PLENARY SPEAKERS

Mark Ablowitz

University of Colorado

Nonlinear waves: from oceans to `optical graphene'

The study of localized waves has a long history dating back to the discoveries in the 1800s describing water waves in shallow water. In both fluid dynamics and nonlinear optics there has been considerable interest in various aspects of localized waves. This lecture will center on the dynamics of nonlinear wave motion in water waves including `line-soliton' interactions, and photonic lattices. In optical lattices with honeycomb backgrounds, novel discrete nonlinear systems will be discussed. Honeycomb lattices appear widely in physics, a notable case being graphene.

Carson Chow

National Institutes of Health

Finite-size Effects in Neural Networks

The dynamics of neural networks have traditionally been analyzed for small systems or in the infinite size mean field limit. While both of these approaches have made great strides, large but finite-sized networks have not been explored as much analytically. Here, I will show how the dynamical behavior of finite-sized systems can be inferred by expanding in the inverse system-size around the mean field solution. The approach can also be used to solve the inverse problem of inferring the effective dynamics of a single neuron embedded in a large network where only incomplete information is available. The formalism I will outline can be generalized to any high dimensional dynamical system.

Sally Morton

University of Pittsburgh

Statistics and Comparative Effectiveness Research

Which healthcare treatment "works best, for whom, and under what circumstances?" (Clancy and Slutsky, 2009). This is the defining question of comparative effectiveness research (CER), which encompasses all patients, including those traditionally underrepresented in clinical research such as individuals with comorbid conditions. CER, as well as the broader area of "patient-centered outcomes research," has received increased attention due to healthcare reform legislation. CER studies may include both the generation of new evidence and the synthesis of existing evidence. As a result, CER methods comprise a variety of statistical design and analysis methodologies such as pragmatic trials, observational studies, propensity scores, and network meta-analysis. In this talk, I will define CER, and briefly discuss its policy origins. From a statistician's perspective and via examples, I will seek to elucidate both CER's promise and challenge in helping patients, clinicians, and policy-makers reach more informed healthcare decisions.

Keith Promislow

Michigan State University

Network Formation and Ion Conduction in Ionomer Membranes

Selective charge transport is an essential step in efficient energy conversion. Ionomer membranes, formed from crosslinked, charged polymers, imbibe solvent to form nanoscaled network structures which lie at the heart of many energy conversion devices. Experimental data shows that the networks are hysteretic, evolving on time scales of minutes and hours, far outside the reach of molecular simulations. We present a novel reformulation of the classical Cahn-Hilliard free energy that permits the inclusion of solvation energy and counter-ion entropy within a continuum model. Gradient flows on the Functionalized Cahn-Hilliard energy show bi-stability of bilayer, pore, and micelle dominated networks. We present several sharp interface reductions of these energies, including classes of curvature driven flows that couple to the underlying structure of the network.

Jane Wang

Cornell University

How do Insects Fly and Turn

Insect's aerial acrobatics results from a concerted effort of its brain, flight muscles, and flapping wings. To understand insect flight, we started from the outer scale, analyzing the unsteady aerodynamics of a flapping wing, and are gradually working toward the inner scale, deducing the control algorithms employed by insects. In this talk, I will first discuss the aerodynamics tricks that a dragonfly employs to hover and fly efficiently. I will then discuss how fruit flies recover from aerial stumbles, and how they make subtle wing movements to induce sharp turns in 40-80ms. This work involves direction numerical simulations, reduced order models for unsteady fluid forces, and analyses of experimental data of insects in free flight.

MINISYMPOSIUM SPEAKERS

Vladimir Ajaev

Southern Methodist University

Rupture of Liquid Films on Structured Surfaces

Liquid transport in microfluidic devices can be enhanced significantly by using microchannels with structured rather than flat walls when gas is trapped between the elements of the structure. Viscous flow in such channels is modeled using the Navier slip condition with the effective slip length that depends on the parameters of the structure. However, since flow in microfluidic devices is usually multiphase, the issue of interaction between drops or bubbles and the channel walls becomes important for determining the overall transport rates. Of particular significance are the conditions of rupture of a thin liquid film separating a drop or a bubble from the structured wall of the microchannel. We develop both linear and nonlinear models of rupture of a liquid film between a gas bubble and a structured wall with gas trapped inside the grooves. Both London- van der Waals disjoining pressure and electrostatic effects are incorporated into the models. Stability criteria are identified as functions of liquid properties and the parameters of the structure. Joint work with C. Ketelaar (SMU) and E.Y.Gatapova and O.A.Kabov (Institute of Thermophysics, Novosibirsk 630090, Russia).

Silas Alben

Georgia Institute of Technology

Interactions between Vortices and Flexible Bodies

Fish often encounter distributions of vorticity while swimming, and can use the interaction to enhance propulsion. We consider models of this phenomenon involving point vortices and flexible bodies. For active swimmers, swimming with a well-defined phase relative to a vortex street can enhance thrust. We calculate thrust-optimizing motions. We also consider the interactions between a single point vortex and passive flexible walls and filaments. We identify traveling-wave solutions for circular and infinite walls. For flexible filaments we find finite-time collisions with a power-law behavior which can be explained using the equations for the coupled system.

Paul Albert

Eunice Kennedy Shriver National Institute of Child Health and Human Development

A Linear Mixed Model for Predicting a Binary Event Under Random Effects Misspecification

The use of longitudinal data for predicting a subsequent binary event is often the focus of diagnostic studies. This is particularly important in obstetrics, where ultrasound measurements taken during fetal development may be useful for predicting various poor pregnancy outcomes. The focus of this paper is on developing a class of joint models for the longitudinal measurements and binary events that can be used for prediction. A shared random parameter model is proposed for linking the two processes together. Under a Gaussian random effects assumption, the approach is simple to implement with standard statistical software. Using asymptotic and simulation results, we show that estimates of predictive accuracy under a Gaussian random effects distribution are robust to severe misspecification of this distribution. However, under some circumstances, estimates of individual risk may be sensitive to severe random effects misspecification. We illustrate the methodology with data from a longitudinal fetal growth study.

Karim Azer

Merck Research Laboratories

Near to the Heart - Physiological Modeling in Cardiovascular Diseases

Blood pressure medications may potentially lower arterial blood pressure in different arteries to varying degrees. Mathematical modeling of the propagation of the pulse in the systemic circulation and understanding drug effects on blood pressure in different arteries may lead to the development of improved therapies for hypertension. In this talk, we provide an overview of the utility of mathematical principles in drug development. We will demonstrate the application of mechanical models of the circulation in hypertension research. Moreover, we will show how characterization of arterial hemodynamics can (1) provide valuable insight into the distribution of pressure in the circulation, (2) aid in the exploration of novel therapies for hypertension, as well as (3) improve understanding of the action of existing ones.

Alexander Barnett

Dartmouth College

Fast Computation of Eigenfrequencies of Planar Domains via the Spectrum of the Neumann-to-Dirichlet Map

We present a new method for the spectrum and eigenfunctions of a planar star-shaped Dirichlet domain. It is `fast' since it is computes a cluster of eigenfunctions (numbering of order the square-root of the eigenvalue) with the effort usually taken to find a single one. For a domain 400 wavelengths across, and relative error 1e-10, the resulting speed-up is 1e3. Its error analysis is rigorous, and it achieves higher-order accuracy than the related `scaling method'. I will also discuss a new technique for evaluation of potential fields close to their source curves. Joint work with Andrew Hassell (ANU).

Andrea Barreiro

Southern Methodist University

Modeling Collective Neural Activity: When are Pairwise Maximum Entropy Methods Good Enough?

Recent experimental studies find that the activity patterns of many neural circuits are well described by pairwise maximum entropy (PME) models which require only the activity of single neurons and neuron pairs even in cases where circuit architecture and input signals seem likely to create a richer set of outputs. Why is this the case? We study spike patterns in a general class of circuits, and attempt to draw general principles about the effects of network architecture and input statistics on the complexity of output spiking patterns. Two significant findings have emerged: in feedforward circuits, responses to unimodal inputs were well described by PME models, while bimodal input signals drove significant departures. Secondly, biophysically motivated recurrence can drive significant departures when added to feedforward circuits.

As a particular application, we investigate the performance of PME models in retinal ganglion cell (RGC) circuits with different architectures and inputs. We find that the distinct filtering properties of parasol cells suppress higher-order interactions by suppressing bimodality in light stimuli, offering a possible mechanism for the remarkable success of PME models in this experimental setting.

Vrushali A. Bokil

Oregon State University

An Analysis of the Uniaxial PML Model For Maxwell's Equations in Dispersive Media

We study the Uniaxial Perfectly matched layer (UPML) model applied to Maxwell's equations in linear dispersive media using energy techniques. We consider the two dimensional TE mode of Maxwell's equations along with single pole Debye and Lorentz polarization models. We obtain uniform in time stability results under certain assumptions on the UPML parameters. We also obtain some energy decay results under additional assumptions on the UPML parameters, indicating the absorbing properties of the UPML model. Next, we consider the discretization of the UPML model using the lowest order edge finite elements. Based on the energy decay results of the continuous model, we investigate the stability of the finite element method for discretizing the UPML model.

Dean Bottino

Hoffmann- La Roche, Inc

A Mathematical Modeling Framework for Antibody-Dependent Cell Mediated Cytotoxicity (ADCC)

Antibody-dependent cell-mediated cytotoxicity (ADCC) is thought to augment the efficacy of IgG1 mAb therapeutics (eg. cetuximab) via the recruitment and activation of CD16+ cells which in turn will mediate tumor cell killing. This observation has led to drug design efforts to intentionally exploit ADCC for enhanced anti-tumor efficacy. For example, GA201 (Roche pRED Oncology) is a humanized and glycoengineered IgG2 anti-EGFR monoclonal antibody (mAb) with enhanced ADCC currently undergoing investigation in phase 2 trials. The dual mechanisms of action of ADCC-enhanced mAbs such as GA201 result in new and challenging drug development questions, for example:

1. Can we quantify the relative contributions of ADCC and target inhibition toward tumor shrinkage?
2. In light of (1), what markers (eg. KRAS mutation status, NK cell function) are predicted to confer sensitivity or resistance to the mAb?
3. Given observed kinetics of CD16+ cell depletion and recovery following administration of the mAb, what is the optimal schedule to optimize ADCC?
4. In the case of combination therapy with an immune-enhancing treatment, what dose and schedule would provide optimal synergy with the mAb's ADCC effect?

We propose a mathematical modeling framework for ADCC with the intention of addressing the questions posed above across several ADCC-relevant therapies. The proposed model would integrate clinically obtainable data sources, for example: FACS counts of (CD16+/56+) cells, NK cell function (CD107a, K562), tumor size (CT scan), mAb concentration in blood, and downstream target inhibition (eg pERK).
Joint work with Micha Levi, Alex Passioukov, Christian Gerdes, Jon Chick, Paul Delmar, Luigi Manenti, and James Rosinski (all Roche employees).

Yassine Boubendir

New Jersey Institute of Technology

About Domain Decomposition Methods for Acoustic Problems

In this talk, I begin by setting the mathematical non-overlapping domain decomposition method for the transmission problem. I'll describe the transmission conditions difficulties and the possible proofs of convergence. The second part will be dedicated to a new quasi-optimal algorithm. It is based on a combination of an appropriate choice of transmission conditions and a suitable approximation of the Dirichlet to Neumann operator.

Jasna Brujic

New York University

From Sphere Packings Towards Biological Tissues

Cell-cell contacts in tissues are continuously subject to mechanical forces due to homeostatic pressure and active cytoskeleton dynamics. While much is known about the molecular pathways of adhesion, the role of mechanics is less well understood. To isolate the role of pressure we present a dense packing of functionalized emulsion droplets in which surface interactions are tuned to mimic those of real cells. By visualizing the microstructure in 3D we find that a threshold compression force is necessary to overcome electrostatic repulsion and surface elasticity and establish protein-mediated adhesion. Varying the droplet interaction potential maps out a phase diagram for adhesion as a function of force and salt concentration. Remarkably, fitting the data with our theoretical model predicts binder concentrations in the adhesion areas that are similar to those found in real cells. Moreover, we quantify the adhesion size dependence on the applied force and thus reveal adhesion strengthening with increasing homeostatic pressure even in the absence of active cellular processes. This biomimetic approach reveals the physical origin of pressure-sensitive adhesion and its strength across cell-cell junctions.

Fioralba Cakoni

University of Delaware

Transmission Eigenvalues in Inverse Scattering Theory

The transmission eigenvalue problem is a new class of eigenvalue problems that has recently appeared in inverse scattering theory for inhomogeneous media. Such eigenvalues provide information about material properties of the scattering object and can be determined from scattering data, hence can play an important role in a variety of problems in target identification. Transmission eigenvalue problem is non-selfadjoint and nonlinear which make its mathematical investigation very interesting. In this lecture we will describe how the transmission eigenvalue problem arises in scattering theory, how transmission eigenvalues can be computed from scattering data and what is known mathematically about these eigenvalues. The investigation of transmission eigenvalue problem for anisotropic media will be discussed and Faber-Krahn type inequalities for the first real transmission eigenvalue will be presented. We conclude our presentation with some recent preliminary results on transmission eigenvalues for absorbing and dispersive media, i.e. with complex valued index of refraction, as well as for anisotropic media with contrast that changes sign. Few numerical examples will be presented showing the applicability of transmission eigenvalues in non-destructive testing.

