PLENARY SPEAKERS

I. David Abrahams

School of Mathematics, University of Manchester, UK

Asymptotic Homogenization and Effective Material Properties in Elasticity and Electromagnetics

The derivation of effective material properties to describe complex materials is ubiquitous in physics, engineering and applied mathematics. For example, for light passing through a crystal the precise detail of the inhomogenous arrangement of atoms can be conveniently 'averaged' into just two macroscopic electromagnetic quantities, the electric permittivity and the magnetic permeability. Many different approaches have been offered to obtain effective, or homogenized, equations to describe the behaviour of materials, and these range from simple engineering methods to mathematically rigorous variational techniques. This overview talk will discuss a number of physical models and several methods for obtaining their effective field equations. As time allows, these will include elastic wave propagation in biological and industrial composite materials, and electromagnetic wave propagation in optical fibres. To illustrate the asymptotic approaches, and the limitations of current methods, recourse will often be made to simple one-dimensional models.

G. Bard Ermentrout

University of Pittsburgh

When the noise is the signal: Stochastic synchronization in neurons

Stochastic synchronization is a mechanism through which correlated noise is able to drive independent oscillators toward synchronization. It has been suggested as a mechanism for cooperative behavior in cellular and neural processes. In this talk I will describe some recent work on how this happens and some optimality principles that underlie stochastic synchrony. I will also discuss recent work on stochastic feedback in the olfactory system and also the role of intrinsic dynamics on the response to noise. Joint work with R.F. Galan, N.N. Urban, S. Marella, and C. Ly.

Frank Hoppensteadt

Courant Institute of Mathematical Sciences, NYU

Multi-scale Methods, Computer Simulations, and Data Mining: Difference Equations and Renewal Equations

Has applied mathematics disappeared behind the computer screen? High level computer languages and high capacity computers for simulation followed by data mining give powerful tools for studying complex systems. The two examples presented here are a system of difference equations from population genetics and a system of Volterra integral equations from demography, both perturbed by random noise. We analyze these systems using averaging methods and then compare the derived solution with computer simulations of the system. In the first case, mathematical analysis guides mining of the simulated solution data base. In the second, mathematical analysis reveals chaotic behavior that confounds the simulation/data mining approach.

Pranab K. Sen

University of North Carolina at Chapel Hill

Whither Biostochastics in Computational Biology and Bioinformatics

Principles of molecular biology, (multi-factorial) genetics, genomics, proteomics, as well as toxicogenomics govern computational biology and bioinformatics; there is ample room for biostochastics to comprehend the basic difference between mathematical determinacy and biological diversity. With the evolution of information technology in conjunction with increasingly faster computer technology, bioinformatics and pharmacogenomics, amidst massive datasets in astounding pace, knowledge discovery and data mining (or statistical learning) tools largely dominate contemporary quantitative assessments. Though the aim is to fathom out the mysteries of disease genes and gene-environment interaction, it often bypasses statistical challenges posed by some thirty thousand genes whose clustered interactions with diseases and environmental stressors are yet to be completely statistically resolved. Excessive cost of carrying out an adequately large and well planned statistical experiment, under a sound statistical design, creates impasses for routine adoption of standard statistical or biomathematical tools.

Some of the biostochastic perspectives in such excessively large dimensional low sample size data models are appraised thoroughly along with some illustrations of some microarray as well as SNP nucleotides models.

Beyond parametrics approaches are high-lighted in these perspectives.

Michael Shelley

Courant Institute of Mathematical Sciences, NYU

TBA

Jean-Marc Vanden-Broeck

University College, London, UK

Studies of Nonlinear Three Dimensional Free Surface Flows

Over the last 200 years important progress has been achieved in the calculations of two dimensional free surface flows. This success is largely based on the fact that two dimensional potential flows can be formulated in terms of complex variables and analytic functions. Three dimensional free surface flows are considerably more difficult to solve because complex analysis is no longer applicable and much larger number of mesh points are needed in numerical simulations. As a result there are much fewer nonlinear three dimensional results. The talk will summarise recent numerical computations which attempt to correct this imbalance. New results on solitary waves, interfacial waves and time dependent free surface flows will be presented and discussed.

INVITED TALKS

Shelley Anna

Carnegie Mellon University

The Dynamics of Tipstreaming in Microfluidic Flow Focusing Devices

Microfluidic devices can successfully produce highly uniform emulsion droplets that are tens of microns in size. Smaller droplets are more difficult to produce due to geometry limitations. We have recently shown that micron-scale droplets can be generated via a tipstreaming-like phenomenon that occurs in microfluidic flow focusing devices when soluble surfactants are present. In this mode of droplet breakup a thin thread is emitted from the tip of a conical interface following the pinchoff of a larger droplet. The thread breaks into discrete, micron-sized droplets. The process is periodic and occurs hundreds of times per second. The thin thread stretches affinely with the centerline velocity downstream and its lifetime depends on the velocity of the outer liquid, the viscosity ratio, and the surfactant mass transport properties. In addition, we observe that the cone angle from which the thread is drawn is insensitive to viscosity ratio but strongly depends on the surfactant properties. We describe a simplified model for the process that we have developed based on an observed symmetric corner flow in the inner liquid during the formation of the thread. Joint work with Lynn M. Walker and Wingki Lee.

Ernest Barreto

George Mason University

Dynamics and Synchronization of Interacting Populations of Oscillators

Many networks of technological, social, and biological interest involve several distinct interacting populations of heterogeneous elements. For example, in neuroscience, neurons can be excitatory or inhibitory, and neurons in each of these classes exhibit a wide range of behaviors. To investigate these kinds of networks, we study multiple interacting Kuramoto systems in which the connectivity is specified by a general matrix. Knowledge of this matrix is sufficient to determine the onset of collective synchronous behavior. We also consider the case of time-dependent coupling among the populations and identify novel mechanisms by which synchronization can arise or be thwarted in such systems.

J. Thomas Beale

Duke University

Numerical Methods for Moving Boundaries in Viscous Fluid Flow

We will describe an approach to computing fluid flow with moving boundaries in which an interface is kept sharp but the fluid motion is computed on a regular grid. Jump conditions at an interface can be imposed naturally through singular integrals. A distinctive feature of this work is a simple, direct method for evaluating a singular or nearly singular integral, such as a layer potential on a curve in 2D or a surface in 3D, which might represent a harmonic function or the velocity in Stokes flow. The nearly singular case occurs when we evaluate at a grid point near the surface. The integral is found by a standard quadrature, using a regularized form of the singularity, with correction terms added for the errors due to regularization and discretization. These corrections are found by local analysis near the singularity. For a surface in 3D, overlapping coordinate grids can be used with reasonable efficiency. In work with John Strain, we have applied this approach to 2D Stokes flow in a periodic box with a moving interface that responds elastically to its stretching. Strain's semi-Lagrangian contouring method is used to move the interface, and Ewald splitting is used for the velocity integral, with the smooth or regularized part computed as a Fourier series. The accuracy of the method was verified with an exact solution of the full problem. The method was formulated to allow for extension to Navier-Stokes flow; it gives the Stokes velocity at regular grid points with periodic boundary conditions. We are currently working with Anita Layton to develop such a method for Navier-Stokes flow with an elastic interface. We expect to find the Stokes velocity at each time, incorporating the jump conditions, and then add a smoother remainder term to the velocity which is computed at regular grid points.

Richard Bertram

Florida State University

Bursting in Pituitary Cells: A Totally Different Animal

Bursting is common in electrically excitable cells, such as neurons and many endocrine cells. The periodic oscillation consists of an episode of action potentials followed by a quiescent phase. The mathematical study of bursting oscillations was motivated by the activity of two cells: the R15 cell of Aplysia and the pancreatic beta-cell. The primary tool for this analysis, developed by John Rinzel, is geometric singular perturbation theory. This tool was used to classify several types of bursting oscillators observed experimentally, as well as many that have not been observed. In this presentation we contrast the dynamics of one of the "classical" bursters, the beta-cell within a pancreatic islet, with the dynamics of cells in the pituitary. These cells, such as somatotrophs and lactotrophs, secrete hormones in accordance with their electrical spiking pattern. An understanding of bursting in pituitary cells poses new mathematical challenges that go beyond the classification schemes that have proven useful for other types of bursters.

