Speaker: Russ Caflisch

Title: Modeling and Simulation for Plasmas with Excitation and Ionization

Abstract:
This talk describes a Monte Carlo simulation method for excitation/deexcitation and ionization/recombination in a plasma. The atoms and ions in the plasma are represented by continuum densities and the electrons by a particle distribution. The wide range of kinetic rates for these processes leads to computational bottlenecks that are overcome by development of acceleration techniques. An additional difficulty is the singularity in the recombination rate for small electron energy which prevents use of the usual acceptance/rejection method. The simulation method is developed for an idealized analytic model of the excitation and ionization cross sections, both in energy and in angle, formulated to be consistent with detailed balance. Numerical results are presented to demonstrate the efficiency of the method on spatially homogeneous problems.

Speaker: Carme Calderer

Title: Gels: modeling, analysis and applications

Abstract:
This presentation deals with models of gels from the point of view of mixture theory. The governing system combines nonlinear elasticity, diffusion, dissipation and also electric effects. We analyze initial, boundary value problems relevant to applications to biomedical and drug delivery devices, and to biological fibers. To address the latter topic, we appeal to anistropy tools from the theory of liquid crystal elastomers. We examine buckling and "peeling" instabilities, which are particularly relevant to predictions on the life cycle of body implantable devices.

Speaker: Rustum Choksi

Title: The Phase Diagram for Microphase Separation of Diblock Copolymers: an approach via a Nonlocal Cahn-Hilliard Functional.

Abstract:
Diblock copolymers are produced by joining two distinct polymer chains, each of a certain monomer species which are thermodynamically incompatible. Phase segregation of these blocks gives rise to an amazingly rich class of nanostructures which allow for the synthesis of materials with tailor made mechanical and chemical properties.

One of the main challenges is to describe and predict the nanostructure given a set of material parameters. A simple model based upon a nonlocal Cahn-Hilliard functional lends itself well to mathematical analysis and numerics. In this talk I will discuss the phase diagram associated with this nonlocal functional. Focusing on certain parameter regimes, a combination of rigorous analysis and numerics will be used in an attempt to characterize minimizers.

Speaker: Yuehua Cui

Title: Large-scale genome-wide association studies via entropy test

Abstract:
Understanding the biological mechanisms that associate genetic variants with complex diseases has been a major task in modern genetical research. Genetic association studies which assess correlations between genetic variants and phenotypic differences in a population level, serve as standard means for this purpose. Recent radical breakthroughs in biotechnology have produced massive amount of large scale genome-wide single nucleotide polymorphisms (SNPs) data, which offer potential prospects in elucidating the genetic etiology of complex diseases. However, the high-dimensional genome-wide SNP data which contain thousands to millions of features across the genome, present daunting challenges in statistical modeling and testing. Traditional analysis by testing each single SNP separately is less efficient and less powerful. Moreover, single SNP analysis suffers from power loss and inflated false positives without considering correlations among SNPs. In this talk, I will present an entropy-based testing procedure by considering SNPs in a gene for an association test. We focus genes as testing units since genes are the functional units in most organisms. The entropy test takes a nonlinear transformation of the joint genotype distribution in both cases and controls, which substantially amplifies association signals and increases testing power. A grouping algorithm based on a penalized entropy measure is proposed to reduce the dimension of the entropy test statistic. Both simulation and real data analysis will be presented to show the utility of the proposed test framework.

Speaker: David Kinderlehrer

Title: New perspectives on texture evolution

Abstract:
Cellular structures coarsen according to a local evolution law, a gradient flow or curvature driven growth, for example, limited by space filling constraints, which give rise to random changes in configuration. Among the most challenging and ancient of such systems are polycrystalline granular networks, especially those which are anisotropic, ubiquitous among engineered materials. It is the problem of microstructure. These are large scale metastable, active across many scales. We discuss recent work in this area, especially the discovery and the theory of the GBCD, the grain boundary character distribution, which offers promise as a predictive measure of texture related material properties. There are many mathematical challenges and the hint of universality.

