects in Crystal Plasticity

Experiments reveal ubiquitous size effects arising during plastic deformation of crystalline solids. At mesoscopic scales, such phenomena are accepted to predominantly stem from dislocation interactions. We report a simple variational toy model that captures Bauschinger and Hall Petch effects as well as typical thin-film size effects. This is accomplished by letting the energy of the microstructure enforce a physically-motivated dislocation saturation limit. The model has further been applied to deformation twinning.

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MS103

Multiscale Problems in Dislocation Theory

One of the hard open problems in mechanical engineering is the upscaling of large numbers of dislocations. The talk treats the derivation of continuum dislocation density models and strain-gradient plasticity models from discrete and semi-discrete dislocations theories. The approach we use is Gamma-convergence. An important tool is a generalisation of the rigidity estimate of Friesecke, James & Müller to fields that are not gradients. We will also discuss progress and open problems in modelling dislocation interactions.

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MS104

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS104
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MS104
Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS104
Title Not Available at Time of Publication

Abstract not available at time of publication.

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TBD, TBD

MS105
Gpu Parallelized Spectral Methods for Phase-Field and Phase-Field-Crystal Models

Abstract not available at time of publication.

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MS105
A Numerical Analysis of the Cahn-Hilliard Equation in a Domain with Non Permeable Walls

In this talk, I will present a joint work with Madalina Petcu (University of Poitiers, France), concerning a numerical analysis of the Cahn-Hilliard equation, for a binary material in a bounded domain. We assume that the walls bordering the material are permeable, which leads us to consider the non usual dynamic boundary conditions recently introduced by G. Goldstein et al. The equation is discretized, using a finite element method for the space and the backward Euler scheme for the time discretization. I will discuss different convergence and stability results, and obtain errors estimates (between the solutions of the discretized and of the continuous problem), depending on whether we assume or relax diffusion along the walls.

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MS105
Convex Splitting Methods for Nonlocal Models of Phase Separation

Abstract not available at time of publication.

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MS105
Two Phase Flow in Porous Media

Abstract not available at time of publication.

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MS106
Energy Driven Pattern Formation in a Non-local Ginzburg-Landau/Cahn-Hilliard Energy

This describes joint work with Sylvia Serfaty and Cyrill Muratov. We study the asymptotic behavior of the screened sharp interface Ohta-Kawasaki energy in dimension 2 using the framework of G-convergence. In that model, two phases appear, and they interact via a nonlocal Coulomb type energy. We focus on the regime where one of the phases has very small volume fraction, thus creating "droplets" of that phase in a sea of the other phase. We consider perturbations to the critical volume fraction where droplets first appear, show the number of droplets increases monotonically with respect to the perturbation factor, and describe their arrangement in all regimes, whether their number is bounded or unbounded. When their number is unbounded, the most interesting case we compute the G limit of the 'zeroth' order energy and yield averaged information for almost minimizers, namely that the density of droplets should be uniform. We then go to the next order, and derive a next order G-limit energy, which is exactly the "Coulombian renormalized energy W" introduced in the work of Sandier/Serfaty, and obtained there as a limiting interaction energy for vortices in Ginzburg-Landau. The derivation is based on their abstract scheme, that serves to obtain lower bounds for 2-scale energies and express them through some probabilities on patterns via the multiparameter ergodic theorem. Without thus appealing at all to the Euler-Lagrange equation, we establish here for all configurations which have "almost minimal energy," the asymptotic roundness and radius of the droplets as done by Muratov, and the fact that they asymptotically shrink to points whose arrangement should minimize the renormalized energy W, in some averaged sense. This leads to expecting to see triangular lattices of droplets.

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MS106
On the Shape of Charged Drops: an Isoperimetric Problem with a Competing Non-local Term.

I will give an overview of my recent work with C. Muratov on the analysis of a class of geometric problems in the calculus of variations. I will discuss the basic questions of existence and non-existence of energy minimizers

for the isoperimetric problem with a competing non-local term and for space dimensions n ¡ 8. A complete answer will be given for the case of slowly decaying kernels in two space dimensions.