Ricardo Carretero

Nonlinear Dynamical Systems group (NLDS) San Diego State University

Matter Wave Vortices: The Quantum Spirograph

Motivated by recent experiments studying the dynamics of configurations bearing a small number of vortices in atomic Bose-Einstein condensates (BECs), we illustrate that such systems can be accurately described by ordinary differential equations (ODEs) incorporating (a) vortex precession induced by the harmonic trap confining the BEC and (b) vortex-vortex interactions. The dynamics is studied in detail at the ODE level, both for the equal and opposite charge vortex pairs. Co-rotating steady states are identified about which perturbations lead to spirographic (epitrochoidal) motion with excellent agreement with experimental observations. A detailed analysis of the ensuing ODEs reveals the possibility of stable asymmetric states bifurcating from symmetric ones. Cases with more than two vortices are also discussed.

Zhiyi Chi

University of Connecticut

Asymptotic Power Equivalence of False Discovery Rate Control and Bayes Classification under Sparsity

The false discovery rate (FDR) control was recently shown to be asymptotically Bayes optimal under sparsity when it is viewed as a type of classification. Since power is a primary concern of the FDR control, while the Bayes risk is a linear combination of Type I error and power that need not have a priori preference to power, an important question is how the FDR control and the Bayes classifier compare in terms of power. Under rather general and easy-to-check assumptions on the null and alternative distributions, we show that the two have asymptotically the same power under sparsity conditions. This is established in a unified way for multiple tests on location, scale, or exponent, as well as for the case where the FDR control is applied region-wise, with results associated with different regions combined afterward. The piecewise FDR control can be used when neither upper-tail nor lower-tail p-values are suitable for multiple testing. The transformations involved in the tests, such as shift in location and scaling, need not be global. Rather, they can be applied to part of the null distribution, resulting in the alternative distribution being a “tilted” or “twisted” version of the null distribution.

Fredric S. Cohen

Rush University Medical Center

Physical Aspects of Biological Membrane Fusion

Fusion between two biological membranes is an essential event in a wide range of continuously occurring processes, such as secretion of neurotransmitters and trafficking of proteins; it is also critical for important sporadic events, such as fertilization of an egg by sperm and viral infection. In membrane fusion, two distinct membranes merge into one, resulting in the continuity of two formerly separated aqueous compartments. A fusion pore is the structure that connects the two membranes and its lumen provides the pathway for exchanges of aqueous contents. The central biophysical problem is to understand how a fusion pore forms and then enlarges. In viral fusion, for example, enlargement must occur if genetic material is to pass from the virus to the cellular interior, initiating infection. Proteins control membrane fusion, but it is the lipids that do the actual fusing. Lipids confer fluidity to the membrane that is necessary for the multiple deformations that occur during fusion. Full fusion proceeds in three main stages: (1) Hemifusion, in which contacting, opposing monolayers of two separate bilayer membranes merge; the four original monolayers have been reduced to two, and a hemifusion diaphragm composed of two monolayers, one from each original bilayer, continues to separate the aqueous compartments; (2) A pore forms in the hemifusion diaphragm; (3) The fusion pore enlarges. Questions and problems in membrane fusion that are amenable to physical and mathematical modeling will be presented. For example, studies that have used continuum membrane mechanics to describe each stage have usually employed equilibrium approaches, whereas membrane fusion is a dynamic process during which energy is dissipated. Also, energy barriers separate the three main stages of fusion, and these transition barriers must be surmounted for fusion to proceed. Membrane proteins provide the necessary sources of energy to overcome these transition barriers, but methodologies that can calculate the height of the barriers need to be developed.

Shibin Dai

Michigan State University

Functionalized Cahn-Hilliard Equation: Competitive Evolution of Bilayers and Pores

The functionalized Cahn-Hilliard equation is introduced as a phase field model to describe the evolution of complex nanoscale structures similar to those observed in Polymer Electrolyte Membrane (PEM) fuel cells. Such complex structures include single layers, bi-layers, pore networks and micelles, etc. We concentrate on the motion of closed bi-layers and pores. Using asymptotic analysis, we analyze their inner structures and derive the leading order normal velocity in different time scales. Also we will show the mechanism under which they compete with each other.

Laurent Demanet

MIT

What type of matrix structure is right for the high-frequency Helmholtz equation?

The Green's function and DtN maps for the high-frequency Helmholtz equation in variable media have a lot of structure, yet our current linear algebra tool kit still has a hard time dealing with it. I will report on some recent numerical experiments involving new preconditioners, or new methods for absorbing boundary conditions.

Sunil K. Dhar

New Jersey Institute of Technology

Bootstrap Tests for Increased Discrimination of New Hemodynamic Variables

Medical practitioners are constantly looking for more efficient ways of measuring patient monitoring data. Clinicians therefore research for new variables with higher variability providing greater discriminative ability between patients. One such method of obtaining new unit-less measurements is through normalizing the variable by its location statistics. Measurements from a minimally-invasive hemodynamic device known as esophageal Doppler monitor are used as the data source for the study. The normalized data makes the process dependent. Hence bootstrap based tests are a necessity for variability evaluation. These bootstrap tests are validated via simulation. The usefulness of these tests is demonstrated for this data on patients who were on mechanical ventilation or underwent surgery.

Julien Diaz

INRIA, France

Stability Analysis of the Interior Penalty Discontinuous Galerkin Method for the Wave Equation

The Interior Penalty Discontinuous Galerkin Method (IPDGM) is probably one of the most efficient Discontinuous Galerkin method for solving the wave equation. However, the appropriate determination of the penalization parameter is still an issue, since a too low value leads to unconditionaly unstable schemes while a too large value severely hampers the CFL condition of the scheme. In the first part of the talk, we show how to determine the penalization parameter in the case of cartesian meshes and we propose an analytical expression of the CFL condition with respect to this parameter. Then, we consider the case of triangular meshes, for which it is not possible to obtain an analytic expression of the penalization parameter. We show, thanks to a numerical study, that it should rather be expressed as a function of the radius of the inscribed circle of the triangles rather than of the radius of the circumscribed circle. Moreover, we propose more accurate expressions based on the angles of the triangles. Finally, we analyze the influence of these different expressions on the CFL condition of the scheme.

Bob Eisenberg

Rush Medical College

Ionic Interactions in Biological Systems: a Variational Treatment

Biology depends on interactions of ions. Interactions with trace concentrations (10^{-6} M) of calcium control most proteins. Interactions of sodium and potassium with ion channels produce nerve signals. Interactions are enormous in highly concentrated solutions (20 M; for comparison, ***solid*** NaCl is 37 M), near DNA, channels, and membranes/electrodes of electrochemical technologies. Classical biochemistry represents solutions as infinitely dilute. Electrostatic theories (Poisson-Boltzmann-PNP) include ions as points, not spheres. Physically based variational methods have not been available for such systems. Now, a general Energetic Variational Approach has been developed by Chun Liu, more than anyone else. Existence and Uniqueness are proven. Incompressible Navier Stokes equations are derived. A variational model of finite ions in solution is available. **If another ion** (magnesium) **or field** (convection) **is included, the resulting Euler Lagrange equations (PNP-delta) automatically describe new interactions with minimal new parameters.** PNP-delta equations have been integrated for ion channels. PNP-delta is a superset of models already used to analyze and predict selectivity of the biologically and medically important (heart) calcium, (nerve) sodium, and (muscle) RyR channels in >100 multicomponent solutions over concentration ranges of 10^6. Numerical inefficiencies are being removed but a great deal remains to be done and many new applications explored.

Jason Fowlkes

Oak Ridge National Laboratory

The Directed Assembly of Linear Metallic Nanoparticle Chains by Nanolithography and Pulsed Laser Induced Dewetting

Directly–assembly via nanolithography and pulsed laser melting was used to assemble nanoparticle chains with precise size and spacing. Specifically, liquid–phase, pulsed laser induced dewetting (PLiD) was used to convert metallic thin film strips into nanoparticle chains exhibiting an unnaturally low deviation in particle size and spacing. Two–dimensional thin film strips retracted into three–dimensional fluid rivulets during the initial stages of dewetting. Next, rivulet break–up ensued forming nanoparticle chains according to a process resembling Rayleigh–Plateau fluid jet destabilization. The resulting mean nanoparticle size and pitch were controlled, yet disperse. However, by imposing a synthetic sinusoidal perturbation onto the edges of initial thin film strips, the dispersion in the final nanoparticle chain was drastically reduced. The sinusoidal perturbations transformed into varicose oscillations on the rivulet surface.

The significant findings reported here are; (1) Synthetic nanoscale varicose perturbations, characterized by a length–scale larger than a critical wavelength, led to a drastic improvement in nanoparticle chain order; (3) Linear stability analysis (LSA) predicted both the rivulet instability development and the critical wavelength required for synthetic perturbations to form ordered chains; (4) Non-linear hydrodynamic simulations reproduced nanoscale features observed during both liquid phase retraction and nanoparticle formation. Joint work with J. Diez (Instituto de Fisica Arroyo Seco, Universidad Nacional del Centro de la Provincia de Buenos Aires (UNCPBA), Tandil, Argentina), L. Kondic (New Jersey Institute of Technology), and Y. Wu, N. A. Roberts, C. E. McCold, P. D. Rack (The University of Tennessee, Knoxville).

Miguel Fuentes-Cabrera

Oak Ridge National Lab

Molecular Dynamics Simulations of the De-wetting on Copper Nanostructures on Graphite

Thin film dewetting can be exploited to self-assemble and organize nanoparticles. To control self-assembly and organization, it is crucial to understand the nanoscale liquid phase dynamics. In this respect, Molecular Dynamics simulations (MD) using a Lennard-Jones (LJ) potential can be a powerful tool. MD simulations employing a LJ potential has been used before to investigate the de-wetting in polymer-like liquids. By comparison, however, there are fewer theoretical studies on the wetting/de-wetting of metallic liquids. In the past two years, we have carried out a research program in which we have investigated the de-wetting of liquid Cu nanostructures on graphite using MD simulations with a LJ potential whose strength and depth varies. Our results have revealed that de-wetting proceeds at the nano-scale in a similar fashion as it does at the macro/microscale, and suggest that it could be harnessed to control the movement of nano-scale objects.

Omri Gat

Hebrew University of Jerusalem

Pulse Dynamics and Synchronization in Externally Seeded Passively Mode Locked Lasers

Abstract: Synchronization is the locking of a self-sustained oscillator frequency to the frequency of an external signal or the mutual locking of two self sustained oscillators. Pulses in mode locked lasers exhibit in the simplest case two independent frequencies, overall phase and timing. We study the dynamics of soliton-like pulses in a passively mode locked laser subject to injection of a weak external pulse. The dynamics is modelled by a subcritical complex Ginzburg-Landau equation with saturable gain. We use soliton perturbation theory to reduce the governing equation to a set of four coupled ordinary differential equations that describe the dynamics of the pulse parameters, amplitude, phase, timing and frequency. We show that timing and overall phase of the pulse lock to the external seed if the injection power is strong enough or the frequency detuning is small enough, and derive the injection-locking phase diagram.

Nathan Gibson

Oregon State University

High Order Finite Difference Methods for Maxwell's Equations in Dispersive Media

We consider models for electromagnetic wave propagation in linear dispersive media which include ordinary differential equations for the electric polarization coupled to Maxwell's equations. We discretize these models using high order finite difference methods and study the properties of the corresponding discrete models. In this talk we will present the stability, dispersion and convergence analysis for a class of finite difference methods that are second order accurate in time and have arbitrary (even) order accuracy in space. Using representative numerical values for the physical parameters, we validate the stability criterion while quantifying numerical dissipation. Lastly, we demonstrate the effect that the spatial discretization order and the corresponding stability condition has on the dispersion error.

Zydrunas Gimbutas

Courant Institute of Mathematical Sciences, NYU

Efficient Algorithm for Rotating Spherical Harmonic Grids with Application to Singular Quadrature

In this talk, we present a fast and accurate algorithm for evaluating singular integral operators on surfaces of spherical topology. The problems of this type arise, for example, in simulating Stokes flows involving slowly deforming particles, and in multi-particle scattering calculations. For smooth surfaces, spherical harmonic expansions are commonly used for geometry representation and the evaluation of the singular integrals is carried out with a high-order quadrature rule on a set of rotated spherical grids. We propose a new algorithm for reducing the computational complexity of applying this quadrature rule from O(p^5) to O(p^4 \log p) for a p-th order expansion. In this scheme, the spherical grids are efficiently interpolated via a hybrid non-uniform FFT, without ever performing spherical transforms. This is joint work with Shravan Veerapaneni.