Speaker: Chun Liu

Title: Energetic Variational Approaches in Complex Fluids: Kinematic Transport

Abstract:
In this talk, we will demonstrate the effects of different kinematic transport in the hydrodynamic models for complex fluids. In particular, we will focus on how to incorporate these properties in the energetic variational framework. We will also show some recent work on the generalized Jeffery's orbits.

Speaker: Cyrill Muratov

Title: Self-induced stochastic resonance: How new non-random behaviors can arise from the action of noise.

Abstract:
It is usually assumed that when a dynamical system is subjected to small random perturbations, its behavior remains essentially unchanged, apart from the noise appearing on top of the otherwise deterministic dynamics. That this is not always the case is dramatically demonstrated by the phenomenon of stochastic resonance, whereby a small but finite amount of noise produces coherent phase locking between an applied periodic signal and the system's dynamical response. Perhaps even more surprisingly, the addition of small noise may produce new coherent behaviors that are fundamentally absent in the dynamics of the noise-free system, i.e, noise can actually play a constructive role in creating dynamics that are essentially non-random. This talk will present an overview of SISR (Self-Induced Stochastic Resonance), a robust mechanism by which such dynamics may emerge out of noise. I will demonstrate SISR in action for systems whose common dynamical feature is excitability. I will show that noise in an excitable system may result in the onset of quasi-deterministic limit cycle oscillations, which, in particular, manifest themselves as pacemakers of target pattens in two-dimensional excitable media. I will argue that one needs to re-examine the role of small noise in modeling the dynamics of complex dynamical systems.

Speaker: Houman Owadi

Title: Homogenization of elasticity equations without scale separation.

Abstract:
We investigate the homogenization of divergence form elliptic(scalar and vectorial, static and dynamic) equations with arbitrary bounded coefficients (in particular in situations where assumptions of scale separation and/or ergodicity are not satisfied). We show the existence of an optimal basis allowing for the approximation of the solutions of these equations with a minimal (optimal given the desired accuracy) number of degrees of freedom and an error constant which is independent of the contrast of the material and the regularity of the domain. We also show how that these results can be extended to less optimal bases (but faster to compute) based on a new class of analytical inequalities analogous to the div curl lemma in homogenization theory. Applications of this work range from reservoir modeling to virtual liver surgery. This is a joint work with Leonid Berlyand.

Speaker: Robert Pego

Title: On statistical self-similarity in clustering and coarsening processes

Abstract:
I will discuss two kinds of clustering phenomena that can lead to self-similar behavior for domain or particle size distributions on large scales. The first is shock-wave clustering in Burgers equation. With random-walk initial data of certain kinds, this is described by Smoluchowski's coagulation equation with additive rate kernel, and we can establish precise criteria for convergence of the solution process to self-similar form. The second is the phenomenon of domain coarsening in the one-dimensional Allen-Cahn PDE. This can be described by a hierarchy of models, leading to a min-driven coagulation process for domain walls on the largest scales. By extending an analysis of Gallay and Mielke for this process, we establish dynamical well-posedness in the space of probability measures, necessary and sufficient conditions for approach to self-similar form, and a Levy-Khintchine representation formula for eternal solutions. This is joint work with Govind Menon and Barbara Niethammer.

Speaker: Peter Smereka

Title: Modeling and Simulation of Heteroeptixial Growth

Abstract:
In this talk I will describe a discrete kinetic Monte Carlo (KMC) model used for the simulation of heteroeptixial growth. Connections of this model with more traditional continuum formulations will be disussed. It will be argued, that despite its apparent simplicity, the KMC model contains all the physics accounted for in most continuum descriptions. However, the KMC model naturally captures physical effects not easily modeled in continuum formulutions such as stochastic effects and nucleation. The KMC model is computationally challenging due the long range nature of elastic interactions. This talk will discuss the Fourier-Multigrid method for fast computation of the elastic displacement field. A technique for obtaining inexpensive upper bounds on transition rates will be presented. Finally, the principle of energy localization is explained which combined with the expanding box method allows one to accurately compute changes elastic energy using local calculations, resulting in a tenfold increase in computation speed. These ideas are combined to allow one simulate heteroeptitaxy using KMC in physically interesting regimes. This is joint work with A. Baskaran, J. Devita, T. Schulze, and G. Russo.