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MS106

Minimality via Second Variation for a Nonlocal Isoperimetric Problem

We discuss the loca lminimality ofcertain configurations for a non local isoperimetric problem used to model microphase separation in diblock copolymer melts. We show that critical configurations with positive second variation are local minimizers of the nonlocal area functional and, in fact, satisfy a quantitative isoperimetric inequality with respect to sets that are L1- close. The link with local minimizers for the diffuse-interface Ohta-Kawasaki energy is also discussed. As a byproduct of the quantitative estimate, we get also new results concerning periodic local minimizers of the area functional.

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MS106

A Double Bubble Solution in a Ternary System with Inhibitory Long Range Interaction

We consider a ternary system of three constituents, a model motivated by the triblock copolymer theory. The free energy of the system consists of two parts: an interfacial energy coming from the boundaries separating the three constituents, and a longer range interaction energy that functions as an inhibitor to limit micro domain growth. We show that a perturbed double bubble exists as a stable solution of the system. Each bubble is occupied by one constituent. The third constituent fills the complement of the double bubble. Two techniques are developed. First one defines restricted classes of perturbed double bubbles. Each perturbed double bubble in a restricted class is obtained from a standard double bubble by a special perturbation. The second technique is the use of the so called internal variables. The advantage of the internal variables is that they are only subject to linear constraints, and perturbed double bubbles in each restricted class represented by internal variables are elements of a Hilbert space. A local minimizer of the free energy in each restricted class is found as a fixed point of a nonlinear equation. This perturbed double bubble satisfies three of the four equations for critical points of the free energy. The unsolved equation is the 120 degree angle condition at triple junction points. Perform another minimization among the local minimizers from all restricted classes. A minimum of minimizers emerges and solves all the equations for critical points.

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MS107

Effective Behavior of Thin Films of Liquid Crystal Elastomers

Abstract not available at time of publication.

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MS107

From Wrinkles to Scars: Universality of Stress Collapse in Confined Crystalline Sheets

Imposing curvature on crystalline sheets leads to distinct types of structural instabilities. The first type involves the proliferation of localized defects that disrupt the crystalline order, whereas the second type consists of elastic modes, such as wrinkles and crumples, which are common also in amorphous sheets. Here we propose a profound link between these types of patterns, encapsulated in a universal, compression-free stress field, which is determined solely by the macro-scale confining conditions.

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MS107

Asymptotics of a Prototype Lattice Energy under an Impenetrability Constraint

We consider the prototype model of particles parameterized on a 2-d triangular lattice linked with mearest neighbouring Lennnard-Jones type interactions in presence of an additional incompenetrability constraint. The positive-determinant constraint indeed mimics the effect of long-range interactions and, as we focus on a surface scaling of the associated energies as the lattice size goes to zero, it limits the ground states to piecewise rigid configurations, i.e. piecewise rotations with an underlying partition of the domain into sets of finite perimeter. We push forward our analysis to determine whether this constraint turns into a (possibly anisotropic) "opening crack" condition along the interfaces. The variational analysis turns out to be rich of features, among these: an opening crack constraint of novel type that take into account both the gradient of the deformation on both sides of the fracture and the orientation of the fracture sites in the reference configuration; additional positive-determinant request on points where more fractures meets (triple points); possible overtaking of the previous conditions by adding "fictitious" micro-fractures.

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MS107

Homogenization of the Kirchhoff Bending Theory for Plates

We carry out the spatially periodic homogenization of Kirchho?s plate theory. The derivation is rigorous in the sense of Gamma-convergence. In contrast to what one naturally would expect, our result shows that the limiting functional is not simply a quadratic functional of the second fundamental of the deformed plate. The limiting functional distinguishes between whether the deformed plate is locally shaped like a cylinder or not. For the derivation we investigate the oscillatory behavior of sequences of second fundamental forms associated with isometric immersions, using two-scale convergence. To do so, we have to treat two-scale convergence in connection with a nonlinear di?erential constraint. Joint work with Stefan Neukamm (MPIS Leipzig, WIAS Berlin.)