Lora Billings

Montclair State University

ADE in Multi-Strain Disease Models

As we increase our resources to fight disease, pathogens become more resilient in their means to survive. One example is antibody-dependent enhancement (ADE), a phenomenon in which viral replication is increased rather than decreased by immune sera. We study the complex dynamics induced by ADE in multi-strain disease models and investigate the effects of vaccine campaigns. In particular, we study the consequences of using single-strain vaccines, which would increase the virulence in other infections.

George Biros

University of Pennsylvania

Numerical Simulation of 2D Fluid Membranes

Fluid membranes are area-preserving interfaces that resist bending. They are models of cell membranes, intracellular organelles, and viral particles. We are interested in developing simulation tools for dilute suspensions of deformable vesicles. These tools should be computationally efficient, that is, they should scale well as the number of vesicles increases. I will discuss methods for the time evolution of vesicles immersed in a Stokesian fluid. I will discuss time-stepping and stability restrictions, and present numerical results that demonstrate the effectiveness of the overall algorithm. This is joint work with Denis Gueyffier (New York University), Shravan K. Veerapaneni (University of Pennsylvania), and Denis Zorin (New York University).

Yassine Boubendir

New Jersey Institute of Technology

Non-Overlapping Domain Decomposition Method and Boundary Element Method for Helmholtz Equation

Domain decomposition (DD) methods provide a significant contribution to modern day simulations. They can allow for seamless coupling between optimally suited numerical schemes and they can also enable simple parallelization strategies. In this talk, we shall first review the difficulties that arise in the optimization of the transmission conditions when applying a non-overlapping DDM to the Helmholtz equation. Then, we shall explain the approach that allows the use of the integral equation method to solve the local problems. In particular, we shall show the flexibility given by this algorithm in the choice of the transmission conditions to improve the effective convergence of the iterative procedure.

Paul Bressloff

University of Utah

Diffusion of Protein Receptors on a Cylindrical Dendritic Membrane with Partially Absorbing Traps

We present a model of protein receptor trafficking within the membrane of a cylindrical dendrite containing small protrusions called spines. Spines are the locus of most excitatory synapses in the central nervous system and act as localized traps for receptors diffusing within the dendritic membrane. We treat the transverse intersection of a spine and dendrite as a spatially-extended, partially-absorbing boundary and use singular perturbation theory to analyze the steady-state distribution of receptors. We compare the singular perturbation solutions with numerical solutions of the full model and with solutions of a reduced one-dimensional model, and find good agreement between them all. We also derive a system of Fokker-Planck equations from our model and use it to exactly solve a mean first passage time (MFPT) problem for a single receptor traveling a fixed axial distance along the dendrite. This is then used to calculate an effective diffusion coefficient for receptors when spines are uniformly distributed along the length of the cable, and to show how a non-uniform distribution of spines gives rise to anomalous subdiffusion.

Javier Cabrera

Rutgers University

A New Data Mining Paradigm for Biopharmaceutical Data

One of the most important questions in the drug industry is to be able to characterize patients who benefit the most from a drug compared to older drugs or to competitive drugs. In the simplest setting we have two treatments A and B and we would like to characterize the patients who benefit from drug A more than from drug B. We measure this benefit with a statistic that computes the difference of mean treatment effect. Usual data mining techniques like recursive partitioning (CART, C4.5) optimize a criterion for partitions of a single population, but in this case we deal with criteria that evaluates partitions of multiple populations.

In this presentation we introduce a new algorithm for recursive partitioning multiple populations. We introduce a set of robust criteria that are suitable for different types of response variable. Our criteria need to be robust because of the complexities of the datasets that we have to analyze that usually consist of combinations of clinical studies from different sources. The result of our analysis is a list of subsets that represents the characteristics of patients that benefit from drug A more than from drug B.

We will illustrate our method by analyzing several clinical studies and characterizing the patients who respond better to one drug over competing treatments. Joint work with Alvir, J., Caridi F., and Nguyen H. (Pfizer Inc.).

Aloknath Chakrabarti

Indian Institute of Science

Scattering of Water Waves by Freely Floating Semi-Infinite Elastic Plates on Water of Finite Depth

A class of mixed boundary value problems (BVPs) arising in the study of scattering of surface water waves by the edges of floating structures comprising of elastic plates, with or without cracks, is examined for analytical as well as numerical solutions. It is observed that the simplest possible method of solution of such BVPs is the one that involves solution of an over-determined system of Linear Algebraic Equations. Such over-determined system of equations are best solved by the method of least squares and numerical results for useful practical quantities such as the "reflection" and "transmission" coefficients are obtained in a straightforward manner. Keywords: Flexural gravity waves, floating elastic plates, cracks, scattering, linear water wave theory, reflection and transmission coefficients and eigenfunction expansion.

Stephen Childress

Courant Institute of Mathematical Sciences, NYU

Inertial Effects in Locomotion at Finite and Large Reynolds Numbers

The classic problem of the swimming of a flexible two-dimensional sheet by propagating waves of constant form is reconsidered at finite and large Reynolds numbers using asymptotic methods. A sheet model for recoil swimming in a perfect fluid is introduced, involving a periodic shape change coupled with oscillating internal masses. The locomotion of this device in a viscous fluid is then analysed using related asymptotic methods in the time domain.

Wooyoung Choi

New Jersey Institute of Technology

Short-Wave Instability of Internal Solitary Waves and a Regularized Long Wave Model

The propagation of large amplitude internal solitary waves in a system of two constant density layers are studied using a strongly nonlinear long wave model. While steady solitary wave solutions of the model show excellent agreement with numerical solutions of the Euler equations and laboratory experiments, a local stability analysis reveals that the time-dependent inviscid model suffers from the Kelvin- Helmholtz instability due to a tangential velocity discontinuity across the interface. To suppress this undesirable short wave instability that is often absent in real experiments, an attempt is made to regularize the model by modifying the short wave behavior of the dispersion relation and introducing the effect of viscosity. Joint work with Ricardo Barros (NJIT) and Tae-Chang Jo (Inha University).

Dharam V. Chopra

Wichita State University

On the Existence and Applications of Balanced Arrays

A balanced array (B-array) of strength t, with m rows (constraints), N columns (runs, treatment-combinations), and with two symbols is merely a matrix T of size $(m \times N)$ with two elements (say, 0 and 1) such that in every $(t \times N, t \leq m)$ submatrix $\overset{*}{T}$ of T, every $(t \times 1)$ vector $\underline{\alpha}$ of weight $i(0 \leq i \leq t;$ the weight of a vector is the number of 1's in it) appears a constant number μ_i (say) times. The number of constraints m and the vector $(\mu_0, \mu_1, -- \mu_t)$ are called the parameters of the array. Clearly the number N of columns is known once we know $\mu_i (i = 0,1,2,..,t)$. If $\mu_i = \mu$ for each i, the B-array is reduced to an orthogonal (O-array) with index set μ. Here we consider the existence of balanced arrays and discuss briefly their applications.
Key words: Balanced arrays, orthogonal arrays, strength of an array, constraints, runs.

Paul Chow

Wayne State University

Asymptotic Solutions of Some Randomly Perturbed Nonlinear Wave Equations

The talk is concerned with the long-time behavior of solutions to some stochastic wave equations with polynomial nonlinearity in three dimensions. In particular we are interested in the questions of global solutions and the asymptotic stability of equilibrium solutions. We will first show by an example that a cubically nonlinear stochastic wave equation may blow up in a finite time in the mean-square sense. Then, under some sufficient conditions, the existence of a global solution and its asymptotic stability will be discussed.