Speaker: Peter Sternberg

Title: Lower dimensional energetic models via Gamma convergence

Abstract:
In this talk I will survey some results on Gamma convergence settings where energies are posed on thin 3d domains. The limiting energies are then defined on either 2d or 1d domains. Examples will largely be drawn from the Ginzburg Landau theory of superconductivity.

Speaker: Richard Tsai

Title: Numerical Multiscale Methods for Nonlinear and Highly Oscillatory ODEs

Abstract: A multiscale method for computing the effective slow behavior of a system of weakly coupled general oscillators is presented. The oscillators may be either in the form of a periodic solution or a stable limit cycle. Furthermore, the oscillators may be in resonance with one another and thereby
generate some hidden slow dynamics. The proposed method relies on correctly tracking a set of slow variables that is sufficient to approximate any variable and functional that are slow under the dynamics of the ODE. The technique is more efficient than exist-ing methods and its advantages are demonstrated with examples. The algorithm follows the framework of the heterogeneous multiscale method.

Speaker: Eric Vanden-eijnden

Title: Transition Pathways of Rare Reactive Events in Complex Systems

Abstract:
The dynamics of biomolecular systems is typically characterized by a wide range of time scales, complicating their study via computer simulations. Of particular difficulty are situations which involve rare reactive events such as conformation changes of macromolecules, nucleation events during first-order phase transitions, chemical reactions, or bistable behavior of genetic switc. The occurrence of these rare events is related to the presence of dynamical bottlenecks of energetic and/or entropic origin which effectively partition the configuration space of the system into metastable basins. The system spends most of its time fluctuating within these long-lived metastable states and only rarely makes transitions between them. The rare events then determine the long-time evolution of the system.

In this talk, I will present a general theoretical framework termed transition path theory (TPT) for the description of rare reactive events and compare it to other approaches such as the classical transition state theory (TST) and the more recent transition path sampling (TPS). I will also show that TPT can used to design efficient numerical algorithms such as the string method for the identification of the pathway, free energy and rate of the rare events. Both the theory and the numerics will be illustrated via examples.

Speaker: Jack Xin

Title: Statistical analysis and computation of time domain blind source separation methods.

Abstract: Blind source separation aims to recover source signals from their mixtures without detailed knowledge of the mixing environment. It arises in many contexts such as cocktail party conversation, brain wave analysis, and biomedical imaging. When signals are time series such as sounds, mixing occurs in time in the form of convolutions. We introduce mixing models and formulate inverse problems based on decorrelation or information maximization in the time domain (without Fourier transform). We present a soft-constrained stochastic gradient descent method, and show its convergence properties as well as computation results.

Speaker: George Yin

Title: Two-Time-Scale Systems Involving Stochastic Discrete Events

Abstract:
In this talk, we study stochastic systems that have a discrete event component modeled as a switching process. Two-time-scale formulations are used to reduce the computational complexity. The processes to be examine include Markov chains, switching diffusion processes, jump-diffusions with switching, and hybrid systems with continuous state dependent switching processes. After motivational examples arising from manufacturing, communication networks, and finance are mentioned, we present asymptotic properties of such processes.

Speaker: Hao-Min Zhou

Title: Fast Numerical Simulations for Stochastic Maxwell Equations with Applications in Photonic Crystal Spectrometer Design.

Abstract: In this presentation, we propose a new stochastic model for general spatially incoherent sources with applications in photonic crystal. The model naturally incorporates the incoherent property and leads to stochastic Maxwell equations. We also propose a fast numerical method based on Wiener Chaos Expansions (WCE), which convert the random equations into coupled system of deterministic equations, so that they can be solved using efficient deterministic methods. In the applications of photonic crystal, the new methods can achieve 2 order of magnitude faster computation time over the standard method.