Mithat Gonen

Memorial Sloan-Kettering Cancer Center, Department of Epidemiology and Biostatistics

Combining Historical and Randomized Controls in Phase II Oncology Trials

Phase II trials in oncology provide a preliminary assessment of efficacy and they are typically single-arm studies with the null hypothesis derived from historical data. As progress in imaging and therapy accelerates the one-sample paradigm is increasingly being questioned. Having a randomized group, while considered ideal, is not yet fully embraced for it results in larger and longer trials. This talk will explore Bayesian ways to combine historical and randomized controls with the goal of justifying unbalanced randomization (smaller control arms) in Phase II trials. Simulation studies with a binary endpoint indicate that the method strikes a balance between single-arm and 1:1 randomized trials. Adaptive randomization

will also be considered to improve efficiency with binary endpoints, but its utility will be limited with time-to-event endpoints which are becoming increasingly popular in Phase II studies.

Boyce Griffith

New York University

Cardiac Fluid-structure and Electro-mechanical Interaction

The heart is a coupled electro-fluid-mechanical system. The contractions of the cardiac muscle are stimulated and coordinated by the electrophysiology of the heart; in turn, these contractions affect the electrical function of the heart by altering the macroscopic conductivity of the tissue and by influencing stretch-activated transmembrane ion channels. To develop a unified approach to modeling cardiac electromechanics, we have extended the immersed boundary (IB) method for fluid-structure interaction, which was originally introduced to model cardiac mechanics, to describe cardiac electrophysiology. The IB method for fluid-structure interaction uses Lagrangian variables to describe the elasticity of the structure, and uses Eulerian variables to describe the fluid. Coupling between Lagrangian and Eulerian descriptions is mediated by integral transforms with Dirac delta function kernels. An analogous approach can be developed for the bidomain equations of cardiac electrophysiology. In the electrophysiological immersed method, interaction between Lagrangian and Eulerian variables happens in a manner that is completely analogous to the corresponding coupling between Lagrangian and Eulerian variables in the conventional IB method for fluid-structure interaction. In this talk, I will describe the IB method for both fluid-structure and electro-mechanical interaction, and I will present applications of this unified methodology to models of heart function that couple descriptions of cardiac mechanics, fluid dynamics, and electrophysiology. Additional applications of the IB method will also be presented.

Wenge Guo

New Jersey Institute of Technology

Further Results on Controlling the False Discovery Proportion

The tail probability of false discovery proportion (gamma-FDP) has received much attention as a measure of false discoveries in multiple testing. Although this measure has received acceptance due to its relevance under dependency, not much progress has been made yet advancing its theory under such dependency in a non-asymptotic setting, which motivates our research in this paper. We provide a larger class of procedures containing the stepup analog of, and hence more powerful than, the stepdown procedure in Lehmann and Romano (2005) controlling the gamma-FDP under the same positive dependence condition assumed in that paper. We offer better alternatives of the stepdown and stepup procedures in Romano and Shaikh (2006a, b) using pairwise joint distributions of the null p-values. We generalize the notion of gamma-FDP making it appropriate in many practical situations where one is willing to tolerate a few false rejections or, due to high dependency some false rejections are inevitable and provide methods that control this generalized gamma-FDP in two different dependence structures. Our theoretical findings are being supported through numerical studies.

Ying Guo

Emory University

Statistical Methods for Assessing Agreement among Correlated Survival Outcomes

Assessing agreement is often of interest in clinical studies to evaluate the similarity of measurements produced by different raters or methods on the same subjects. One of the challenging topics in agreement studies is how to account for censored or truncated observations such as those observed in survival data. Another special feature related to measuring agreement in survival studies is the need to assess the agreement among a subgroup of subjects who survive beyond a specific time point. In this talk, we present a system of new statistical methods for assessing agreement for correlated multivariate survival outcomes. Our agreement methods can accommodate both discrete and continuous survival times. Nonparametric as well as parametric estimation approaches have been proposed. We also develop new time-dependent agreement methods which allow us to measure agreement on a subpopulation of interest by conditioning on subjects' survival status. The time-dependent measures can help reveal how the strength of agreement evolves along the time among survivors remaining in the study. The proposed agreement methods can be applied to bivariate and multivariate survival outcomes. Simulation studies are conducted to evaluate the performance of the proposed methods. A real data example from a prostate cancer study is used to illustrate the methods.

Greg Hayrapetyan

Carnegie Mellon University

Geometric Evolution of Interfaces in the Functionalized Cahn-Hilliard Equation

The functionalized Cahn-Hilliard energy (FCH) is a novel higher-order energy that serves as a model for network formation in solvated, functionalized polymers. Leading order minimizers of this energy include new bi-layer solutions with homoclinic cross sections. An overview of the reduction of the gradient flow of (FCH) to the sharp interface evolution is presented.

Daniel Heitjan

University of Pennsylvania School of Medicine

Real-Time Prediction in Clinical Trials: A Statistical History of REMATCH

Randomized clinical trials often include one or more planned interim analyses, during which an external monitoring committee reviews the accumulated data and determines whether it is scientifically and ethically appropriate for the study to continue. With survival-time endpoints, it is often desirable to schedule the interim analyses at the times of occurrence of specified landmark events, such as the 50th event, the 100th event, and so on. Because the timing of such events is random, and the interim analyses impose considerable logistical burdens, it is worthwhile to predict the event times as accurately as possible. Prediction methods available prior to 2001 used data only from previous trials, which are often of questionable relevance to the trial for which one wishes to make predictions. With modern data management systems it is often feasible to use data from the trial itself to make these predictions, rendering them far more reliable. This talk will describe work that some colleagues and students and I have done in this area. I will set the methodologic development in the context of the trial that motivated our work: REMATCH, a randomized clinical trial of a heart assist device.

Johan Helsing

Lund University

On the Polarizability and Capacitance of the Cube

An electrostatic solver is constructed for problems on domains with cuboidal inclusions. A particular characteristic of the solver is that it takes advantage of sharp edges and corners, rather than being a victim of them. In this way we circumvent the need to round sharp geometric features slightly -- a common practice which leads to complications as new length-scales are introduced and, in extreme cases, to radically different solutions. Our solver can be used to compute the polarizability of a dielectric cube in a dielectric background medium at virtually every permittivity ratio for which it exists. For example, polarizabilities accurate to between five and ten digits are obtained (as complex limits) for negative permittivity ratios in minutes on a standard workstation. In passing, the capacitance of the unit cube is determined with unprecedented accuracy. Some aspects of polarizabilities and their representing measures are also clarified, including limiting behavior both when approaching the support of the measure and when deforming smooth domains into a non-smooth domain. Finally, stepping down to two dimensions, we show a high-resolution animation illustrating how the effective permittivity of an array of dielectric squares evolves as the geometry approaches that of a dielectric checkerboard. The talk is based on joint work with Graeme Milton, Karl-Mikael Perfekt, and Ross McPhedran.

Mark Hoefer

North Carolina State University

Dispersive Shock Waves in Eulerian Fluids

Normal and oblique nonstationary dispersive shock waves (DSWs) for the one and two-dimensional isentropic Euler equations regularized by dispersion are constructed using Whitham averaging. Under modest assumptions, the jump conditions and admissibility criteria for weak DSWs are determined in terms of a general pressure law and the sign of the dispersion. Large amplitude DSWs are constructed for several particular dispersive fluids including superfluids (Bose-Einstein condensates and ultracold Fermions) and "optical fluids" modeled by the generalized Nonlinear Schrodinger equation as well as fully nonlinear shallow water waves with surface tension modeled by the generalized Serre equations. The one-dimensional shock tube problem and the M-θ-β diagram for oblique DSWs are addressed. Numerical simulations compare favorably with the symptotic results in the weak to moderate amplitude regimes and reveal the breakdown of the asymptotic theory when the DSW experiences cavitation.

Christel Hohenegger

University of Utah

Dynamics of Active Suspensions Near Boundaries

One of the challenges in modeling the transport properties of complex fluids (e.g. many biofluids, polymer solutions, particle suspensions) is describing the interaction between the suspended micro-structure with the fluid itself particularly in the vicinity of solid boundaries. I will focus on understanding the dynamics of semi-dilute active suspensions, like swimming bacteria or artificial micro-swimmers and illustrate the role of the domain geometry in driving the flow and the large-scale instabilities. Finally, I will discuss the difficulties of imposing appropriate boundary conditions in a kinetic model of these active suspensions.

Theodoros Horikis

University of Ioannina

Solitons in Mode-locked Lasers

Ultrashort pulses have many important applications, ranging from communications and optical clock technology, to high-order harmonic generation, extreme physics, and even measuring of the fundamental constants of nature. One of the techniques used to produce ultrashort pulses is mode locking in laser systems. Mode-locked lasers have been studied for many years, with origins dating back more than four decades. However, due to their complicated dynamics it is only in recent years that researchers have begun to better understand and utilize their true potential. We will present a model system that describes the physical properties of these lasers. This model exhibits mode locking capabilities in all dispersive regimes (normal and anomalous), i.e., general initial pulses evolve to stable localized solutions. Both bright and dark solitons are found. Remarkably, the same model can be used to study the bright soliton dynamics in a normally dispersive laser. It is found that pulses exist for wide choices of the parameters, the only requirement being sufficient gain. Moreover, these pulses are essentially solitons of the classical nonlinear Schrodinger equation. Using perturbation theory evolution equations are found for the pulse amplitude, velocity, position. The same theory is extended for non decaying (dark) pulses.

Chyi-Hung Hsu

Johnson & Johnson

Improving Clinical Study Design and Understanding via Modeling and Simulation

Sample size calculations for and overall design of clinical trials have since long relied on the statistical power for hypothesis test paradigm. This is true also for early development and dose-ranging studies, even though the key questions to be addressed in such studies are more of an estimation nature than related to testing a pre-determined hypothesis. Many reasons have contributed to this "Phase 3 view" of clinical drug development, including software availability and methodological training/knowledge. Modeling and simulation (M&S) approaches have freed statisticians and modelers from the "power calculation" dogma for trial design, allowing better understanding of the true underlying goes of the trial and appropriately tailoring the design to them. This talk will discuss the M&S view of study design, using examples from real trials to motivate and illustrate the key ideas.

Boaz Ilan

University of California-Merced

Dark Solitons, Dispersive Shock Waves and Their Transverse Instabilities

Transverse instabilities of dark solitons for the (2+1)-dimensional defocusing nonlinear Schrodinger / Gross-Pitaevskii equation are considered. Asymptotics and computations of the linearized equation yield the dispersion relation, which, in turn, yields the separatrix for the transition between convective and absolute instabilities of dark solitons. The implications for stationary and non-stationary oblique dispersive shock waves are elucidated. Our results have application to controlling dispersive shocks, which are being studied in Bose-Einstein condensates and nonlinear optics. Joint work with Mark Hoefer.

Badal Joshi

Duke University

Identifying Multistationarity in Chemical Reaction Networks Based on Reaction Network Structure

Chemical reaction networks are used as models of biological systems such as gene regulatory networks and metabolic networks. The existence of multiple steady states is a necessary condition for a reaction network to act as a biomolecular switch, therefore determining which networks permit multiple steady states is an important theoretical problem. We present new conditions to preclude multistationarity based on the network structure. We also give new sufficient conditions for a reaction network to allow multiple steady states for some parameter values by defining certain minimal reaction networks called atoms of multistationarity. Furthermore, we give complete characterization of one reaction atoms of multistationarity. This is joint work with Anne Shiu.

Shilpa Khatri

University of North Carolina at Chapel Hill

Settling of Porous Particles in Density Stratified Fluids: Analysis and Experiments

Marine snow, composed of organic and inorganic matter, plays a major role in marine carbon cycling. Most of these macroscopic particles are extremely porous, allowing diffusion of salt from the ambient fluid to affect the density and therefore the settling of these particles. In a first approximation, these particles can be modeled as spheres. This talk will present a study of the effect of porosity and salt diffusion in the dynamics of a sphere settling under gravity in a salt-stratfied fluid. For linear stratification in viscosity dominated regimes, an explicit solution for the sphere's position in time is derived. For more general ambient fluid stratification, the sphere's position can be solved for numerically, under the asymptotic assumptions about the typical time scales of diffusion and settling. A discussion about the competing effects of entrainment and diffusion will be included. A parametric study of the settling behaviors and preliminary comparisons with experiments will be presented.

Mikhail Khenner

Western Kentucky University

Analysis of a Model for Dewetting of the Pulsed Laser-melted Thin Metallic Films

Self-organized nanoparticle arrays from pulsed laser induced dewetting in thin metallic films can be used to manufacture complex multifunctional surfaces that can be applied to existing technologies such as surface Raman sensing or magnetic data storage devices, but can also enable a host of new applications that are generally based on sensing, detecting or manipulating charge, electromagnetic signals, and magnetization. This presentation will describe the long-wave nonlinear PDE model of self-organization in the time-periodically melted single-layer and bilayer films. In the presence of intermolecular interactions with the substrate and between the layers, the in-plane non-uniformity of heating due to beam interference, and thermocapillary effects, the liquid flow in the film gives rise to surface and interface deformation and film dewets into nanoparticle arrays with well-defined length scales and composition. We used stability analysis and computations of film height dynamics to determine dependencies of key quantities of interest (particle spacing, morphology, composition) on physical and process parameters. This theoretical exploration is a step toward predictively make multifunctional surfaces in new systems. Joint work with Sagar Yadavali (Department of Chemical and Biomolecular Engineering, The University of Tennessee, Knoxville) and

Ramki Kalyanaraman (Department of Chemical and Biomolecular Engineering, Department of Materials Science and Engineering, Sustainable Energy Education Research Center, The University of Tennessee, Knoxville).