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MS108

An Optimization Based Atomistic-to-Continuum Coupling Method

Atomistic-to-continuum (AtC) coupling methods aim to combine the efficiency of continuum models with the accuracy of the atomistic models necessary to resolve local features. We present a new AtC method which seeks to minimize the error between the atomistic and continuum displacement fields over a suitably defined overlap region. We provide an error analysis of the method in the context of a 1D linear system with next-nearest neighbor interactions.

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MS108

Energy-Based Atomistic-to-Continuum Coupling

I will discuss the recent advances in the construction and analysis of the energy-based atomistic-to-continuum coupling.

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MS108

Numerical Analysis of the Blended Quasicontinuum Method

The energy-based Blended Quasicontinuum method (BQCE) is an atomistic-to-continuum coupling used to simulate defects such as cracks and vacancies in crystalline materials. I will present a numerical analysis of BQCE. I will then explain how the analysis can be used to choose optimal approximation parameters for the implementation of BQCE. I will also explain how the analysis leads to novel continuum models which can be used in versions of BQCE for materials which have multi-lattice structure.

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MS108

Consistent Atomistic/Continuum Coupling Methods

Atomistic/continuum coupling methods are a class of coarse-graining techniques for the efficient simulation of atomistic systems with localized defects. I will show that for general simple crystal lattices, patch test consistency is a necessary and sufficient condition for the first-order consistency of an energy based coupling method. We will construct consistent coupling energy functional by geometric reconstruction on the interface in 2D and 3D. I will remark on the stability of the method.

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PP1

Algorithm for Linear Programming Involving Interval Constraints

In real optimization, we meet the criteria of useful outcomes increasing or expenses decreasing and demands of lower uncertainty. Therefore, we usually formulate an optimization problem under conditions of uncertainty. In this paper, a new method for solving linear programming problems with Interval coefficients in the objective function and the constraints based on preference relations between intervals is investigated. To illustrate the efficiency of the proposed method, a numerical example is presented.

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PP1

Constitutive Models for the Macroscopic Response and Microstructure Evolution in Particle-Reinforced Elastomers at Finite Strains

This study presents the application of recently proposed, homogenization estimates (Avazmohammadi and Ponte Castañeda; J. Elasticity, 2012) for hyperelastic composites consisting of an incompressible matrix and aligned, rigid spheroidal particles, subjected to general (3-D), finite-deformation loadings. The major results of this study include: (1) the particles tend to orient themselves with the largest tensile loading axis, (2) the rotation of particles has

a significant impact on the macroscopic response and can lead to loss of strong ellipticity.

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PP1

Multi Stage Approach to Extract Microstructural Information in X-Ray Microtomography Images: Case Study of Fully Lamellar Titanium Alloy

(α+β) titanium alloys are widely used in the industry. An important materials science aspect is the understanding of their microstructural properties in relation to damage. No other nondestructive 3D techniques than X-ray microtomography can provide these information, provided the use of 3D image processing. The current work concentrates on the fully lamellar microstructure and uses directional filter bank, edge preserving smoothing combined with discrete geometry analysis to separately segment α-lamellar colonies and β grain boundaries.

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PP1

Quasi-Equilibrium Off-Lattice Kinetic Monte Carlo of Heteroepitaxy

We present an off-lattice kinetic Monte Carlo algorithm in $(1+1)$-dimensions that drives surface diffusion by a chemical potential gradient. Interactions between atoms are defined by the Lennard-Jones potential which removes the lattice restriction on atomic positions enforced by lattice based models. The method is validated by simulations of heteroepitaxial growth, annealing of strained bilayer systems and a qualitative verification of Stoney's formula.

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PP1

A Second Order Minimality Criterion for Free Discontinuity Problems

We present a sufficient condition for local minimality for a free discontinuity problem, in the context of a variational model for epitaxial growth of strained elastic films. We generalize previous results to the three dimensional case and to nonlinear elastic energies, deriving a minimality criterion expressed in terms of a suitable notion of second variation of the functional involved. Applications to the study of stability of flat morphologies are shown.

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PP1

A Quantitative Second Order Minimality Criterion for Cavities in Elastic Bodies

We consider a functional which models an elastic body with a cavity. We show that if a critical point has positive second variation then it is a strict local minimizer. We also provide a quantitative estimate.