Michael D. Collins

Rensselaer Polytechnic Institute

Physics of an Avian Controversy

After being feared extinct for many decades, there have been recent reports by ornithologists of Ivory-billed Woodpecker in Arkansas and Florida. Although physical evidence has been obtained at both sites, this topic has remained controversial due to the fact that many ornithologists lack experience in evaluating evidence that falls short of a clear image. Due to the difficulty of obtaining evidence of this extremely rare and wary species, efforts to determine locations where small populations survive will benefit from the development of expertise in evaluating low-quality videos, audio recordings, and other forms of evidence. This type of analysis involves basic physics, such as motion dynamics, flight mechanics, sonograms, and bark adhesion. Applications to data from Arkansas and Florida as well as data obtained by the author will be discussed.

Pam Cook

University of Delaware

Steady and Transient Flows of Entangled Polymeric and Micellar Solutions

Surfactant molecules (micelles) can self-assemble in solution into long flexible structures known as wormlike micelles. These structures entangle, forming a dense network and thus exhibit viscoelastic properties similar to entangled polymer melts. In contrast to ‘inert’ polymeric networks, wormlike micelles continuously break and reform leading to an additional relaxation mechanism and the name ‘living polymers’. Experimental studies with both classes of entangled fluids show that shearing flows exhibit spatial inhomogeneities, 'shear-banding'. The formulation of a new class of constitutive models (denoted VCM) is presented along with the model predictions. These models form a class of two-species elastic network models which can capture, in a self-consistent manner, micellar breakage and reforming as well as non-affine tube deformation and chain disentanglement through coupling between the microstructural conformations and the macroscopic stress. In steady state shear analysis of the full inhomogeneous flow field of these models shows localized shear bands that grow linearly in extent across the gap as the apparent shear rate is incremented. Time-dependent predictions under Large Amplitude Oscillatory shear (LAOS), along with phase plane and Pipkin diagrams of the flows are used to explore the complex model dynamics and to discriminate between various existing models. Portions of this work were done with support of NSF-DMS under DMS#0405931 and DMS#0406590. Joint work with Lin Zhou (University of Delaware) and Gareth McKinley (Massachusetts Institute of Technology).

Sharon Crook

Arizona State University

Modeling Activity-Dependent Changes in Dendritic Spine Structure

Recent evidence indicates that the morphology and density of dendritic spines are regulated during synaptic plasticity. High-frequency stimuli that induce long-term potentiation have been associated with increases in the number and size of spines. In contrast, low-frequency stimuli that induce long-term depression are associated with decreases in the number and size of spines. Decreases in spine density also occur due to excitotoxicity associated with very high levels of activity such as during seizures. This activity-dependent structural plasticity exists over a vast range of time scales, from minutes to days or weeks. In this work, performed in collaboration with Steve Baer, we extend previous modeling studies to include calcium-mediated spine restructuring. The models are based on the standard dimensionless cable equation for the changes in membrane potential in a passive dendrite. Additional equations characterize the activity-dependent changes in spine shape along the dendrite. We use computational studies to investigate the interactions between the many activity-dependent spines and to reveal the impact of their collective dynamics on the output properties of the dendrite.

Steven A. Cummer

Duke University

Cloaking and Other Material-Based Manipulations of Acoustic Waves

It was recently shown [Pendry et al., Science, 2006] how coordinate transformations of Maxwell's equations can be interpreted in terms of an electromagnetic material in the original coordinates with transformed permittivity and permeability values. Consequently, the bending and stretching of electromagnetic fields specified by coordinate transformations can be implemented with electromagnetic materials, enabling unexpected and interesting solutions such as electromagnetic cloaking. We have recently shown, through several different approaches, how this same concept can be extended to realize arbitrary manipulations of acoustic waves, including cloaking, using materials with very specific properties. This presentation will summarize the related concepts of transformation optics and transformation acoustics and will discuss approaches for engineering composite materials

with the properties needed to realize in practice the applications that have been thus far only been conceived on paper.

Linda J. Cummings

University of Nottingham

Fluid Dynamics and Crystal Deposition in Stented and Catheterised Urinary Tracts

A ureteric stent is a slender polymer tube that can be placed within the ureter (the muscular tube that conveys urine from the kidney to the bladder) to relieve a blockage due, for example, to a kidney stone in transit, or to external pressure from a tumour. A urinary catheter can be placed similarly within the urethra (the muscular tube conveying urine from the bladder out of the body), either again to relieve a blockage, or to allow control of urination in incontinent patients or those recovering from surgery.

Several clinical complications are associated with each of these biomedical devices. Both become encrusted, over time, with salts that precipitate out from the urine. Such encrustation is often associated with infection and the presence of bacterial biofilm on the device and, if severe, can make removal of the device difficult and painful. Ureteric stents are also associated with urinary reflux: retrograde flow of urine back towards the kidney. This arises because the presence of the stent prevents proper function of the sphincter between ureter and bladder that normally closes off when bladder pressure rises. Such reflux can expose the kidney to dangerously high pressures, and increase the risk of renal infection, both of which can lead to long-term damage.

We have been involved in an interdisciplinary study of these processes, with colleagues from Medical & Surgical Sciences and Materials Engineering. We present mathematical models of the reflux and encrustation processes, and consider the implications for device design and clinical practice.

Manisha Desai

Columbia University

Multiple Imputation to Reduce Selection Bias in Molecular Epidemiology Studies with Non-Ignorably Missing Data

The majority of molecular epidemiologic studies contain missing data because of the nature of their data collection. The issue of missing data is often not addressed. Furthermore, a complete-case analysis is the typical approach chosen to answer the research question, presumably for its computational ease and accessibility. Such complete-case analyses may be biased, however, particularly if the missing data are non-ignorably missing or not missing at random (NMAR). For example, if genomic data are available only on tumors that are large enough to provide DNA samples and if tumor size is related to the genomic information, the data are likely to be NMAR. We use simulated data to compare the complete-case approach to a multiple imputation (MI) approach, another accessible method, when the data are NMAR. We find that MI methods can reduce the bias relative to a complete-case analysis in the presence of auxiliary data even though the NMAR assumption has been violated. We apply both methods to data from the Long Island Breast Cancer Study Project. We conclude that using MI methods in addition to a complete-case analysis will allow investigators to assess how sensitive their findings are to assumptions about selection bias. For example, if inferences are comparable between complete-case and MI methods, it is less likely that selection bias, while always present in observational epidemiology, can explain the findings.

Gerhard Dikta

Aachen University of Applied Sciences, Campus Jülich

The Bootstrap in Binary Model Diagnostics

Consider a binary regression model, where the conditional expectation of the binary variable given an explanatory variable belongs to a parametric family. To check whether a sequence of independent and identically distributed observations of these variables belongs to such a parametric family, we use Kolmogorov-Smirnov and Cramér von Mises type tests which are based on maximum likelihood estimation of the parameter and on a marked empirical process introduced by Stute. We study a new resampling scheme of the bootstrap in this setup to approximate the critical values belonging to these tests. Furthermore, this approach is applied to simulated and real data. In the latter case we check parametric model assumptions of some right censored data sets. These checks are necessary if one wants to apply a semiparametric approach to analyze the censored data.

Rabia Djellouli

California State University at Northridge

Performance Assessment of a New Class of Local Absorbing Boundary Conditions for Elliptical-Shaped Boundaries in the Low Frequency Regime

New approximate local DtN boundary conditions are proposed to be applied on elliptical- or prolate-spheroid exterior boundaries when solving respectively two- or three-dimensional acoustic scattering problems by elongated obstacles. These new absorbing conditions are designed to be exact for the first modes. They can be easily incorporated in any finite element parallel code while preserving the local structure of the algebraic system. Unlike the standard approximate local DtN boundary conditions that are restricted to circular- or spherical-shaped boundaries, the proposed conditions are applicable to exterior elliptical-shaped boundaries that are more suitable for surrounding elongated scatterers because they yield to smaller computational domains. The mathematical and numerical analysis of the effect of the frequency and the eccentricity values of the boundary on the accuracy of these conditions, when applied for solving radiators and scattering problems, reveals - in particular- that the new second-order DtN boundary condition retains a good level of accuracy, in the low frequency regime, regardless of the slenderness of the boundary.