Mark Kramer

Boston University

Multi-scale Seizure Dynamics: Analysis and Models

A seizure represents an extreme deviation from normal brain activity. In this talk, we will consider some characteristics of the seizure as observed across spatial and temporal scales in human patients. We will focus in particular on the slowing rhythmic activity of the seizure, and the coupling between brain regions that evolves during the seizure. These results will motivate discussion of a mathematical model consistent with the stereotyped dynamics observed at seizure termination.

Guillaume Lajoie

University of Washington

Spike Time Reliability of Temporally Driven Neural Networks in Balanced Regimes

If the same sensory stimulus is presented multiple times to a neuronal network, how similar are the spike trains that it evokes? This question of the reproducibility, or reliability, of stimulus-induced spike times has a long history in neuroscience. Here, we contribute new results on how features of spiking network dynamics constrain this reliability. We focus on networks with sparse, random connectivity and balanced excitation and inhibition. Such networks have attracted great interest, as they reproduce the irregular firing that typifies cortical activity. For several models of neural dynamics, this activity is known to be chaotic, with extremely strong sensitivity of spike outputs on tiny changes in a network's initial conditions [VanVreeswijk and Sompolinsky, 1996, Monteforte and Wolf, 2010, London et al., 2010]. These chaotic networks are by definition unreliable. Here, our goal is to understand whether this is essentially always the case, or whether there are non-chaotic – and hence reliable – varieties of balanced networks as well. We consider sparse networks of inhibitory and excitatory neurons, modeled as phase variables, randomly coupled and driven by independent temporally structured inputs. We explore the impact of two key parameters. The first is the amplitude of a signal impinging on the network. The second is the superthreshold vs. subthreshold state of the individual cells – that is, whether they are in mean-driven vs. fluctuation-driven regimes. We show that both parameters strongly impact network reliability. In particular, a range of networks with moderate signal amplitudes and excitable single-cell dynamics exhibit sustained irregular activity that is not chaotic. Such networks reliably respond to a given input, with high spike timing accuracy on several trials with distinct initial conditions. These same networks become unreliable when individual cells come closer to superthreshold states, connecting with results for sparse recurrent networks in the literature.

Shingyu Leung

Hong Kong University of Science and Technology

A Grid Based Particle Method for Solving Partial Differential Equations on Evolving Surfaces and Modeling High Order Geometrical Motion

We develop numerical methods for solving partial differential equations (PDE) defined on an evolving interface represented by the grid based particle method (GBPM). We propose implicit time discretization methods for the advection–diffusion equation where the time step is restricted solely by the advection part of the equation. We also generalize the GBPM to solve high order geometrical flows including surface diffusion and Willmore-type flows. The resulting algorithm can be easily implemented. Without any computational mesh or triangulation defined on the interface, we do not require remeshing or reparametrization in the case of highly distorted motion or when there are topological changes. One application is image processing with total variation (TV) regularization on manifolds. Another interesting application is to study locally inextensible flows governed by energy minimization. We introduce tension force via a Lagrange multiplier determined by the solution to a Helmholtz equation defined on the evolving interface. Extensive numerical examples are also given to demonstrate the efficiency of the proposed approach.

Bo Li

Department of Mathematics and the NSF Center for Theoretical Biological Physics
University of California, San Diego

Modeling and Simulation of Biomolecular Interactions with Solute Mechanics and Implicit Solvent

Biomolecular interactions determine the conformation, dynamics, and functions of an underlying biological system. Accurate and efficient modeling of such interactions is challenging due to the enormous number of atoms and molecules in the system, and their multiscale mechanical relaxation and chemical reactions. In this talk, a novel variational implicit-solvent approach to the biomolecular relaxation is introduced. The key in this approach is the coupling of solute molecular mechanical interactions with solute-solvent van der Waals and electrostatic interactions in an effective Hamiltonian of solute particles and the solute-solvent interfaces. Robust numerical relaxation methods are described. Extensive computational results with comparison with molecular dynamics are presented to demonstrate the success of this new approach in capturing the hydrophobic interaction and dry-wet fluctuation between multiple equilibrium states. Related mathematical and numerical issues are discussed.

Jichun Li

University of Nevada - Las Vegas

Recent Advances in Numerical Modeling of Electromagnetic Wave Propagation in Metamaterials

Since the first successful construction of negative index metamaterials in 2000, there is a growing interest in the study of metamaterials due to their potential applications in areas such as design of invisibility cloak and sub-wavelength imaging. In this talk, I'll first give a brief introduction to the short history of metamaterials. Then I'll focus on the mathematical modeling of metamaterials, and discuss some time-domain finite elemental schemes we developed in recent years. Finally, I'll conclude the talk with our cloak simulation and some open issues for further exploration.

Tai-Chia Lin

National Taiwan University

A New Approach to the Lennard-Jones Potential and a New Model: PNP-delta Equations

A class of approximate Lennard-Jones (LJ) potentials with a small parameter is found whose Fourier transforms have a simple asymptotic behavior as the parameter goes to zero. Amazingly, when the LJ potential is replaced by the approximate LJ potential, the total energy functional becomes simple and exactly the same as replacing the LJ potential by a delta function. Such a simple energy functional can be used to derive the Poisson-Nernst-Planck delta (PNP-delta) equations, a new mathematical model for the LJ interaction in ionic solutions. Stability and instability conditions for the 1D PNP-delta equations with the Dirichlet boundary conditions for one anionic and cationic species are expressed by the valences, diffusion constants, ionic diameters and coupling constants. This is the first step to study the dynamics of solutions of the PNP-delta equations.

Georgi Medvedev

Drexel University

The Geometry of Spontaneous Spiking in Neuronal Networks

We study electrically coupled networks of excitable neurons forced by small noise. Using the center manifold reduction, techniques for randomly perturbed dynamical systems, and elements of algebraic graph theory, we derive a variational problem, which provides a clear geometric picture of the network dynamics. In particular, we describe the evolution of spontaneous patterns starting from uncorrelated activity for very weak coupling, and progressing through formation of clusters, and waves, to complete synchrony for stronger coupling. The variational analysis is complemented by the stability analysis of the synchronous state in the strong coupling regime. The stability estimates reveal the contribution of the network connectivity to its synchronization properties. This work is motivated by the experimental and modeling studies of the ensemble of neurons in the Locus Coeruleus, a nucleus in the brainstem involved in the regulation of cognitive performance and behavior.

Laura Miller

University of North Carolina

Using 3D Numerical Simulations and Physical Models to Understand the Role of Wing Flexibility in Tiny Insect Flight

A vast body of research has described the complexity of flight in insects ranging from the fruit fly, *Drosophila melanogaster*, to the hawk moth, *Manduca sexta*. The smallest flying insects have received far less attention, although previous work has shown that flight kinematics and aerodynamics can be significantly different. In this presentation, three-dimensional direct numerical simulations are used to compute the lift and drag forces generated by flexible wings to reveal the aerodynamics of these tiny fliers. Results are validated against dynamically scaled physical models. At the lowest Reynolds numbers relevant to insect flight, the relative forces required to rotate the wings and fling them apart become substantially greater. Wing flexibility can reduce these forces and improve efficiency in some situations.

Peter Minev

University of Alberta

A New Class of Massively-parallel Direction Splitting Techniques for the Incompressible Navier-Stokes Equations

A new direction-splitting-based fractional time stepping for solving the incompressible Navier-Stokes equations will be discussed. The main originality of the method is that the pressure correction is computed by solving a sequence of one one-dimensional elliptic problem in each spatial direction. The method is unconditionally stable only in case of simple geometries. Therefore, it requires some adjustments in case of flows in geometries of a complex shape which will also be discussed. Finally, some results of various flow problems will be presented.

Nilima Nigam

Simon Fraser University

Fast Methods for Boundary Integral Equations on Compact Manifolds

Models describing physical or biological phenomena constrained to evolve on subsurfaces of compact manifolds can be reformulated in terms of integral equations. Examples of such models include point vortices moving on the surface of the earth, or polar-driven chemotactic migration on cell membranes during mitosis. The use of integral equation strategies in this context is fairly new, and requires a careful examination of the relevant parametrices for the elliptic operator of concern. In this talk we first describe reformulations of a boundary value problem for the Laplace-Beltrami operator in terms of layer potentials. We then describe a class of methods based on the fast multipole method.

Sean Nixon

University of Vermont

Perturbations of Dark Solitons

A direct perturbation method for approximating dark soliton solutions of the nonlinear Schrödinger equation under the influence of perturbations is presented. The problem is broken into an inner region, where core of the soliton resides, and an outer region, which evolves independently of the soliton. It is shown that a shelf develops around the soliton which propagates with speed determined by the background intensity. Integral relations obtained from the conservation laws of the nonlinear Schrödinger equation are used to approximate the depth and velocity of the perturbed soliton as well as the shape of the shelf. To determine the shift in the perturbed soliton's position the first order correction term must be solved for completely. The analysis is developed for both constant and slowly evolving backgrounds. A number of problems are investigated including linear and nonlinear damping type perturbations.

Sarah Olson

Worchester Polytechnic Institute

Coupling Biochemistry, Mechanics, and Hydrodynamics to Model Sperm Motility

Sperm are known to exhibit two distinct types of motility. One is characterized by constant amplitude, symmetrical waveforms. The other is characterized by asymmetrical waveforms, corresponding to an increase in calcium concentration within the flagellum. The goal of this work is to model sperm swimming in a viscous, incompressible fluid using the method of regularized Stokeslets. The mechanical forces are due to passive stiffness properties and active bending moments are a function of the local calcium concentration. Results showing emergent waveforms, swimming speeds, and trajectories will be compared to experimental data. The hydrodynamic interactions of multiple sperm will also be presented and compared to experimental data, where sperm trains and vortices are often seen.

Matthew Paoletti

University of Texas at Austin

Propagating and Evanescent Internal Waves in Nonuniform Stratifications

Authors: M. S. Paoletti and Harry L. Swinney

In a stratified fluid, an internal wave transports momentum and energy as a propagating disturbance restored by buoyancy forces. Internal waves generated by tidal flow over ocean topography are thought to play a crucial role in oceanic mixing, which affects global climate patterns. We present experimental and computational studies of the propagation of internal waves in an exponentially stratified fluid that models the deep ocean. The buoyancy frequency profile N(z) (proportional to the square root of the density gradient) smoothly varies by nearly an order of magnitude over the fluid depth, rather than being constant or piecewise-constant as in prior studies. The stratification is characterized by a turning depth z_c, where $N(z_c)$ is equal to the wave frequency ω and $N(z<z_c) < \omega$. Downward propagating internal waves reflect from the turning depth and become evanescent below. The energy flux below the turning depth is shown to decay exponentially with a decay constant given by the horizontal wavenumber at the turning depth. The vertical velocity fields of the incoming and reflected waves above the turning depth agree within a few percent with a previously untested theory by Kistovich and Chashechkin [J. App. Mech. Tech. Phys. **39**, 729-737 (1998)].

Edsel A. Pena

University of South Carolina

Some Recent Developments in the Analysis of Recurrent Event Data

In this talk I will discuss some recent developments in the analysis of recurrent event data. Recurrent events are prevalent in studies in many areas, notably in biostatistics and public health, reliability and engineering, and in the social sciences. I will discuss models for recurrent event data and describe inference methods based on observations of the recurrent event. In particular, I will focus on informative censoring models, recurrent event settings with competing risks, and possibly touch on nonparametric Bayesian estimation of the inter-event distribution with recurrent event data. The results presented here are based on joint work with Akim Adekpedjou, Laura Taylor, and Fazlur Rahman.

Bijan Pesaran

New York University

A Sequential Probability Ratio Test to Detect Behavioral Events in Neuronal Activity

The timing of neural responses to ongoing behavior is an important measure of the underlying neural processes. Neural processes are distributed across many different brain regions and measures of the timing of neural responses are routinely used to test relationships between different brain regions. Testing detailed models of functional neural circuitry underlying behavior depends on extracting information from single trials. Despite their importance, existing methods for analyzing the timing of information in neural signals on single trials remain limited in their scope and application. We develop a novel method for estimating the timing of information in neural activity that we use to measure selection times, when an observer can reliably use observations of neural activity to select between two descriptions of the activity. The method is designed to satisfy three criteria: selection times should be computed from single trials, they should be computed from both spiking and local field potential (LFP) activity, and they should allow us to make comparisons between different recordings. We develop the procedure for binary and multiclass discrimination using example recordings of spiking and LFP activity in the frontal and parietal cortices of monkeys performing a range of behavioral tasks. We propose that this method is a general and practical framework for the analysis of signal timing in the nervous system.