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PP1

Morphological and Mechanical Properties of Entangled Triblock Copolymer Gels

A novel dissipative particle dynamics model which includes a modified segmental repulsive potential was used to elucidate the morphological/mechanical properties of triblock copolymer gels. The micelle size, distance between micelles, and the bridge fraction were calculated as a function of concentration, where only a strong dependence on concentration was observed for micelle size. The cross-link and entanglement contribution to the modulus were extracted from deformation simulations and were found to qualitatively agree with theoretical predications.

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PP1

Use of Sensitivity Analysis and Error Analysis to Implement Recursively Self-Consistent Programs

To conquer slowly and unstably oscillatory phenomena produced by stimulating recursively self-consistent calculation, invented scaling approaches, which stop the propagation errors of the recursive iterations, eliminate or reduce the possibilities of producing the oscillatory calculations. To grant a better practical solution at the next step of optimization processes, exploring primary errors is helpful to understand the sensitive mechanisms of the invented scal-

ing approaches.

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PP1

A Quasistatic Evolution Model for Perfectly Plastic Plates Derived by Gamma Convergence

The subject of this poster is the rigorous derivation of a quasistatic evolution model for a linearly elastic - perfectly plastic thin plate. As the thickness of the plate tends to zero, we prove via G-convergence techniques that solutions to the three-dimensional quasistatic evolution problem of Prandtl-Reuss elastoplasticity converge to a quasistatic evolution of a suitable reduced model. In this limiting model the admissible displacements are of Kirchhoff-Love type and the stretching and bending components of the stress are coupled through a plastic flow rule.

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PP1

Modeling Collective Chemical Effects in Carbon Nanotube Growth

We model and simulate collective chemical effects in the growth of populations of carbon nanotubes. When carbon deposits on the catalyst during growth, growth-enhancing gases are produced. We model the partial pressure of these gases using a diffusion equation and couple with a growth model developed by Puretzky, et al. [Applied Physics A, 2005]. We fit parameters to our model by comparing computer simulations with experimental results for growth of patterned carbon nanotube "forest" microstructures.

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PP1

Electro-active Polymer Composites at Finite Deformations: Effective Behavior and Stability Analysis

In this poster we present homogenization estimates for the effective response of electro-active polymer composites (EAPCs), consisting of a family of aligned rigid fibers firmly embedded in an ideal dielectric matrix and undergoing finite strains. Using such homogenization estimates, we investigate the effect of microstructural parameters on the electro-mechanical response of dielectric actuators made of fibrous EAPCs. We also study the effect of electromechanical instabilities and dielectric breakdown on the performance of such actuators.

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PP1

Electron Transport in Thin Semiconductor Gas Sensors

The aim of this work is to derive, from a kinetic description, a SHE model (for Spherical Harmonics Expansion) for electron transport in semiconductor gas sensor. Electron transport in the thin semiconductor gas sensors is modeled by a collisionless Boltzman equation subject to a periodic array of localized scatters modeling the periodic heterogeneities of the semiconductors material. The localized scatters may not conserve the electron number, and then a localized electronic charge have been manifested to reveal the localized absorption phenomenon. The limit of a large number of periodicity cells combined with a large time asymptotics leads to a homogenized diffusion equation (SHE model) with a non vanishing second term which represents the absorption term. The rigorous proof relies on fine estimates on the operator modeling the localized scatters.

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PP1

Spectra of Functionalized Operators Arising from Hypersurfaces

Functionalized energies, such as the Functionalized Cahn-Hilliard, model phase separation in amphiphilic systems, in which interface production is limited by competition for surfactant phase, which wets the interface. This is in contrast to classical phase-separating energies, such as the Cahn-Hilliard, in which interfacial area is energetically penalized. In binary amphiphilic mixtures interfaces are characterized by bilayers, which divide the domain of the dominant phase, A, via thin layers of phase B formed by homoclinic connections. We characterize the center-unstable spectra of the second variation of the Functionalized energy and obtain resolvent estimates to the operators associated with gradient flows of the Functionalized energies. This is an essential step to a rigorous reduction to a sharp-interface limit.