Brent Doiron

University of Pittsburgh

Microcircuits and Macrodynamics in Cortical Processing

Cortical rhythms are modulated by both stimuli structure and subject attention, however, the cortical architectures and synaptic dynamics that permit rhythm modulation are unknown. We present paired recordings from an auditory cortex slice preparation that shows that fast spiking interneurons project weaker inhibition to nearby pyramidal cells than they do to distant pyramidal cells. Incorporating this experimental observation into a network of spiking model neurons permits spatially localized feed-forward input to recruit intense gamma-band oscillations (~40 Hz) across the network, while spatially diffuse inputs produce far less gamma activity. Using the timescale separation between the rhythm dynamics and a slow feed-forward inhibition we compute a mean field theory that replicates the spatially selectivity of the network rhythm.

Donald Drew

Rensselaer Polytechnic Institute

Random Spatial Networks: A Biological Solution to the Structure/Transport/Connection Problem

Spatial networks are collections of fibers occupying a spatial region. The network is called random if we are interested in an ensemble of equivalent such networks, where the positions of the individual fibers are not identical but have some statistical "sameness." Examples of random statistical networks include microtubule structures, capillaries, neurons, and trees. Each of these networks has a function that it can fulfill by producing a realization out of an ensemble of such networks having certain properties. For example, a microtubule network that is responsible for cell integrity must support the forces that maintain the cell shape; capillaries must deliver and/or absorb chemical species to the surrounding matrix. We discuss microscale (individual fiber) and structural (probability density function) models to describe random spatial networks. so as to relate network statistical structure to assembly dynamics of individual network fibers, and to determine the biological functionality of the network from network statistical properties. In addition, network assembly, disassembly, and interactions with the surroundings during network formation and structure can add to the understanding of the biochemistry and biophysics of fiber formation and guidance.

We shall focus on axonogenesis. Axons are the propagation elements in neurostructures in all higher species. During formation of the brain and nervous system, axons are generated by extension of processes from neural cells with dynamics determined at the growth cone. The progress of the growth cone is determined by the response of surface receptors to gradients of signaling molecules. Surface structures bind the signaling molecules, leading to changes in the assembly of the actin/microtubule structure that drives axonal growth cone motion. In this paper we introduce a two-dimensional stochastic model which captures the random behavior of axon growth to simulate axonal trajectories for cells in a homogeneous medium. We use data to evaluate the standard deviation of the angle changes on the axonal trajectories and to verify the validity of the structure of the stochastic differential equations for the axonal trajectories. For the model of growth of axons, Analyze trajectory data consisting of measurements of the position of the axon tip at different frames in the time sequence of micrographs. This data shows that the axon tip changes direction randomly, but the data is noisy due to the data collection procedures. We develop algorithms to filter out noise while maintaining the underlying dynamics of the axon growth process. We perform statistical analyses on relevant variables generated from our filtered data. We present Monte Carlo simulations of stochastic differential equation systems.

Alan Elcrat

Wichita State University

Axisymmetric Vortices with Swirl

This talk is concerned with finding solutions of the Euler equations by solving elliptic boundary value problems for the Bragg-Hawthorne equation. These flows are axisymmetric and have a swirl component out of the mereanal plane. (In order to set the context for the results obtained we first sketch previous results for two dimensional flows and axisymmetric flows without swirl.) Theoretical results have been given for problems with swirl and general classes of profile functions f, h by successive replacements for L=rf() + h() , and showing that the iterants converge montonically to a solution. The solutions obtained depend on the initial guess, which can be thought of as prescribing level sets of the vortex. When a computational program was attempted these monotone iterations turned out to be numerically unstable, and a stable computation was acheived by fixing the moment of the cross section of a vortex in the merideanal plane. We obtain famillies of vortices related to vortex rings with swirl, Moffatt's generalization of Hill's vortex and tubes of vorticity with swirl wrapped around the symmetry axis. The vortices are embedded in either an irrotational flow or a flow with shear, and we deal with the transition from no swirl in the vortex to flow with only swirl, a Beltrami flow. Joint work with Bengt Fornberg (University of Colorado) and Ken Miller (Wichita State University).

Richard B. Evans

Rensselaer Polytechnic Institute

Convergence of Galerkin Approximations for Differential Eigenvalue Problems with Derivative Discontinuities

The eigenfunctions and eigenvalues of the depth separated underwater acoustic wave equation in a two layer waveguide with a piecewise continuous density and sound speed profile are approximated using the Galerkin method based on a two layer waveguide with piecewise constant density and sound speed. The convergence of the Galerkin approximation, to the eigenpairs, is demonstrated for the case when the derivative discontinuity of the eigenfunctions at the interface between the two layers is chosen to be the same in both problems.

Nina Fefferman

Princeton University

Evolutionary Epidemiology In Silico: Endogenous Social Structure and Disease Defense

In the study of infectious disease dynamics, contact network structures based on social organization of a population have been shown to drastically affect the robustness of a population to disease threats. Especially in natural populations, species with the same susceptibility to a disease can display drastically different social structures. We'll use computational experimentation to explore how drastic the impact of social organizational strategies can be to endogenous disease defense.

Jayanta Ghosh

Purdue University

Motivation and Convergence of Two "New" Fast Algorithms for Estimating the Mixing Distribution in Mixture Models

High dimensional mixture models have become very important in Bioinformatics. One major area of application is to microarray data on expression of thousands of genes. The most difficult part of inference is the estimation of the mixing distribution, the rest of inference is fairly straightforward. More details appear below. Given the parameters t_i, i = 1,2,...n, the observed random variables are independent with density $p(x/t_i)$. In the gene expression problem the t_i is the effect of the ith gene. In the mixture model,the t_i's are iid with distribution f(t). If we integrate out the t_i's, the x_i's are iid with density p_f(x) = integral of p(x/t)f(t)dt. The density f is called either a prior for t or a mixing density. Our inference problem is to estimate f nonparmetricly given iid x_i's with density p_f(x). We discuss properties of a relatively new and very fast algorithm for a NP Empirical Bayes estimate by Newton and its average over permutations of data. These estimates are compared with NP MLE and NP Bayes estimate. We also provide motivation through Stochastic Approximation and prove convergence.

Thomas Hagstrom
The University of New Mexico

Accurate Numerical Methods for Time-Domain Scattering Problems

We report on our progress in developing accurate numerical solvers for time-domain scattering problems. Topics to be addressed include:

(i.) Theory and experiments with convergent local radiation boundary condition sequences on polygonal artificial boundaries, as well as their possible use for multiple scattering applications and for scattering by potentials: in particular we prove that by using complete plane wave expansions optimal complexity estimates can be obtained. The approximations and error estimates follow from a nontraditional representation of solutions of the wave equation in a half-space.
(ii.) High-resolution difference methods on structured, composite grids: we show that high-order one-sided difference formulas required at boundaries can be stabilized via the introduction of simple mesh modifications. Issues related to the development of discrete energy estimates are discussed. We also consider the development of optimized difference formulas using band-limited basis functions. Implementation within the Overture framework is also considered.

Jingfang Huang
University of North Carolina at Chapel Hill

Krylov Deferred Correction Methods for Time Dependent Partial Differential Equations

In this talk, we discuss a new class of numerical methods for the accurate and efficient integration of time dependent partial differential equations. Unlike traditional method of lines (MoL), the new Krylov deferred correction (KDC) accelerated method of lines transpose (Mol^T) first discretizes the temporal direction using Gaussian type nodes and spectral integration, and the resulting coupled elliptic system is solved iteratively using Newton-Krylov techniques such as Newton-GMRES method, in which each function evaluation is simply one low order time stepping approximation of the error by solving a decoupled system using available fast elliptic equation solvers. Preliminary numerical experiments show that the KDC accelerated MoL^T technique is unconditionally stable, can be spectrally accurate in both temporal and spatial directions, and allows optimal time step sizes in long-time simulations. Numerical experiments for parabolic type equations including the Schrodinger equation will be discussed.