Derick R. Peterson

University of Rochester

Local Polynomial Density Estimation with Interval Censored Data

A survival time T is interval censored if only its current status is observed at several monitoring times. We provide an estimator with pointwise confidence limits for any derivative of the distribution of T, assuming that the observed monitoring times are independent of T. Our estimator is a standard local polynomial regression smoother applied to the pooled sample of N dependent current status observations. We show that the proposed estimator has a normal limiting distribution identical to that of a smoother applied to N i.i.d. current status observations. Thus local bandwidth selection techniques and pointwise confidence limit procedures for standard nonparametric regression perform properly despite the dependence in the pooled sample. Our results also imply that, for a large number of subjects, each additional monitoring time for subjects already monitored actually carries as much or more information for estimation of the survival function as a monitoring time for a new, independent subject. We investigate the practical performance of our proposed data-driven density estimator in a simulation study. Joint work with Mark J. van der Laan.

Mary Putt

University of Pennsylvania

Determining Changes in Blood Flow when the Baseline Function is Modeled with a Smoothing Spline

In an animal model, the extent and duration of the reduction in blood flow in solid tumors appears to be a key determinant of subsequent response to therapy. Estimating the change-times corresponding to the initial reduction and the subsequent stabilization of flow is challenging because the baseline blood flow is may not be well fit by a parametric model. We modeled the data using a smoothing spline for the baseline curvature and a parametric component to add a linear decrease in flow at the change-points. While generalized cross validation (GCV) is commonly used as a criterion for choosing the smoothing parameter in similar partial spline models where the change-times are known, we found that GCV-based estimates of the change times in the blood flow data have substantial bias and variance. Minimizing GCV tends to yield models that under-smooth the data; here, accurate identification of the change-times is of little importance to the overall fit. We propose a data-driven modification to GCV that potentially re-weights the model fit and complexity terms based on a comparison with a model without change-points. Results from both simulation and tumor biology studies suggest that this adaptive GCV yields substantial improvement in estimation of the change-times and the function at the change-times.

Hermann Riecke

Northwestern University

Stimulus Decorrelation by Adaptive Neurogenetic Networks in Olfaction

A common first step in sensory processing is contrast enhancement. It is thought to aid subsequent processing steps like stimulus discrimination and storage. Thus, in olfaction it has been observed that this initial processing, which is performed by the olfactory bulb, increases the differences between the representations of similar stimuli. Due to the high dimensionality of odor space the activity patterns elicited by even simple odors are quite complex. It is therefore natural to assume that the connectivity of the neuronal networks achieving this task will reflect this complexity and may be the result of an experience-dependent process. Motivated by the experimental observation of a substantial neuronal turn-over in the largest interneuron population of the olfactory bulb--a turn-over that persists even into adulthood - we investigate neuronal networks that adapt their connectivity through the random addition of new neurons and their activity-dependent removal. We show that such networks can indeed learn to decorrelate effectively the representations of similar stimuli. The decorrelation results from a normalization of the stimulus representations and the mutual inhibition of highly co-active principal neurons. The model makes predictions for the impact of the training protocol on the ability of animals to discriminate certain types of mixtures. Joint work with Siu Fai Chow.

Jerónimo Rodríguez

University of Santiago

Retarded Potentials and Discontinuous Galerkin Methods with Upwind Fluxes for Transient Wave Propagation on Unbounded Domains

This work deals with the numerical simulation of transient wave propagation on unbounded domains containing localized heterogeneities. We will decompose the computational domain in two non-overlapping sub-domains; one of them (the interior sub-domain) being bounded and containing all the defaults, the other one (the exterior sub-domain) assumed to be homogeneous and unbounded. In previous studies, in the frame of the scalar wave equation, the authors proposed a hybrid method based on the retarded potential method in the exterior domain (on the artificial boundary) and a non-dissipative discontinuous Galerkin (DG) method in space (using centered fluxes) combined with explicit second order finite differences in time (leap frog scheme) in the interior. The coupling was specially built to ensure by construction a discrete energy identity (consistent with the usual energy conservation satisfied by the exact solution) yielding to the stability of the numerical method under the usual CFL condition on the interior domain, that is, the stability condition was not affected by the transparent boundary condition. Moreover, the coupling technique allowed to use a smaller time step in the interior domain leading to quasi-optimal discretization parameters for both methods.

Since the DG discretizations based on centered fluxes provide sub-optimal rates of convergence (mainly for equations involving convective terms) it is desirable to include the possibility of using upwind fluxes. The leap frog scheme used for the previous study being unstable in presence of dissipative terms, the authors propose a time discretization of the interior equations being explicit, conditionally stable and allowing the presence of dissipative terms. We propose a new global discretization allowing to couple the novel interior approximation with the retarded potential method that is stable by construction. The efficiency of the method will be discussed through some numerical experiments for the scalar wave equation.

Rolf Ryham

Fordham University

Qualitative and Modeling Aspects for Ionic Fluid PDE

The study of electrolytes and their applications to biology is related to the ability of a biological membrane to act as a barrier between ionic solutions. These processes are mathematically challenging to study because they involve physical forces on multiple scales and predicting the time course is more consequential than the equilibrium end states. This talk will show how such fluid mechanical and electrostatic interactions are formulated in terms of variational derivatives of energy functionals, thereby providing a tool for deriving and studying more complicated scenarios. Recent theoretical results characterizing the long term behavior of solutions is also described.

Sanat Sarkar

Temple University

Capturing the Severity of Type II Errors in High-Dimensional Multiple Testing

Multiple testing methods controlling false discoveries are useful statistical tools for analyzing data from many modern scientific investigations, such as brain imaging, microarray analysis, astronomy, atmospheric science, and many others. A number of such methods have been proposed in the literature. However, they have been developed without addressing the following issue that is of importance in high-dimensional multiple testing with sparse signals: Miss-detecting a strong signal is often a more severe error than miss-detecting a weak signal, with the severity getting larger as the signal gets stronger. In this talk, a new, optimal multiple testing method controlling false discoveries is proposed addressing this issue from a Bayesian decision theoretic point of view.

Leonardo E. Silbert

Southern Illinois University

Finite Compressibility of Jammed and Glassy Matter

The jamming point signals the transition between mechanically stable and unstable states for systems far from thermodynamic equilibrium and is often described in the language of critical phenomena. Interestingly, however, many of the properties characterising the jamming transition are either independent of dimensionality or dependent on interaction potential. These features distinguish the jamming transition from a regular thermodynamic phase transition and associated critical phenomena. Indeed, the onset of mechanical stability in hard sphere packings has been referred to as an inverted critical point. One particular feature that has promoted this idea is a specific structural signature termed hyperuniformity, or the suppression of long wavelength density fluctuations. Hyperuniformity presents itself as an anomalous feature (as compared with traditional fluids) in the low-wavenumber region of the static structure factor and has been shown to connect with dynamical properties of a jammed packing. Through the use of large-scale computer simulations of amorphous materials we determine the generality of this anomalous property, finding that such long-wavelength structural features provide a generic indicator of the mechanically stable state not only in jammed, sphere-packings, but also in model glassy systems.

Debajyoti Sinha

Florida State University

Semiparametric Bayesian Survival Analysis using Models with Log-linear Median

For the analysis of survival data from clinical trails, we present two novel semiparametric survival models with log-linear median regression functions. Our models are useful alternatives to the popular Cox (1972) model and linear transformation models (Cheng et al., 1995). Compared to existing semiparametric models, our models have many important practical advantages, including interpretation of the regression parameters via the median and the ability to address heteroscedasticity of survival response. We demonstrate that our modeling techniques facilitate the ease of prior elicitation and computation for both parametric and semiparametric Bayesian analysis of survival data. We illustrate the advantages of our modeling, as well as model diagnostics, via reanalysis of a small-cell lung cancer study. Results of our simulation study provide further guidance regarding appropriate modelling in clinical trial.

Wenguang Sun

University of Southern California

False Discovery Control in Large-Scale Spatial Multiple Testing

In this talk I discuss a unified theoretical and computational framework for false discovery control in multiple testing of spatial signals. We consider both point-wise and cluster-wise spatial analyses, and derive oracle procedures which optimally control the false discovery rate, false discovery exceedence and false cluster rate, respectively. The implementation of the oracle procedures is very challenging in practice, especially on a continuous spatial domain. Hence we develop a class of data-driven procedures, based on a finite approximation strategy, to mimic the oracle procedures. Our data-driven procedures are asymptotically valid and can be effectively implemented using Bayesian computational algorithms for analysis of large spatial data sets. In particular, we discuss how to summarize the fitted spatial models using posterior sampling to address related multiple testing problems. Numerical results show that our data-driven procedures lead to more accurate error control and enhanced power than conventional methods. The proposed methods are demonstrated for analyzing the time trends in tropospheric ozone in eastern US.

Johannes Tausch

Southern Methodist University

Solution of Shape Optimization Problems for the Heat Equation using the Parabolic Fast Multipole Method

The talk is concerned with the solution of inverse shape optimization problems for the heat equation. The goal is to determine the shape of an inclusion or a heat source from measurements of temperatures and heat fluxes on the exterior boundary. These shape identification problems can be formulated as the minimization of a least-squares cost functional for the difference of computed and measured boundary data. The shape gradient of the cost functional is computed by means of the adjoint method. Thus a gradient based nonlinear Ritz-Galerkin scheme can be applied to discretize the shape optimization problem. The state equation and its adjoint are boundary value problems of the heat equation, which are reformulated as parabolic boundary integral equations. The direct evaluation of discretized thermal potential operators has $O(N^2 M^2)$ cost, where N is the number of temporal and M is the number of spatial nodes. The complexity can be reduced to nearly $O(N M)$ operations by using a parabolic version of the Fast Multipole Method. Here, sources and evaluation points are clustered in space and time and cluster interactions are computed efficiently by an eight variate Chebyshev expansion of the heat kernel. The talk will conclude with some examples of reconstructed shapes.

Peter Thomas

Case Western Reserve University

Phase Resetting in an Asymptotically Phaseless System: On the Phase Response of Limit Cycles Verging on a Heteroclinic Orbit

Rhythmic behaviors in neural systems often combine features of limit cycle dynamics (stability and periodicity) with features of near heteroclinic or near homoclinic cycle dynamics (extended dwell times in localized regions of phase space). Proximity of a limit cycle to one or more saddle equilibria can have a profound effect on the timing of trajectory components and response to both fast and slow perturbations, providing a possible mechanism for adaptive control of rhythmic motions. Reyn showed that for a planar dynamical system with a stable heteroclinic cycle (or separatrix polygon), small perturbations satisfying a net inflow condition will generically give rise to a stable limit cycle (Reyn, 1980; Guckenheimer and Holmes, 1983). Here we consider the asymptotic behavior of the infinitesimal phase response curve (iPRC) for examples of two systems satisfying Reyn's inflow criterion, (i) a smooth system with a chain of four hyperbolic saddle points and (ii) a piecewise linear system corresponding to local linearization of the smooth system about its saddle points. For system (ii), we obtain exact expressions for the limit cycle and the iPRC as a function of a parameter $\mu>0$ representing the distance from a heteroclinic bifurcation point. In the $\mu\to 0$ limit, we find that perturbations parallel to the unstable eigenvector direction in a piecewise linear region lead to divergent phase response, as previously observed (Brown, Moehlis and Holmes, 2004). In contrast to previous work, we find that perturbations parallel to the stable eigenvector direction can lead to either divergent or convergent phase response, depending on the phase at which the perturbation occurs. In the smooth system (i), we show numerical evidence of qualitatively similar phase specific sensitivity to perturbation. Having the exact expression for the iPRC for the piecewise linear system allows us to investigate its stability under diffusive coupling. In addition, we qualitatively compare iPRCs obtained for systems (i) and (ii) to iPRCs for the Morris-Lecar equations near a bifurcation from limit cycles to a saddle-homoclinic orbit.

Anna-Karin Tornberg

KTH, Royal Institute of Technology

Spectrally Accurate Fast Summation Methods Applied to Stokes Flow

In microfluidic applications, the Reynolds number is often very small, and the dynamics of the fluid can be described by the Stokes equations, which can be reformulated as a boundary integral equation. Numerical simulations based on boundary integral formulations can be accelerated using a fast summation method. I will present a spectrally accurate FFT based Ewald method for this purpose. For electrostatics, this new method is compared to the established so-called SPME method for triply perodic domains, and is found to compare favourably, especially regarding memory. I will discuss also the extension of our spectral Ewald method also to the case of planar periodicity (periodic in two of the three dimensions), a case for which no fast Ewald methods previously existed for Stokes. The performance of the method will be illustrated and its application to simulations of e.g. fiber suspensions will be discussed.