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PP1

A Density Result for GSBD and Its Application to the Approximation of Fracture Energies

We present an approximation result for functions $u : \Omega \to R^n$ belonging to the space $GSBD(\Omega) \cap L^2(\Omega, R^n)$ with $e(u)$ square integrable and $H^{n-1}(J_u)$ finite. The approximating functions u_k are piecewise continuous functions such that $u_k \to u$ in $L^2(\Omega, R^n)$, $e(u_k) \to e(u)$ in $L^2(\Omega, M^{n\times n}_{sym})$, $H^{n-1}(J_{u_k} \triangle J_u) \to 0$, and $\int_{J_{u_k} \cup J_u} |u_k^{\pm} - u^{\pm}| \wedge 1 dH^{n-1} \to 0$. As an application, we provide the extension to the vector-valued case of the Γ-convergence result in $SBV(\Omega)$ proved in [Ambrosio L., Tortorelli V.M., On the approximation of free discontinuity problems, Boll. Un. Mat. Ital. 6, 105-123].

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PP1

Zero Transmission in Waveguides with Thin Structured Membranes

Structured membrane devices, sometimes known as membrane metamaterials, can exhibit unusual and surprising wave scattering properties. I will present resent work on a particular such device consisting of a waveguide in which sound waves interact with a thin elastic membrane. With a proper choice of membrane structure the device will completely reflect incoming waves for certain frequencies. Using a new simplified model, this effect can be understood in a precise way.

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PP1

Domain Wall Motion in Magnetic Nanowires: An Asymptotic Approach

We study the motion of domain walls in a magnetic nanowire under the influence of small applied magnetic fields, material anisotropy, and applied electric current. The Landau–Lifshitz–Gilbert equation is linearized about a static solution and the magnetization dynamics investigated via a perturbation expansion. We compute leading order behaviour, propagation velocities, and first order corrections of both travelling waves and oscillatory solutions, and find bifurcation points between these two types of solutions.

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PP1

Tubes of Maximal Probability and Transition Pathway Sampling

We are studying how a collection of atoms, governed by Brownian dynamics, undergoes a conformational change. When the encountered energy barrier is much larger than the thermal energy of the atoms, the transition is a rare event. We probe the free energy landscape and directly sample such rare transition paths in an efficient manner using a Hybrid Monte Carlo method. This method includes thermal fluctuations and thus conserves the sample's thermodynamic significance. To interpret the data generated by direct sampling of the paths, we explore a novel method that approximates the physical measure with a Gaussian measure that can be viewed as a tube that encloses the vast majority of the paths. The optimal parameters are then determined by minimizing the asymmetric KullbackLeibler divergence between the two measures. The extracted parameters define the tube center and its width. We present results for a particle moving in several multi-welled two-dimensional potentials.

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PP1

***mystic* and Uncertainty Quantification in Materials Design, Analysis, and Failure**

We have developed a rigorous mathematical framework for quantifying uncertainty (*OUQ*), and a robust software (*mystic*) for solving high-dimensional global optimization problems. *Mystic* provides tools for constraining design space and targeting unique solutions, including suites of standard and statistical constraints, and constraints for legacy data and coupled or surrogate models. *Mystic* has been used in large-scale calculations of materials failure under hypervelocity impact and elasto-plastic failure in structures under seismic ground acceleration, among others.

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PP1

Mathematical and Computational Methods for the Analysis of Low-Energy Electron Microscopy/Diffraction of Graphene and Other Semiconductors

We present a computational method, using density-functional theory (DFT), to calculate low-energy electron microscopy (LEEM) spectra of semiconductor thin-films, including graphene. We solve Schrodinger equation boundary value problems with a Bloch wave matching approach using self-consistent potentials via DFT to approximate LEEM spectra better than previous model-potential methods in the lowest energy range. We compare results to experiment and discuss well-posedness and associated issues in obtaining the solution sets needed for matching at higher-energies.

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PP1

Renormalized Energy and Dynamics of Screw Dislocations with Antiplane Shear

We describe the dynamics for a system of screw dislocations subject to anti-plane shear. Variational techniques allow us to find minimizers for the energy functional associated with the system of dislocations in an elastic medium. Building on a model due to Cermelli and Gurtin, a weak notion of solutions (in the sense of Filippov) to ordinary differential equations is used to solve the dynamics problem. Some examples of interesting scenarios complement the presentation.