John Klein
Medical College of Wisconsin

Direct Regression Models for Survival Parameters Based on Pseudo-Values

Recently we have investigated the use of pseudo-values from a jackknife statistic constructed from a simple summary statistic as a way of direct regression modeling of survival probabilities. These pseudo-values, based on the difference between the complete sample and leave-one-out estimator, are used in a generalized estimating equation to obtain estimates of model parameters. The approach can be applied to direct regression modeling of the survival function over time, the cumulative incidence function for competing risk data, the restricted mean survival time, the mean quality of life, and the probabilities in a multistate model. We illustrate many of these techniques using bone marrow transplant data from the Center for International Blood and Marrow Transplantation.

Charles Knessl

University of Illinois at Chicago

Applications of Applied Mathematics Methods to the Analysis of Algorithms and Tree Properties

Many problems in analyzing trees and algorithms lead to solving difference, differential and/or integral equations. There are 3 broad classes of methods for solving these: (1) exact solutions (transforms, generating functions) (2) numerical solutions and (3) asymptotic approximations. Within the latter there are two classes of techniques: (I) methods for evaluating integrals and sums: Laplace, stationary phase and saddle point methods; Euler-MacLaurin and Poisson summation formulas; and (II) singular perturbation methods: WKB and ray methods, matched asymptotic expansions, multiple scale and averaging methods, homogenization. The second class of methods has not been used much in algorithm analysis. We show how these methods can be used to get interesting new results for certain classic problems, such as the QUICKSORT algorithm, heights of various digital trees, heights of binary trees, and enumeration problems relating to counting binary trees by number of nodes and path length. We also consider enumeration of binary trees, while distinguishing left and right paths. This leads to interesting connections with certain classic non-linear differential equations, called Painleve transcendents. This is joint work with Wojtek Szpankowski of Purdue.

John Kolassa

Rutgers University

Conditional Saddlepoint Approximations for Non-Continuous and Non-Lattice Distributions

We present saddlepoint approximations to the distribution of a statistic arising as a possibly complicated non-linear function of a random vector, conditional on the event that some components of the random vector lie in an interval. We prove that these approximations have typical saddlepoint relative error behavior subject to far milder regularity conditions than the presence of a density. We apply these approximations to approximations to the Beta distribution when expressed as the distribution of a gamma random variable conditioned on the sum of two gamma variables, and to the distribution of the Wald statistic in a logistic regression. Joint work with John Robinson.

Trine Krogh-Madsen

Weill Cornell Medical College

Termination and Resetting of Reentrant Cardiac Activity

Implantable cardioverter defibrillators (ICDs) have become standard therapy for many patients at risk for reentrant ventricular tachycardias. By applying one or more series of suprathreshold stimuli, the antitachycardia pacing modality of ICDs successfully terminates ventricular tachycardia in up to 90% of attempted trials. However, many aspects of why antitachycardia pacing is successful are unknown.

We conducted numerical simulations to investigate the dynamics of reentry termination, and have in particular studied situations where

(1) the stimulus site is located at some distance away from the reentrant loop, and

(2) the reentrant circuit is sufficiently short that a bifurcation to repolarization alternans occurs.

In the first case, we show that when applying a single stimulus there exists a critical distance below which termination of reentry occurs over a range of values for the timing of the stimulus. This behavior is in fact predicted by a discontinuous window in the phase resetting curve. Above this critical distance, however, termination of reentry due to a single stimulus is impossible.

In the second case, we found that reentry termination is very much facilitated when the ring size is such that there is alternans. The main determinant of the ability to terminate is the spatial gradient of recovery time that the induced waves encounter. Based on these findings, we propose novel algorithms for antitachycardia pacing.

Rachel Kuske
University of British Columbia

Transients + instabilities + noise = structure?

Transient or unstable behavior is often ignored in considering long time dynamics in the deterministic world. However, stochastic effects can change the picture dramatically, so that the transients can dominate the long range behavior. Coherence resonance is one relatively simple example of this transformation, and we consider others such as noise-driven synchronization in networks, fluctuations in disease dynamics, and response reliability due to stochastic forcing. The questions that arise in these contexts illustrate the influence of multiple time scales, where the interaction of noise with slow and fast time scales plays a key role in transitions. Furthermore, identifying the cooperation of both discrete and continuous aspects in the dynamics is necessary to understand and predict these phenomenon. Additional insight is obtained by seeking the remnants of the underlying bifurcation structure visible through the noise, as well as highlighting nearly deterministic dynamics in the phase plane that survive in the random context.

Michelle Lacey
Tulane University

A Sharp Error Probability Estimate for the Reconstruction of Phylogenetic Quartets

Phylogeny reconstruction is the process of inferring evolutionary relationships from molecular sequences. Despite the continued development of advanced algorithms, the assessment of phylogenetic accuracy remains a challenging problem, particularly when the sequence alignments under consideration include only a few hundred positions. For this reason, new tools are needed to assist researchers in the prediction and evaluation of phylogenetic performance.

Regardless of the method selected, the quality of estimated trees depends on the strength of the phylogenetic signal contained in the data, and this, in turn, is directly related to the length of the aligned sequences and the evolutionary distances among the taxa. While it is intractable to consider the probabilistic analysis of an entire n-taxa tree, it is reasonable to focus on bounding the error associated with subsets of four taxa, known as quartets. We present a probabilistic analysis of quartet accuracy for the one-parameter Jukes-Cantor model for nucleotide substitution, deriving a sharp error estimate as a function of the quartet branch lengths and the number of nucleotide positions available. These estimates may be employed to select the subset of quartets that are associated with a low error probability, indicating the phylogenetic clades which are resolved with a high degree of statistical confidence.

Ming-Chih Lai
National Chiao Tung University

An Immersed Boundary Method for the Simulation of Interfacial Flows with Insoluble Surfactant

In this talk, an immersed boundary method is proposed for the simulation of two-dimensional fluid interfaces with insoluble surfactant. The governing equations are written in an usual immersed boundary formulation where a mixture of Eulerian flow and Lagrangian interfacial variables are used and the linkage between these two set of variables is provided by the Dirac delta function. The immersed boundary force comes from the surface tension which is affected by the distribution of surfactant along the interface. By tracking the interface in a Lagrangian manner, a simplified surfactant transport equation is derived. The numerical method involves solving the Navier-Stokes equations on a staggered grid by a semi-implicit pressure increment projection method where the immersed interfacial forces are calculated at the beginning of each time step. Once the velocity value and interfacial configurations are obtained, surfactant concentration is updated using the transport equation. Moreover, a new symmetric discretization for the surfactant concentration equation is proposed that ensures the surfactant mass conservation numerically. The effect of surfactant on drop deformation in a shear flow is investigated in detail.

Rachel Levy
Harvey Mudd College

Settling of Particles in a Slurry Flow down an Inclined Plane

The profile of a viscous liquid flowing down an inclined plane can be modeled using lubrication theory by a hyperbolic conservation law. The solution has a leading shock and trailing rarefaction. After an initial transient, the position of the shock scales ~ $t^{1/3}$. If small spherical particles with density greater than that of the fluid are added to create a slurry, the profile of the flow changes. This flow can be modeled by a hyperbolic system for the film height and particle concentration. The new model still shows a leading order scaling of the shock position ~ $t^{1/3}$ but with a different constant than the one in the model of pure fluid flow.

An important factor differentiating a slurry flow from pure fluid flow is the settling of the particles in the liquid. We explore the effect of different models for the particle settling on analytical and computational results for the model. The goal is to capture qualitative differences observed experimentally in slurry flows with different particle concentrations. This is joint work with Natalie Grunewald (UCLA) and Andrea Bertozzi (UCLA), with acknowledgments to B. Cook, T. Ward, C. Wey and A.E. Hosoi.