Catalin Turc

Case Western Reserve University

Approximations of Singular Solutions of PDEs in Domains with Corners and Edges by Solutions of PDEs in Nearby Smooth Domains

We present a new algorithm based on integral equation formulations for the solution of constant-coefficient linear partial differential equations (PDEs) in two and three dimensional domains with corners and edges. In these cases, the integral-equation solutions may become unbounded at singular boundary points (corners and edges), and the singular behavior of solutions may be complicated. When integral equations of the second kind are used (e.g. combined field integral equations for scattering problems), the unbounded nature of solutions poses a significant challenge to solvers based on collocation methods as cancellations of infinite quantities ought to be accounted for. We present a method that (1) produces extremely close approximations to non-smooth boundaries by smooth boundaries, namely, the boundaries that result by rounding the corners and edges; (2) constructs appropriate meshes and singular/nearly-singular quadrature rules so that the solutions of the boundary integral equations on the arbitrarily sharp rounded boundaries are computed with high-order accuracy and short computational times; and (3) retrieves the solutions of the PDEs in singular domains by taking limits of solutions of the boundary integral equations on the arbitrarily sharp rounded boundaries produced per points (1) and (2). We present a variety of theoretical and numerical results that illustrate the efficiency of the method. Joint work with A. Anand (IIT Kanpur, India), O. Bruno (ACM Caltech), J. Ovall (Kentucky), and Luke Voss (CWRU).

Qi Wang

University of South Carolina

Modeling and Simulation of Biofilms and Fusion of Multicellular Aggregates

In this presentation, I will discuss a paradigm for developing mathematical models for hydrogels applicable to biofilms and cellular aggregates. This modeling framework is based on a kinetic theory accounting for molecular level thermo and hydrodynamics of active cells and nutrient molecules. When scaled-up, it yields some of the well-known field phase models for multiphase fluid problems. Model predication in 2-D and 3-D in various flow and geometric conditions will be discussed. A parallel Lattice Boltzmann Methods has been developed to complement the mesoscopic kinetic theory modeling and continuum level simulation, which could provide an alternative means to study complex biological fluids.

Kyle Wathen

Johnson & Johnson Research and Development

Utilizing Safety and Efficacy Data in a Phase II Study to Select the Best Treatment for a Phase III Study

When planning a phase III clinical trial it is often difficult to select the best treatment from among several candidate treatments or doses based on limited safety data from phase I and efficacy data on a different set of patients from phase II. In this talk I will present a clinical trial design that utilizes two safety measures and a separate efficacy outcome. There is prior belief that all three outcomes may be correlated and thus this approach provides an opportunity to better understand the outcome structure and will provide superior information for planning the phase III study. In this design an initial set of patients is randomized among all treatments and after the initial stage patients will be adaptively randomized to all treatments that remain admissible. This design employees a Bayesian framework to monitor both safety outcomes and the efficacy outcome for the entire trial. In addition, a Bayesian approach is used to adapt the randomization to favor the treatment(s) that, on average, have superior interim results. In this talk I will present the design details as well as a simulation study to better understand how this approach will perform in practice.

Brian Wetton

University of British Columbia

A General Framework for High Accuracy Solutions to Energy Gradient Flows from Material Science Models

A computational framework is presented for materials science models that come from energy gradient flows that lead to the evolution of structure involving two or more phases. The models are considered in periodic cells and standard Fourier spectral discretization in space is used. Implicit time stepping is used, and the resulting implicit systems are solved iteratively with the preconditioned conjugate gradient method. The dependence of the condition number of the preconditioned system on the size of the time step and the order parameter in the model (that represents the scaled width of transition layers between phases) is investigated. The framework is easily extended to higher order derivative models, higher dimensional settings, and vector problems. Several examples of its application are demonstrated. A comparison to time-stepping with operator splitting (into convex and concave parts) is done.

Matthieu Wyart

New York University

Geometrical Analysis of Suspension Flows near Jamming

The viscosity of suspensions was computed early on by Einstein and Batchelor in the dilute regime. At high density however, their rheology remains mystifying. As the packing fraction increases, steric hindrance becomes dominant and particles move under stress in a more and more coordinated way. Eventually, the viscosity diverges as the suspension jams into an amorphous solid. Such a jamming transition is reminiscent of critical points: the rheology displays scaling and a diverging length scale. Jamming bear similarities with the glass transition where steric hindrance is enhanced under cooling, and where the dynamics is also observed to become more and more collective as it slows down. In all these examples, understanding the nature of the collective dynamics and the associated rheology remains a challenge. Recent progress has been made however on a related problem, the unjamming transition where a solid made of repulsive soft particles is isotropically decompressed towar d vanishing pressure. In this situation various properties of the amorphous solid, such as elasticity, transport or force propagation, display scaling with the distance to threshold. Theoretically these observations can be shown to stem from the presence of soft modes in the vibrational spectrum, a result that can be extended to thermal colloidal glasses as well. Here we focus on particles driven by shear at zero temperature. We show that if hydrodynamical interactions are neglected an analogy can be made between the rheology of such a suspension and the elasticity of simple networks, building a link between the jamming and the unjamming transition. This analogy enables us to unify in a common framework key aspects of the elasticity of amorphous solids with the rheology of dense suspensions, and to relate features of the latter to the geometry of configurations visited under flow.

Yuan Xiong

Novartis Pharmaceuticals Corporation

A Systems Modeling Approach to Understanding the Mechanisms of Salt Sensitivity in Essential Hypertensive Patients and the Effect of Salt Sensitivity on Blood Pressure Response to Antihypertensive Agents

Salt sensitivity (SS) is common among hypertensive patients, particularly in Asian populations. The underlying physiological mechanisms of SS are incompletely understood. Differences in the blood pressure (BP) dose response to antihypertensive agents have been observed in global clinical studies, and it is possible that SS may play a role in these differences. An integrative physiological model of hypertension was used to investigate the mechanisms of SS, and the effect of these mechanisms on the BP response to antihypertensive agents. The Guyton model of blood pressure regulation was extended to include a detailed model of the renin-angiotensin-aldosterone system (RAAS), and to include hypertensive virtual patients (VPs) with a range of underlying disease mechanisms. The effects of many classes of antihypertensives have been calibrated in the model. To test mechanistic hypotheses that may explain SS, simulations and statistical analyses were carried out using a cohort of essential hypertensive VPs. Further, the BP responses of both SS and non-SS VPs to various RAAS-targeting agents were simulated and characterized. Four mechanisms were identified to contribute to SS, including decreased distal or proximal tubule sodium reabsorption rates, decreased glomerular ultrafiltration coefficient, or increased peripheral resistance. Each mechanism independently caused mild SS, and combining mechanisms resulted in an additive effect. Differentiated BP responses to antihypertensives in SS and non-SS groups have been predicted by the model. This study confirmed a generally accepted fact that the differences in the sensitivity to salt in essential hypertension patients lead to diverse therapeutic BP response to antihypertensives such as diuretics and RAAS blockers. To further explore the mechanistic factors contributing to SS, a systematic approach was used based on a large-scale mechanistic model. Further simulations indicated that these factors accounts for the different therapeutic BP response to antihypertensives observed in clinical studies.

Sara Zahedi

Uppsala University

A Nitsche Method for a Stokes Interface Problem

We present a finite element method for the Stokes equations involving two immiscible incompressible fluids with different viscosities and with surface tension. The interface separating the two fluids does not need to align with the mesh. Jump conditions on the interface are imposed weakly using a stabilized Nitsche type formulation. The method is based on the so called P1 iso P2/P1 element, which is an inf-sup stable element where the pressure is approximated by continuous piecewise linear elements and the velocities by continuous piecewise linear elements on a mesh obtained by splitting each triangle into four subtriangles. The proposed finite element method allows for discontinuities along the interface with optimal a priori error estimates. A stabilization procedure is used which ensures that the method produces a well conditioned stiffness matrix independent of the location of the interface relative to the grid.

Ying Zhang

University of Iowa

A Nonparametric Least-squares Estimation Method for Tumor Growth Function with Interval Censored Observations

The study of tumor growth has been an active area in cancer research for last several decades. The estimation of tumor growth function defined as the expected tumor size over time is a challenging task, as the tumor onset time is often not exactly observed but only known to be within an interval obtained from two adjacent examination times in a series of tumor screening times. In this project, we develop a nonparametric least-squares estimation procedure for the tumor growth function in the context that the tumor onset time is subject to interval censoring. We show that this procedure leads to a consistent estimate and is robust against underlying model for the tumor growth. Extensive simulation studies are carried out to validate the proposed method and a real-data application from the SEER (Surveillance, Epidemiology, and End Results) program of the NCI (National Cancer Institute) is used to demonstrate the method.

Zhigang Zhang

Memorial Sloan-Kettering Cancer Center

A Class of Transformed Mean Residual Life Models under Right Censoring

The mean residual life function is an alternative to the survival function or the hazard function of a survival time in practice. It provides the remaining life expectancy of a subject surviving up to t. In this study, we propose a class of transformed mean residual life models for fitting survival data under right censoring. To estimate the model parameter (potentially time-varying), we make use of the inverse probability of censoring weighting approach and develop a system of estimating equations. Both asymptotic and finite sample properties of the proposed estimators are established and the approach is applied to two real life data sets collected from a clinical trial. We also considered the efficiency and double robustness of our estimator, and developed a model checking technique for some special cases of the transformation models.

Yi Zhu
Tsinghua University
Nonlinear Waves in Shallow Honeycomb Lattices
The linear spectrum and corresponding Bloch modes near Dirac points are studied and employed to describe wave envelope dynamics in shallow honeycomb lattices. Using perturbation theory, the dispersion relation is found to have three-fold degeneracy to leading order with eigenvalue splitting at the following two orders; i.e., the three-fold eigenvalue splits into single and double values. The nonlinear dynamics of the envelope depends on different asymptotic balances whereupon a three-level nonlinear Dirac-type equation or a two-level nonlinear Dirac equation are derived. The analysis agrees well with direct numerical simulations.

CONTRIBUTED TALKS

Adrianna Gillman

Dartmouth College

A New Direct Solution Technique for Two-dimensional Quasi-periodic Fields

Accurate numerical modeling of periodic scattering problems is important for many applications including solar cells, diffraction gratings, acoustics absorbers, and photonic crystal slabs. Recently, a new integral representation for quasi-periodic scattering problems that achieves spectral accuracy has been developed. This representation avoids the blow-up of the quasi-periodic Green's function at so-called Wood anomalies by restricting the exterior domain to a quasi-periodic strip and using the free-space Green's function. Upon discretization, the integral representation leads to a linear system of size N+M where N is the number of boundary nodes and M is the number of periodizing unknowns. Solving this system can be computationally prohibitive for complicated geometries and near resonances, even when using a Fast Multipole Method to accelerate iterative methods. In this talk, we present a new direct solution technique which utilizes the robust fast direct solvers developed for one-dimensional integral equations. Since M is O(1), the result is a method with computational cost that grows linearly with N. Each additional solve is less expensive than the first. This is important for problems with multiple right-hand sides that often arise in design problems where there are multiple incident angles.

This work is done in collaboration with Alex Barnett.

Fangxu Jing

Georgia Institute of Technology

Optimization of Two-link and Three-link Snake Like Locomotion

We analyze two-link (or three-link) 2D snake like locomotions and discuss the optimization of the motion. The snake is modeled as two (or three) identical links connected via hinge joints and the relative angles between the links are prescribed as periodic actuation functions. An essential feature of the locomotion is the anisotropy of friction coefficients. The dynamics of the snake is analyzed numerically, as well as analytically for small amplitude actuations of the relative angles. Cost of locomotion is defined as the ratio between distance traveled by the snake and the energy expenditure within one period. Optimal conditions of the highest efficiency in terms of the friction coefficients and the actuations are discussed for the model.

Joint work with Silas Alben.

Pilhwa Lee

University of Connecticut Health Center

Modeling Collective Cell Migration: Wound Healing and Cancer Metastasis

We do modeling for collective migration of epithelial tissues. Individual crawling cells on 2D substrate are represented by dipole-stress with their polarity in continuum. Cell-cell and cell-substrate interactions are realized by viscoelastic relaxation and viscous drag forces, respectively. This framework is applied to the mechanisms of wound healing and cancer metastasis. We show that the wound closure is essentially mechanical and the integrin up-regulation and cadherin down-regulation are sufficient in the metastatic transition in cancer.

Nick Lowman

North Carolina State University

A Characterization of Dispersive Shock Waves in the Magma Equation

In one-dimension and under reasonable simplifications and assumptions, the full governing equations of subterranean vertical magma transport reduce to a degenerate nonlinear third-order dispersive partial differential equation for the fluid porosity with two variable parameters. For an arbitrary initial step and physical parameter values, the properties of magma dispersive shock waves (speeds, leading amplitude) are constructed asymptotically. Results are corroborated by comparisons with robust, accurate numerical simulations for long-time evolution.