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PP1

On Modeling Plane-Strain Fracture Using Strain-Limiting Theory of Elasticity

In this work we study the problem of plane-strain fracture in the setting of a strain-limiting theory of elasticity. Recently Rajagopal and Walton used a new class of such models to study anti-plane strain fracture. Using asymptotic analysis of the model near the tip of crack, they showed that both stress and strain vanish at the crack-tip, and the crack separation displacement has a cusp-shaped profile. The purpose of present study is to extend this previous analysis to the setting of plane-strain fracture. In joint work with K. Gou, K. R. Rajagopal and J. R. Walton, we employ a combination of asymptotic and numerical techniques to show that both stress and strain vanish at the tip of the crack.

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PP1

Connection of Kinetic Monte Carlo Method for Surfaces to the Burton-Cabrera-Frank Model

There are many questions concerning the underlying physical processes and theoretical assumptions that yield the Burton- Cabrera-Frank (BCF) model of step-flow. We formally derive the BCF theory from an atomistic, kinetic Monte Carlo model of the surface in 1+1 dimensions with one step. Our analysis (i) shows how the BCF theory describes a surface with a low density of adsorbed atoms, and (ii) establishes near-equilibrium conditions ensuring that the theory remains valid for all times.

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PP1

Evolution Results for Epitaxially Strained Thin Films

We consider the evolution equation with curvature regularization that models the motion of a two-dimensional thin film by evaporation-condensation on a rigid substrate. The film is strained due to a mismatch between the crystalline lattices of the two materials and the film surface anisotropy is taken into account. The author established short time existence, uniqueness, and regularity of the solution using De Giorgi's minimizing movements to exploit the L^2-gradient flow structure of the fourth order parabolic equation. This seems to be the first analytical result for the evaporation-condensation case in the presence of elasticity.

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PP1

A Model for Crack Growth with Branching and Kinking

We study an evolution model for fractured elastic materials in the 2-dimensional case, for which the crack path is not known a priori. We introduce some general assumptions

on the fracture sets structure suitable to allow for kinking and branching to develop. We define the front of the fracture and its velocity. By means of a time-discretization approach, we prove the existence of a continuous-time evolution that satisfies an energy inequality and a stability criterion.

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PP1

Behavioral Modeling of Corundum under the Effect of Porosity Rate

Corundum Known for its relatively high hardness, its other characteristics depend on the rate of porosity that varies depending on the manufacturing process. One of the characteristics to consider is the value of the tensile stress in a standard test to failure as a function of the force applied and the rate of porosity. In this study, to analyze the simultaneous effect of two parameters, we used the statistical method of design of experiments.

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PP1

Practical Modelling of Statistical Nanocomposite Optical Coating Materials for Filter and Absorber Specifications: Oscillator Model, Mixing Model and Spectral Moments Approaches

Metal-dielectric nanocomposites are candidate materials for applications in optical coatings when in the specification tailored optical absorption behaviour is required. In order to make such nanocomposite coatings accessible to commercial coating design and characterization software, reliable mathematical modelling of the dispersion of the composites effective optical constants is essential. We present different possible approaches and discuss their relative use for optical characterization or design tasks at practically relevant examples (beamsplitters, color filters, decorative coatings).

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PP1

Nonlinear Solvers for Dislocation Dynamics

We present results of applying accelerated fixed point and Newton nonlinear solvers for implicit integration of dislocation dynamics simulations in the ParaDiS code. In particular, we compare performance of fixed point and Anderson accelerated fixed point methods for large-scale, parallel simulations looking at parallel efficiency, algorithmic scalability, and robustness. Preliminary results show significant speedup using the acceleration methods. These methods will also be compared with a Newton iteration.

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PP1

Collective Behavior of Walls of Dislocations

We try to understand plastic behavior of metals by upscaling the micro-mechanics of dislocations. We consider a highly simplified dislocation network, which leads to our microscopic model being a one dimensional particle system, in which the interactions between the particles are singular and non-local. Finally, we derive the effective equations by means of Gamma-convergence on the space of probability measures.

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