Timothy Lewis
University of California, Davis

Global Bifurcations and the Appearance of a One-Dimensional Spiral Wave in Excitable Media

Excitable media can support a “fast” stable traveling pulse, which appears through a saddle-node bifurcation accompanied by a “slow” unstable traveling pulse. Furthermore, the uniform rest state is stable. We provide numerical evidence that, near the saddle-node bifurcation, the threshold between the rest state and fast pulse consists of the stable manifold of the slow pulse. However, further away from the saddle-node bifurcation, the threshold involves an unstable periodic solution that has been referred to as a 1D spiral wave. We discussion the implications of these results in the context of cardiac arrhythmias. This work is in collaboration with Eric Cytrynbaum (Dept. of Mathematics, UBC).

Regina Liu
Rutgers University

Mining Massive Text Data: Classification and Tracking Statistics

We present a systematic data mining procedure for exploring large free-style text datasets to discover useful features and develop tracking statistics (often referred to as performance measures or risk indicators). The procedure includes text classification, construction of tracking statistics, inference under error measurements and risk management. The main difficulty in deriving this inference scheme is the accounting for misclassification errors, for which we propose two types of approaches: "plug-in" and "projection" methods. We also consider the bootstrap calibration for fine tuning. Finally, as an illustrative example, the proposed data mining procedure is applied to analyzing an FAA inspection report repository to show its utility in aviation risk management or general decision-support systems.

Although most illustrations here are drawn from aviation safety data, the proposed data mining procedure applies to many other domains, including, for example, mining free-style medical reports for tracking medical errors. This is joint work with Daniel Jeske, Department of Statistics, UC Riverside.

Ji Meng Loh
Columbia University

Accounting for Spatial Correlation in the Scan Statistic

The spatial scan statistic has been widely used in epidemiology as a tool to identify hotspots or clusters in the occurrence of diseases. An underlying assumption of the procedure is the independence of disease incidence between different locations. However, it is sometimes more realistic (e.g. for contagious diseases) to have correlation in the disease counts of neighboring regions. Using a simulation study and a data example, we show that when spatial correlation or overdispersion is present, the spatial scan statistic identifies significant disease clusters too frequently. We relate this issue of excessive false positives to similar work in Efron (2004; 2007). Finally, we introduce a simple procedure to obtain modified p values of identified clusters that account for observed correlation in the data. We show how this procedure helps to reduce the number of false positives, and how it changes the results of our data analyses.

References:
Efron (2004) Large-Scale Simultaneous Hypothesis Testing: The Choice of a Null Hypothesis. JASA, 99, 96-104
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John Lowengrub
University of California-Irvine

Multiscale Models of Solid Tumor Growth and Angiogenesis

We present and investigate models for solid tumor growth that incorporate features of the tumor microenvironment including tumor-induced angiogenesis. Using analysis and nonlinear numerical simulations, we explore the effects of the interaction between the genetic characteristics of the tumor and the tumor microenvironment on the resulting tumor progression and morphology. We account for variable cell-cell/cell-matrix adhesion in response to microenvironmental conditions (e.g. hypoxia) and to the presence of multiple tumor cell species. We focus on glioblastoma and quantify the interdependence of the tumor mass on the microenvironment and on the cellular phenotypes. The model provides resolution at various tissue physical scales, including the microvasculature, and quantifies functional links of molecular factors to phenotype that for the most part can only be tentatively established through laboratory or clinical observation. This allows observable properties of a tumor (e.g. morphology) to be used to both understand the underlying cellular physiology and to predict subsequent growth or treatment outcome, thereby providing a bridge between observable, morphologic properties of the tumor and its prognosis.

Donald Ludwig
University of British Columbia

Mathematical Bioeconomics of Environmental Change

The classic theory of bioeconomics can be extended to apply to problems of climate change and other large environmental changes. If potential changes are great enough, it is by no means clear that steady economic growth is assured. A re-examination of economic uncertainty provides support for policies that prevent or mitigate environmental damage.

Marianthi Markatou
Columbia University

Analysis of Variance of Cross Validation Estimators of the Generalization Error of Computer Algorithms

We bring together methods from statistics and machine learning to study the problem of estimating variances of cross validation estimators of the generalization error of computer algorithms. Providing an estimator of the variance of the cross validation estimator of the generalization error is a difficult problem, particularly if one wants to take into account various sources of variability. We provide a general framework which allows us to treat this problem as a problem in approximating the moments of a statistic. For the simple problem of predicting the sample mean and in the case of smooth loss functions, we show that the variance of the cross validation estimators of the generalization error is a function of the moments of the random variables Y, Z where Y denotes the cardinality of the intersection of two different training sets and Z denotes the cardinality of the intersection of two different test sets. We extend these results to regression, kernel regression and classification, and illustrate the methods through a health services research example on the hospital length of stay of patients that have undergone colon cancer surgery.

Victor Matveev

New Jersey Institute of Technology

Non-Synchronous Dynamics in Non-Weakly Coupled Inhibitory Networks of Type-I Oscillators

Synchronization of excitable cells coupled by reciprocal inhibition is a topic of significant interest due to the important role that inhibitory networks play in the generation and regulation of coherent rhythmic activity in a variety of neural systems. While recent work revealed the synchronizing influence of inhibitory synaptic interaction in the case of weak coupling, it is known that strong coupling can destabilize phase-locked firing. In particular, Maran and Canavier (2007) observed stable non phase-locked states in non-weakly coupled Wang-Buzsaki model neurons, whereby the firing order of the two cells changes in each cycle of the oscillation. We find that such dynamics is a more general property of a wider class of type-I excitable cells coupled by strong inhibition, and can also be achieved with simpler Morris-Lecar (ML) oscillators. While alternating-order firing has been previously characterized as near-synchronous dynamics, we show that the stable phase difference between the spikes of the two ML cells can constitute as much as 70% of the unperturbed oscillation period. We derive conditions for existence and stability of such alternating-order firing in a homogeneous network in terms of the phase resetting properties of the coupled cells, and show their implications for the biophysical properties of the coupled cells. Finally, we examine the conditions under which the bistability between synchronous and alternating-order firing can be achieved. These results may be relevant for the study of central pattern generators, many of which contain two-cell subnetworks coupled by reciprocal inhibition.

Colleen Mitchell

University of Iowa

Do Neurons Have Sharp Time Windows?

In order to study how n to 1 convergence sharpens timing information, we have used a simple time-window (TW) model in which the target neuron fires the first time it has received m action potentials in the previous ε milleseconds. Although the TW is convenient for proving theorems and Monte-Carlo simulations, it is a natural question whether it represents well the physiological reality. We first present simulations that show, in the case $n = 3$, $m = 3$, that the Hodgkin-Huxley model has a very sharp time window but the leaky integrate-and-fire model (LIF) does not. Simulations also show that other non-linear models including quadratic-integrate-and-fire (QIF), the theta model, and the Fitzhugh-Nagumo model also have sharp time window behavior. We then give a complete analytical treatment of the LIF and QIF models to explain why the first does not have a sharp time window but the second does. This suggests that TW neurons may give a better approximation to physiological reality than LIF neurons.

Kannan Natarajan

Novartis Pharmaceutical Corporation

Statistical Challenges in Drug Development

A major challenge in drug development is faster and efficient development to get much needed drugs to our patients, especially with life threatening diseases like cancer, quicker and with good quality data. The talk will focus on current statistical issues in 3 main areas of development: assessment of optimal biologic dose with proof of concept, confirmation of benefit vs. risk, and life cycle management.

In the dose assessment phase, the use of Bayesian or adaptive methods have gained traction, particularly to utilize prior knowledge from either pre-clinical dosing and/or dosing information from patients in previous cohorts. However, most of the current statistical methods are focused on either safety or efficacy and not on the early assessment of both risk and benefit. The confirmatory phase often involves a Phase II followed by a Phase III. Issues at this stage range from the appropriate choice of control drug (if any), integrating information from Phase II and Phase III, and safety signal assessment. Post marketing surveillance for further characterization of safety has issues ranging from data collection to appropriate methods for integrating this data with that of controlled trials.

Examples from oncology drug development will be provided with the current statistical methods, highlighting the issues and unmet need where appropriate.