Kellen Petersen

New York University

Use of the String Method to Find Minimal Energy Paths of Droplets on Superhydrophobic Surfaces

Interest in superhydrophobic surfaces has increased due to a number of interesting advances in science and engineering. Here we use a diffuse interface model for droplets on topographically and chemically patterned surfaces in the regime where gravity is negligible. We then apply the constrained string method to examine the transition of droplets between different metastable/stable states. The string method finds the minimal energy paths (MEPs) which correspond to the most probable transition pathways between the metastable/stable states in the configuration space. In the case of a hydrophobic surface with posts of variable height and separation, we determine the MEP corresponding to the transition between the Cassie-Baxter and Wenzel states. Additionally, we realize critical droplet morphologies along the MEP associated with saddle points of the free-energy potential and the energy barrier of the free energy. We analyze and compare the MEPs and free-energy barriers for a variety of surface geometries, droplets sizes, and static contact angles ranging from partial wetting to complete wetting. We also introduce an unbiased double well potential in the diffuse interace model by introducing a chemical potential that is fixed for a given simulation. We find that the energy barrier shifts toward the Wenzel state along the MEP as the height of the pillars increases in the topographically patterned case while a shorter energy barrier exists and is more centered along the MEP for pillars of shorter height. More importantly, we demonstrate the string method as a useful tool in the study of droplets on superhydrophobic surfaces by presenting a numerical study that finds MEPs in configuration space, critical droplet morphologies and free-energy barriers which in turn give us a greater understanding of the free-energy landscape.

Jeffrey Pohlmeyer

New Jersey Institute of Technology

Mathematical Model of Growth Factor Driven Haptotaxis and Proliferation in a Tissue Engineering Scaffold

We investigate the effect of growth factor based haptotaxis and proliferation in a perfusion tissue engineering bioreactor, in which nutrient-rich culture medium is perfused through a 2D porous scaffold seeded with cells. Our goal is to model the effect of impregnating the scaffold with a non-diffusible growth factor to which cells respond haptotactically, and which also enhances proliferation. We model these processes on the timescale of cell proliferation, which typically is of the order of days. While a quantitative representation of these phenomena requires more experimental data than is yet available, qualitative agreement with preliminary experimental studies is obtained, and appears promising.

Xiaolin Wang

Georgia Institute of Technology

A Numerical Study of Vorticity Enhanced Heat Transfer

The Glezer lab at Georgia Tech has found that vorticity can improve heat transfer efficiency in electronic hardware. Vortices are able to enhance the forced convection in the boundary layer and fully mix the heated fluid with cooler core flow. Some recent experiments showed the possibility of using a vibrated reed to produce vortices in heat sinks. In this work, we simulate both the fluid and the heat transfer process in a 3-dimensional plate fin heat sink. We propose a simplified model by considering flow and temperature in a 2-D channel, and extend the model to the third dimension using a 1-D heat fin model. We simulate periodically steady-state solutions. We show that the total heat flux transferred from the plate to the fluid can be improved with vortices given the same input power. A possible optimal solution for the largest heat transfer efficiency is proposed for the physical parameters of a real computer heat sink. We discuss the effect of the important parameters such as Reynolds number and thermal conductivities.

Ying Wang
University of Minnesota

A Continuum Mathematical Model of Endothelial Layer Maintenance and Senescence

In this talk, I will introduce a continuum mathematical model, which describes the dynamics of large endothelial cells (EC) populations of the endothelium using a system of differential equations for the number densities of cells of different generations starting from endothelial progenitors to senescent cells, as well as the densities of dead cells and the holes created upon clearing dead cells. The proposed model describes the aging of the endothelium as being driven by cellular senescence, with a rate that does not necessarily correspond to the chronological aging of a person. It is shown that the age of the endothelium depends sensitively on the homing rates of EC progenitor cells. (Joint work with Baltazar D. Aguda and Avner Friedman)

POSTERS

Sonia Bandha and M.C. Bhattacharjee

New Jersey Institute of Technology

Managing Warranty Costs with Variable Usage Rates

The majority of research literature on modeling and optimization of warranty servicing costs assume a constant and known usage rate of the product by its customers. Such an assumption is unrealistic for many moderately high value items with a substantial sales volume (such as new automobiles) where the product's use profile may at best be statistically known in terms of a usage rate distribution. We consider such a formulation under standard two-dimensional warranties (max allowable accumulated use, or attaining a specified age of the product, whichever occurs first) for some widely used warranty servicing policies. The impact of the intensity of use on product lifetime is modeled using a "Copula" approach that allows a choice of dependency structures. Application of the Copula approach in the warranty context is illustrated with a uniformly distributed usage rate and AFT (Accelerated Failure Time) model with Weibull lifetime conditional on the rate of use. Since the expected warranty costs cannot usually be expressed in a directly computable closed analytic form; numerical integration in two dimensions and "simulated annealing" methods are used to derive computational solutions for the optimal values of the decision parameters in the warranty servicing policy.

Irina Berezovik

Fordham University

Control of Lipidic Pore Dynamics by Aqueous Viscosity

A new theory, to our knowledge, is developed that describes the dynamics of a lipidic pore in a liposome. The equations of the theory capture the experimentally observed three-stage functional form of pore radius over time—stage 1, rapid pore enlargement; stage 2, slow pore shrinkage; and stage 3, rapid pore closure. They also show that lipid flow is kinetically limited by the values of both membrane and aqueous viscosity; therefore, pore evolution is affected by both viscosities. The theory predicts that for a giant liposome, tens of microns in radius, water viscosity dominates over the effects of membrane viscosity. The edge tension of a lipidic pore is calculated by using the theory to quantitatively account for pore kinetics in stage 3, rapid pore closing. This value of edge tension agrees with the value as standardly calculated from the stage of slow pore closure, stage 2. For small, submicron liposomes, membrane viscosity affects pore kinetics, but only if the viscosity of the aqueous solution is comparable to that of distilled water. A first-principle fluid-echanics calculation of the friction due to aqueous viscosity is in excellent agreement with the friction obtained by applying the new theory to data of previously published experimental results. Joint work with Rolf Ryham and Fredric Cohen.

Carlos Borges

Worcester Polytechnic Institute

Multi-frequency Iterative Integral Equations Method for the Shape Reconstruction of an Acoustically Sound-soft Obstacle using Backscattering

We present a method of solving the problem of obtaining a reconstruction of a planar acoustically sound-soft obstacle from the measured far-field pattern generated by plane waves with a fixed incidence and varying frequencies. We solve iteratively the problem for each frequency, from the lowest to the highest, using as an initial guess the solution given by the previous frequency. We present numerical results showing the benefits of our approach.

Todd Caskey, Albi Kavo, Mandeep Singh, and David J. Horntrop
New Jersey Institute of Technology

Variance Reduction Techniques for Stochastic Differential Equations

Stochastic differential equations are essential to modeling many physical phenomena including option prices in mathematical finance. The stochastic simulation of the quantities of interest is done using repeated realizations of Monte Carlo methods. However, these methods are well known for converging slowly with an order of only 1/2 in terms of the number of realizations. Therefore, there is an increasing need for variance reduction in order to improve efficiency of Monte Carlo simulations. Here we use control variates to improve the computational efficiency. The results presented demonstrate the magnitude of the achieved variance reduction. This research was completed as part of the NSF-sponsored CSUMS program for undergraduate research.

Feiyan Chen
New Jersey Institute of Technology

The Goodness-of-fit Tests for Geometric Models

We propose two types of goodness-of-fit tests for geometric distribution and for a bivariate geometric distribution called BGD (B&D), based on their probability generating function (PGF). The first type is a special-case application of the general testing procedure for discrete distributions proposed by Kocherlakota and Kocherlakota (1986) (K&K). The second type utilizes the supremum of the absolute value of the standardized difference between the PGF's MLE and its empirical counterpart as the test statistic. The second type test is an improvement over the first one. We compare the empirical critical points of the first type of test with their asymptotic values, and calculate the critical points of the second type of test using simulation for various sample sizes and parameters. We simulate the empirical significance level of our proposed tests. Also we make power comparisons of our proposed tests with the Chi-square tests and with those in Best and Rayner (2003) in the univariate case. Real data sets will be used to illustrate the proposed methods for the goodness-of-fit of the geometric models.

Daniel Fong
New Jersey Institute of Technology

An Asymptotic Theory of Laminar Premixed Flames in Dense Fluids

We derive an asymptotic theory of laminar premixed flames in high density fluids in the limit of large activation energy. The model is intended to provide insights into the structure and dynamics of deflagration waves in high pressure, dense fluids where normal Fickian diffusion is limited. In such cases, particularly under conditions exceeding the thermodynamic critical point of the fluid, the primary mode of species transport is through thermal-diffusion, i.e. the Soret effect. Such a model for diffusive transport is considered, and we derive a model with an explicit dependence on the Soret effect for a one-step overall reaction. The density is assumed sufficiently high to adopt a constant density formulation. The local reaction-diffusion structure is found to be fundamentally different from that of an ideal gas with Fickian diffusion, which results in new conditions relating the equations for thermal and mass transport in the bulk flow. The model is used to investigate the basic structure of planar flames, as well as their stability. Stability boundaries are identified that mark the transition from planar to either steady, spatially periodic structures, or time-dependent modes of propagation. The combined effects of the Soret diffusion coefficient and Lewis number are discussed. Furthermore, a weakly nonlinear analysis of the derived model is carried out, resulting in a modified Kuramoto-Sivashinsky (K-S) equation. Joint work with John Bechtold.

Natasha Cayco Gajic
University of Washington

An Analysis of the Emergence of Critical Activity in Feedforward Neural Networks

Recent experimental and computational evidence has suggested that the brain may operate at a critical state characterized by complex dynamics, signicant higher-order correlations, and optimal computational properties. We investigate the emergence of critical activity in a homogeneous, feedforward neural network of McCullochs-Pitts neurons. By applying an eigenstructure analysis of a mean-field Markov chain model, we are able to explain geometrically this complexity. We extend this analysis to more realistic models that include inhibition and noise.

Shengyan Gao, Jay N. Meegoda, and Liming Hu

New Jersey Institute of Technology

Simulation of Dynamic Two-Phase Flow during Air Sparging

Air sparging (AS) is an in-situ soil/groundwater remediation technology, which involves the injection of pressurized air/oxygen through an air sparging well below the zone of contamination. Characterizing the mechanisms governing movement of air through saturated porous media is critical for the design of an effective cleanup treatment system. In this research, micromechanical investigation was performed in order to understand the physics of air migration and subsequent spatial distribution of air at pore scale during air sparging. The void space in the porous medium was first characterized by pore network consisting of connected pore bodies and bonds. One methodology of extracting pore network from the simulated packing of spheres was proposed and employed to extract main structural properties of the random packing of spheres. Modified Delaunay tessellation (MDT) in conjunction with modified Nelder-Mead method was used to characterize the void space of the simulated packing. The Biconical Abscissa Asymmetric CONcentric (BACON) bond was used to describe the connection between two adjacent pore bodies. Then a rule-based dynamic two-phase flow model was developed and applied to the pore network model. A forward integration of time was performed using the Euler scheme. For each time step, the effective viscosity of fluid was calculated based on fractions of two phases in each bond and capillary pressures across the menisci was considered to compute the pressure field. Finally, the developed dynamic model was used to study the rate-dependent drainage during air sparging. The effect of the capillary number and geometrical properties of the network on the dynamic flow properties of two-phase flow including residual saturation, spatial distribution of air and water, dynamic phase transitions, and relative permeability-capillary pressure curves were systematically investigated. Results showed that all the above information for describing the two-phase flow during air sparging are not intrinsic properties of the porous medium, but are affected by the two-phase flow dynamics and spatial distribution of each phase, providing new insight to air sparging.

Md.Shahadat Hossain, Bhavin Dalal, Sathish Kumar Gurupatham, Ian Fischer, and Pushpendra Singh

New Jersey Institute of Technology

Thin Films with Self-Assembled Monolayers Embedded on Their Surfaces

We have recently shown that the capillarity-based process for self-assembling particle monolayers on fluid-liquid interfaces can be improved by applying an electric field in the direction normal to the interface. The electric field gives rise to repulsive dipole-dipole forces among the particles causing them to move apart, and thus move freely without blocking one another. The latter allows for the formation of virtually defect-free monolayers with long-range order. In this paper, we present a technique for freezing these expanded monolayers onto the surface of a flexible thin film. The technique involves assembling the monolayer on the interface between a UV-curable resin and a fluid which can be air or another liquid, and then curing the resin by applying UV light. The monolayer becomes embedded on the surface of the solidified resin film.

Yogesh Joshi

Kingsborough Community College

Exponentially Decaying Discrete Dynamical Systems

There are numerous phenomena in the biological and ecological sciences whose discrete evolution can be effectively modeled by exponentially decaying discrete dynamical systems (ED3S). A discrete Pioneer-Climax population model is an example for ED3S. It is not difficult to show that these exponentially decaying dynamical systems have attracting sets that can have remarkable properties. For example, the attractor may be a strange attractor – a set with non-integer fractal dimension on which the dynamics is chaotic and variations in the parameter can cause bifurcations that change the fundamental nature of the chaotic regimes.

Tao Lin

New Jersey Institute of Technology

An Inverse Method for Estimating Sound Speed in Stratified Ocean

The focus of my work is to develop a new inverse method for estimating geoacoustic properties in shallow water environments, in particular the sound-speed profile. In this work, I implement Stickler's method and then investigate two problems that are not addressed in previously published work. The first problem is the lack of a fast and accurate numerical algorithm for solving the nonlinear trace formula. The second is the consideration of noise in the data used as input to the inverse problem.