David P. Nicholls

University of Illinois at Chicago

Spectral Stability of Traveling Water Waves

The motion of the free surface of an ideal fluid under the effects of gravity and capillarity arises in a number of problems of practical interest, consequently, the reliable and accurate numerical simulation of these "water waves" is of central importance. Recently, an efficient, stable, and high-order Boundary Perturbation scheme for simulating these traveling water waves (due to the author and F. Reitich) has been extended to address the equally important topic of their dynamic (spectral) stability. In this talk we will discuss this algorithm and present new results on the "motion" of the spectrum of the linearized water wave equations as the traveling waveform is varied. In particular, we will focus upon the radius of convergence of a Taylor series expansion of the spectral data and its possible connection to spectral instability of traveling water waves.

Nilima Nigam

McGill University

Integral Equation Methods and Vortex Motion on Spheres

While studying the motion of point vortices constrained to move on the surface of a sphere with islands, one is lead naturally to the Dirichlet problem for the Laplace-Beltrami problem. One method for solving this problem involved stereographic projection onto the place, followed by conformal mapping strategies. We present instead a boundary integral strategy which is flexible and applicable for island boundaries which are non-smooth. We then discretize this BIE using a Galerkin strategy. Numerical experiments validating the method are presented. We also discuss other problems which may be considered in this framework. This is joint work with Simon Gemmrich and Olaf Steinbach.

Robert O'Malley

University of Washington

Doing Asymptotics Using the Renormalization Group Method

The renormalization group method has been presented as a universal technique. We will indeed suggest its versatility by examining some diverse examples of its application.

Lev A. Ostrovsky

Zel Technologies/University of Colorado

Theoretical Models of Strongly Nonlinear Internal Waves

It is now a common knowledge that internal gravity waves in the ocean are typically nonlinear and often strongly nonlinear so that the classical weakly nonlinear models such as the Korteweg-de Vries (KdV) and Benjamin-Ono (BO) equations and their modifications can be inapplicable. Along with direct numerical simulations (often very time-consuming), a significant interest is attracted to the attempts to construct simplified models describing propagation of a given internal mode in the horizontal plane. In the works by Miyata and Choi-Camassa, model equations for strong internal waves in a two-layer fluid similar to the weakly nonlinear Boussinesq-type equations were suggested. Ostrovsky and Grue suggested unidirectional models similar to the KdV and BO equations. These models combine strong nonlinearity and weak dispersion that are in principle contradictory for solitons for which these two factors are balanced by definition. Although, a consistent description of strongly nonlinear processes in the form integrated over depth is, strictly speaking, impossible, the 2-D and 3-D models can provide satisfactory approximation in many cases. Along with a brief review of the existing theories, here we suggest a Hamiltonian description without expansion of a dispersive term. This form secures conservation of mass and energy and can be readily extended to include different small and slow factors such as sloping bottom, dissipation, and cylindrical divergence. Some specific solutions for realistic oceanic conditions are presented and applied to observational data.

John Pelesko

University of Delaware

Dynamics of Electrostatic MEMS

In 1968, in the context of investigating fundamental questions in electrohydrodynamics, G.I. Taylor studied the electrostatic deflection of elastic membranes. Utilizing soap film as the membrane material and applying a fixed high voltage potential difference between two supported circular membranes, Taylor showed experimentally that at a critical voltage the two membranes snap together and touch. That is, the equilibrium state where the membranes remained separate that existed at smaller voltages either became unstable or failed to exist. This instability is familiar to researchers in the MEMS (microelectromechanical systems) and NEMS (nanoelectromechanical systems) fields where it is known as the "pull-in" instability. In fact, in an interesting historical coincidence H.C. Nathanson and his coworkers studied this instability in the context of a primitive MEMS device at roughly the same time as Taylor was conducting his studies. Nathanson is responsible for the "pull-in" nomenclature and the analysis of a mass-spring model of this effect. Taylor, in conjunction with R.C. Ackerberg developed and numerically analyzed a more accurate membrane based model of electrostatic deflection. Recently, a rigorous analysis of this model was completed. Surprisingly, even this simple model of electrostatic deflection contains a rich solution set exhibiting a bifurcation diagram with infinitely many folds. In this talk, we provide an overview of recent results on the interaction of elastic membranes with electrostatic fields. We discuss a re-creation of the Taylor experiment, some new experimental results and discuss the relevance of this research to MEMS and NEMS systems.

Edsel A. Peña

University of South Carolina, Columbia, SC

Modeling and Analysis of Recurrent Events

Recurrent events arise in many scientific areas: biomedical and public health; reliability and engineering; actuarial settings; economic, sociological, and political settings. In this talk I will discuss issues of stochastic modeling of recurrent event data and the statistical inference concerning the parameters of such models. I will indicate unique and intrinsic features that lead to some difficulties with the handling of recurrent event data, specifically the impact of the sum-quota accrual scheme, which leads to both informative and dependent censoring. I will also discuss computational and efficiency issues pertaining to the statistical inference of the model parameters. Some illustrations will be performed with biomedical data.

Thomas M. Roberts

Air Force Research Laboratory

Efficient Ranking of Polyomino-based Antennas

We recently found superior sidelobe suppression in phased arrays when using identical, non-overlapping subarrays--also known as polyominoes--that fill rectangular apertures exactly. Such apertures are said to be tiled.

Further studies using months of computer time prompted us to be more efficient in finding arrays that have low sidelobes. With that motivation, and using 200 numerical examples, we will show clear, systematic differences in sidelobes based mainly on the type used in tiling. Joint work with Scott G. Santarelli and Robert J. Mailloux.

Anton Schick

Binghamton University

Rates of Convergence for Estimators of Convolutions of Densities

The goal of this talk is to give an overview of various types of convergence results for estimating the convolution of a density with itself. The estimator of this convolution is a local U-statistic based on a random sample from the base density. The surprising fact

is that under rather mild assumptions on the base density this estimator has a convergence rate of the order root-n, pointwise and in various norms, and (functional) central limit theorems can be proved in the corresponding normed spaces. Key to these results are integrability conditions on the base density.
A violation of these conditions results in slower rates of convergence. The behavior of the local U-statistic is now similar to that of kernel estimators with the customary trade-off between bias and variance terms. These slower rates of convergence, however, are still faster than the optimal rates of convergence for kernel estimators based on a sample from the convolution.

Sebastian Schreiber
University of California, Davis

Cycling in Space: Persistence of Rock-Scissor-Paper Metapopulations

In the past decade, several empirical studies have shown that the children's game of rock-scissor-paper occurs in natural systems. For instance, different strains of E.coli that produce and/or resist toxins can generate an intransitive dominance relationship. For this system, persistence of all three strains requires that the strains have localized dispersal. To better understand how spatial heterogeneity, dispersal rates, and strategic asymmetries influence local and global persistence, I introduce a general class of spatial evolutionary games and an approach to analyze them. The analysis applied to the rock-scissor-paper version of these games suggests how different forms of spatial and strategic heterogeneity can promote persistence at different rates of dispersal.

Jie Shen
Purdue University

Efficient and Stable Spectral Methods for the Helmholtz Equation in Exterior Domains

I shall present an efficient and stable spectral algorithm and their numerical analysis for the Helmholtz equation in both two- and three-dimensional exterior domains. The algorithm couples a boundary perturbation technique with a well-conditioned spectral-Galerkin solver based on an essentially exact Dirichlet-to-Neumann operator. Error analysis with explicit dependence on the wave number as well as ample numerical results will be presented to show the accuracy, stability, and versatility of this algorithm.