Te-Sheng Lin

New Jersey Institute of Technology

Instabilities of Thin Fluid Films

We study instabilities of Newtonian films within the framework of lubrication approximation. It is found that, under destabilizing gravitational force, a contact line, modelled by a commonly used precursor film model, leads to free surface instabilities without any additional natural or excited perturbations. In addition, there is also a coupling between the surface instabilities and the transverse (fingering) instabilities, lead to complex behaviors. All the observed phenomena are characterized by a single parameter D=(3Ca)^(1/3)cot(a), where Ca is the capillary number and a is the inclination angle. Variation of D leads to change in the wavelike properties of the instabilities, allowing us to observe travelling wave behavior, mixed waves, and the wave resembling solitary ones.

Yang Liu

Drexel University

Properties of Discrete Delta Functions and Convergence of the Immersed Boundary Method

Many problems involving internal interfaces can be formulated as partial differential equations with singular source terms. Numerical approximation to such problems on a regular grid necessitates suitable regularizations of delta functions. We study the convergence properties of such discretizations for constant coefficient elliptic problems using the immersed boundary method as an example. We show how the order of the differential operator, order of the finite difference discretization, and properties of the discrete delta function all influence the local convergence behavior. In particular, we show how a recently introduced property of discrete delta functions-the smoothing order-is important in the determination of local convergence rates.

Gavin Lynch

New Jersey Institute of Technology

The Control of the False Discovery Rate in Fixed Sequence Multiple Testing

Controlling the false discovery rate (FDR) is a powerful approach to multiple testing. However, existing FDR controlling procedures typically order the tests based on the p-values, incurring a large multiple testing penalty. If, instead, the ordering of the tests is fixed based on prior knowledge then the critical constants can be made much larger. In this presentation, we present the first known procedures for controlling the FDR in fixed sequence multiple testing. First, we consider the conventional fixed sequence method, where the procedure stops on the first acceptance, under any dependence and independence. Then we extend the method and develop procedures that stop on the kth acceptance. This extension accounts for any potential mistakes in the ordering of the tests. Simulation studies show that these procedures can be a powerful alternative to the well-known Benjamini-Hochberg procedure.

Manman Ma

New Jersey Institute of Technology

A Numerical Method for Electro-osmotic Flow with Moving Boundaries

Electrokinetics has wide applications in analytical chemistry, microfluidics and other related fields, We consider a viscous drop suspended in an electrolyte with a steady electric field applied. Both the drop and

the suspending fluid are electrolytes and electrokinetic effects have to be taken into account. The Debye layer that appears adjacent to the charged surface because of ions diffusion makes the problem different from the classical model for perfect conductors or leaky dielectrics. Asymptotic methods are utilized to solve leading order time dependent problem for layer potential and charge density. We have solved the leading order time dependent problem and numerical steady state problem for potential. For drop deformation, we intend to use the slenderness of the layer to develop a fast and accurate 'hybrid' or multiscale numerical method that incorporates a singular perturbation analysis of the boundary layer into a boundary integral numerical solution of the free boundary problem.

Kyle Mahady

New Jersey Institute of Technology

Volume of Fluid Simulations of the Breakup of a Rivulet

Consider a finite rivulet of fluid. As the rivulet retracts, fluid accumulates at the edges and, under suitable circumstances, may break off into separate drops. We simulate the dynamics of retracting rivulets in two and three dimensions using the full Navier Stokes equations with Volume of Fluid interface tracking. The stability of the retraction is compared with the predictions of linear stability analyses in the infinite case.

Tony Mastroberardino

Penn State Erie, The Behrend College

Mixed Convection in Viscoelastic Flow due to a Stretching Sheet

The study of the fluid mechanics due to a stretching surface in a fluid at rest is an important aspect of various industrial applications. For instance, in polymer extrusion processes, the extruded material passes between two solid blocks into a region containing fluid at rest that cools the sheet and alters its mechanical properties. In this presentation, I will perform an analysis of a mathematical model describing the aforementioned process in which the ambient fluid is non-Newtonian and the effects of mixed convection are taken into consideration. The governing partial differential equations for the fluid flow and temperature are reduced to a nonlinear system of ordinary differential equations which are solved analytically using the homotopy analysis method (HAM).

Dawid Midura

New Jersey Institute of Technology

Acceleration of the Convergence of Non-overlapping Domain Decomposition Methods Using the Cross-point Technique

We are interested in applying non-overlapping domain decomposition method to the Helmholtz equation. This requires the use of the cross-point technique which consists of preservation of continuity of the finite element space at the nodes shared by more than two subdomains. In this work we extend the technique to nodes located at the artificial interfaces with an aim to improve the convergence of the resulting iterative method.

Elizabeth Munch

Duke University

Using Metrics on Vineyards to Analyze Primate Group Fission and Fusion Patterns

Computational topology has become an increasingly useful tool in data analysis. Given a point cloud, we can use simplicial complexes like the Vietoris-Rips complex or the Cech complex for increasing radii and watch how the topology of the space changes. This allows us to differentiate between noise, which are classes that appear and disappear quickly, and the important topological features of the underlying space. This process yields a persistence diagram, which is a 2-dimensional representation of the birth and death time of each topological feature.

If we instead have a dynamic point cloud, the cloud at each time gives a persistence diagram. When these diagrams are stacked up, we call the resulting construction a vineyard. The vineyard can be used to understand something about the changing behavior of the dynamic point cloud.

We use vineyards to understand primate group fission and fusion patterns by building an agent based model (ABM) to approximate the behaviors seen in vito. However, we want a quatitative way to compare the approximations seen in the ABM to the true data. As such, we have defined a metric on the vineyards to be able to compare the results of one to the other. Most importantly, this metric satisfies various notions of stability so that we can be sure a slight change in the point cloud gives vineyards which are close in the sense of our metric.
This work is joint with John Harer, Anne Pusey, Susan Alberts, and Ian Gilby.

Naga Musunuri, Bhavin Dalal, Md.Shahadat Hossain, Ian Fischer, and Pushpendra Singh

New Jersey Institute of Technology

Dispersion of Particles on Fluid-Liquid Interfaces

When powders containing small particles, e.g., glass, flour, pollen, etc., come in contact with an air-liquid interface, they disperse in a manner that appears explosive. This is due to the fact that when a particle comes in contact with an interface the capillary force pulls it inwards causing it to accelerate to a relatively-large velocity in the direction normal to the interface. The motion of the particle is inertia dominated, and so it oscillates vertically about its equilibrium position before coming to a stop. The flow induced near the interface due to the adsorption of a particle is away from the particle and directly below is towards the particle. The former causes nearby particles to move away. The rate of dispersion depends on the parameters such as the size of particles, the viscosities of the fluids, the interfacial tension and the contact angle.

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A Modeling Study of Conductance Co-regulation in Neuronal Models

Rhythmic oscillation in neurons can be characterized by various attributes such as the oscillation period and duty cycle. The values of these features depend on the levels of the participating ionic currents, and can be characterized by the values of their corresponding conductances. Recent experimental and theoretical work has shown that the values of certain attributes can be maintained constant for different combinations of conductances, referred to as correlated conductances, defining specific level sets. In this work we use modeling, dynamical systems tools and numerical simulations to investigate the biophysical and dynamic mechanisms responsible for maintaining a constant period for different sets of correlated conductances in two neuron models that include representative currents typically found in neurons. We find that maintenance of constant spiking and oscillation periods involves not only balanced changes in the maximal conductances, but also a compensation mechanism that involves different effective time scales of the evolution of the different ionic currents due to their particular dynamics and voltage dependencies.

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Nonparametric Bayes Estimation of Inter-Event Distribution with Recurrent Event Data

Nonparametric Bayes estimation of the inter-event time survivor function governing the time to occurrence of recurrent event in the presence of censoring is of interest. For the i-th unit, denote the successive interoccurrence time of a recurrent event by {T_ij, k=1, 2, 3,} and the end of monitoring time by Y_i. Assume that {T_ij , i=1, 2,..., n ; j=1, 2,} and {Y_i , i=1, 2,..., n } are i.i.d. nonnegative random variables with common distribution function F and G, respectively,and with Y_i and {T_ij } mutually independent. In our Bayesian approach we let F has prior measure P, which is a Dirichlet processes with parameter alpha. There are nonparametric non-Bayes methods of estimating F in the literature, for example, Pena et al. (JASA, 2001), and also nonparametric Bayes estimation methods; for instance, Sethuraman and Hollander's nonparametric Bayes estimation for repair models (JSPI, 2009) and Susarla and Van Ryzin's (JASA, 1976) Bayesian estimation of survival function for single event complete and censored observations. Susarla et al. derived a Bayesian extension of the Kaplan-Meier (Product-Limit) estimator. Following Susarla et al.'s approach, we derive nonparametric Bayesian estimator of F of the survival function in recurrent event settings. The estimator can be viewed as Bayesian extension of the nonparametric PL type estimator (proposed by Pena et al.). One can view PL type estimator as a special case of the Bayes estimator when alpha(R^+) tends 0). By simulation studies, we demonstrate that the PL type estimator has smaller bias but higher root-mean-squared errors than those of the Bayes and the empirical Bayes estimators. Even in the case of mis-specification of the prior distribution parameter alpha. Bayes estimators and empirical Bayes estimators have smaller root-mean-squared errors than PL type estimator, which is an indication of robustness of the Bayes estimators. The Bayes estimators are smoother than Pena et al. (JASA, 2001) non-Bayes estimators. Graphical comparison shows that the Bayes and non-Bayes estimates of survival function tend to be close. This work is under the supervision of my advisor Professor Edsel A. Pena. Research is supported by National Science Foundation (NSF) Grants DMS-1106435.

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The Microstructure Evolution in Density Relaxation by Tapping

Density relaxation is modeling using both Monte Carlo and discrete element simulations to investigate the effects of regular taps applied to a container having a planar floor filled with monodisperse spheres. Results suggest the existence of a critical tap intensity which produces a maximum bulk solids fraction. We find that the mechanism responsible for the relaxation phenomenon is an evolving ordered packing structure propagating upwards from the plane floor.

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Optimal Finite Difference Grids for Elliptic and Parabolic PDEs with Applications

In many applications one observes rapid change of the solution in the boundary region. Accurate and numerically efficient resolution of the solution close to the moving boundaries is considered to be an important problem. We propose the optimal grids method to efficiently obtain the NtD and DtN maps with spectral accuracy for nonuniform boundary data. Method is applied to the model elliptic boundary value problem and parabolic initial value problem in the semi-infinite domains. We show that the described special choice of the discretization grid steps provides a spectral convergence order of the solution at the boundary. Using the suggested approach we are able to achieve the exponential convergence of the boundary Neumann-to-Dirichlet maps. Optimal grids method increases the convergence order without increasing the stencil size of the finite-difference scheme.

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Tapping Dynamics for a Colume of Particles and Beyond

The dynamics of a vertical stack of particles subject to gravity and a sequence of small, periodically applied taps is considered.

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Modeling History-dependence of Conduction Delay in a Non-myelinated Axon

Conduction delay in axons is a function of the axon morphology, its passive membrane properties and voltage-gated ionic currents. Although conduction delay is usually assumed to be constant, indicating perfect temporal fidelity, recent work has shown that the conduction delay of each action potential depends on the prior short- and long-term history of activity in the axon (Ballo & Bucher, 2009). Experimental measurements in the motor axon of the pyloric dilator (PD) neuron of the lobster *H. americanus* examined conduction delay using Poisson random stimuli applied at different mean rates (Bucher et al, SfN 287.3, 2010). These measurements showed that both the mean value and the variance of conduction delay increases as a function of stimulus time until these values reach a steady state at about the 5th minute post stimulation. Additionally, even at steady state, conduction delay has a nonlinear relationship with instantaneous frequency (f_{inst}): it is higher at small or large values of f_{inst} but has a minimum at f_{inst} ~45 Hz.

We use a model of the PD axon to examine the role of different ionic currents in shaping the history dependence of conduction delay. In addition to the Hodgkin-Huxley leak, fast sodium and delayed-rectifier potassium currents, this model incorporates voltage-gated ionic currents, such as a transient potassium current I_A and a hyperpolarization activated inward current I_h, that have been characterized in this axon. We find that adding a Na^+/K^+ pump with slow (τ=90 sec) time constant results in an increase of the mean value and the variance of conduction delay with stimulus time, as observed in the experiments. Additionally, the presence of the Na^+/K^+ pump in our model also results in the decrease of conduction delay as a function of f_{ints}, which shows the local minimum that also observed in the experiments. Furthermore, similar to experimental observations, temporal fidelity is improved as I_h is increased. The model provides a quantitative tool to describe the effects of nonlinear currents on temporal fidelity of conduction delay in a non-myelinated axon. Grants: NIH MH60605 and NS58825

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Threshold Phenomena in Reaction-Diffusion Problems

We study the Cauchy problems for bistable nonlinear reaction-diffusion equations by using energy methods. We prove the one-to-one relation between long time behavior of solution and the limit value of energy. Moreover, for a suitable monotone one-parameter family of initial data, there exists a sharp transition between extinction and propagation.