Arthur Sherman
National Institutes of Health

Bifurcation Analysis of the Dual Oscillator Model for Pancreatic Beta-Cell Calcium Oscillations

The dual oscillator model describes the metabolic and electrical oscillations that combine to drive insulin secretion from the beta-cells of the pancreatic islets of Langerhans. The metabolic and electrical subsystems are each postulated to be able to oscillate independently but also to interact with each other. A heuristic diagrammatic reduced model has been developed for pedagogical purposes but has turned out to be useful for predicting behaviors of the full mathematical model. The heuristic model treats each of the two oscillators as a relaxation oscillator, with silent, oscillatory, and fully on modes and thresholds for transitioning between the modes that are dependent on the glucose concentration applied to an islet. Depending on the relative positions of the thresholds of the two, a variety of patterns of behavior can be obtained, essentially all of which are found experimentally. Conversely, most of the observed patterns correspond to some such arrangement. Here we put the heuristic model on a firmer footing by constructing appropriate bifurcation diagrams of the electrical system with external forcing from the metabolic system. We use the diagrams to investigate the relative contributions in different parameter regimes of bursting oscillations driven by hysteresis of the electrical subsystem, and hence in principle resettable by brief electrical perturbations and sensitive to ion channel noise, vs. oscillations externally imposed by the metabolic subsystem, and hence resistant to both resetting and noise.

Gregory D. Smith

The College of William and Mary

Moment Closure for Local Control Models of Calcium-Induced Calcium Release in Cardiac Myocytes

I will describe a probability density approach to modeling local control of Ca-induced Ca release in cardiac myocytes [Williams et al. Biophys. J. 92(7):2311--28, 2007] consisting of coupled advection-reaction equations the time-dependent probability density of subsarcolemmal subspace and junctional sarcoplasmic reticulum [Ca] conditioned on Ca release unit (CaRU) state. When coupled to ODEs for the bulk myoplasmic and network SR [Ca], a realistic but minimal model of cardiac excitation-contraction coupling is produced that avoids the computationally demanding task of resolving spatial aspects of global Ca signaling, while accurately representing heterogeneous local Ca signals in a population of diadic subspaces and junctional sarcoplasmic reticulum depletion domains. I will introduce a computationally efficient method for approximately simulating such whole cell models that begins with a derivation of a system of ODEs describing the time-evolution of the first and second moments of the probability density functions for local [Ca] jointly distributed with CaRU state. This open system of ODEs is then closed by assuming an algebraic relationship that expresses the third moment in terms of the first and second moments. In simulated voltage-clamp protocols using four-state CaRUs that respond to the dynamics of junctional SR depletion, this "moment closure approach" to modeling local control of excitation-contraction coupling produces high-gain Ca release that is graded with changes in membrane potential, a phenomenon not exhibited by so-called "common pool" models. Benchmark simulations indicate that the moment closure approach is 9000 times more computationally efficient than corresponding Monte Carlo simulations and leads to nearly identical results. [This project is joint work with Marco A. Huertas, George S. B. Williams, Eric A. Sobie, and M. Saleet Jafri.]

Marc K. Smith

Georgia Institute of Technology

The Vibration of an Inviscid Incompressible Sessile Drop

The fundamental frequencies and modes of vibration of a free spherical drop of inviscid incompressible fluid were computed 129 years ago by Lord Rayleigh. The analysis was possible because of simplifications resulting from the use of spherical coordinates. These simplifications don't occur for a sessile drop, i.e., when the drop is supported on a horizontal planar surface, except for the case of a hemispherical drop. The present work describes an integrated analytical and numerical technique for the computation of the fundamental frequencies and modes of vibration of a supported sessile drop. Spherical coordinates are used to describe the interface shape, but the flow field inside the drop is computed numerically using the finite element method. Combining these techniques produces a linear eigenvalue problem that is solved numerically. Results will be presented for sessile drops with different contact angles without gravity and compared to experimental data. The extension of this technique to sessile drops with gravity will also be discussed.

Christian Stucchio

Courant Institute of Mathematical Sciences

Stable Outgoing Wave Filters for Anisotropic Waves

In this talk I present a new type of open boundary conditions, the phase space filter. Based on modern scattering theory, the basic idea is to identify in phase space the region corresponding to outgoing waves and filter them before they reach the computational boundary. I'll discuss Schrodinger, (Anisotropic) Maxwell and Molecular Dynamics models. The method is stable for all linear waves. It is local in time and pseudo-local in space, and imposes few restrictions on the interior solver and coordinate system.

Sundar Subramanian

New Jersey Institute of Technology

Survival and Hazard Function Estimation for the Missing Censoring Indicator Model

In survival studies, death certificate information can be missing, or incidental and fatal occurrences may be indistinguishable for some subjects, leading to missing censoring indicators. For the framework of right censored data with missing censoring indicators, we describe several non- and semi-parametric survival and hazard function estimators arising from two different representations of the cumulative hazard function, and provide a comparison study of their asymptotic variances. When the parametric model is properly specified, the semi-parametric estimators provide gains in efficiency, as one would expect. Frequently in practice, however, a practitioner has to balance bias inherent in a parametric misspecification with the corresponding lack of efficiency due to a nonparametric choice. We also discuss this aspect. The efficacy of the proposed procedures is investigated through several simulation studies and some illustrations are provided.

Charles Tier

Illinois Institute of Technology

Asymptotic Approximations to Models of Financial Derivatives

In recent years there has been growing interest in more sophisticated models for pricing financial derivatives that go beyond the Black-Scholes-Merton Model. The new pricing models try to include more real-world market details that are not accounted for in the Black-Scholes-Merton theory. We will consider models in which the volatility of the underlying financial asset is no longer constant but may be a deterministic or stochastic function. Unfortunately, exact, closed form solutions for the price of financial derivatives based on these new models are not known, so we will use asymptotic methods such as the ray method from geometric optics to develop simple, useful formulas for them. We will discuss derivatives such as variance swaps and options on interest rate derivatives.

Catalin Turc

University of North Carolina-Charlotte

Fast, High-Order, Well-Conditioned Algorithms for the Solution of Three-Dimensional Acoustic and Electromagnetic Scattering Problems

We present a novel computational methodology to produce fast and very accurate solutions of acoustic and electromagnetic problems in small numbers of Krylov-subspace iterative solvers. At the heart of our approach are integral equation formulations that exhibit excellent spectral properties. In the case of scattering from perfectly conducting structures, and just as the classical Combined Field Integral Equation (CFIE), our equations result from representations of the scattered fields as a combination of magnetic- and electric-dipole distributions on the surface of the scatterer. In contrast with the classical equations, however, our electric-dipole operators involve use of certain types of regularizing operators whose design is based on the pseudodifferential calculus on manifolds. We call the resulting equations Regularized Combined Field Integral Equations (CFIE-R). Unlike the CFIE, the CFIE-R are well-conditioned equations; careful selection of coupling parameters, further, yields CFIE-R operators with excellent spectral distributions---with closely clustered eigenvalues--so that small numbers of iterations suffice to solve the corresponding equations by means of Krylov subspace iterative solvers such as GMRES. We present a high-order Nystrom approach based on use of partitions of unity and high-order integration schemes that produces high-order algorithms for acoustic and electromagnetic scattering problems. A variety of numerical results demonstrate that, for a given accuracy, the new equations can give rise to order-of-magnitude reductions in computational costs over those resulting from previous approaches.

Barbara Wagner

Weierstrass Institute, Germany

On the Wavelength of the Contact-Line Instability of Dewetting Fronts

We investigate the stability of the contact line of a dewetting thin liquid film on a hydrophobised substrate, taking account of large slippage. We derive a sharp-interface model for the rim of the thin film via matched asymptotic expansions and derive the eigenvalues from a linear stability analysis of the reduced model. Our findings are compared to our numerical simulations for the full lubrication models and experimental results.

Thomas Ward

University of California-Los Angeles

Electrohydrostatically Driven Flows in Microscale Geometries

Viscous fluid flow control in confined geometries (at dimensions less than the capillary length) such as porous media are of interest to emerging fields, such as micro (MEMS) and nano-electromechanical systems (NEMS). If fluids in these devices are driven by pressure, and/or motor driven constant flow-rate pumping then they lack a certain degree of control that is desirable for high precision and robust experimentation. Recently, researchers have been studying the possibility of driving precision motion of fluids in porous media by using electrically driven flow phenomenon to overcome some of the shortcomings of their flow-rate and/or pressure driven flow counterparts. Here, the theoretical analysis and experiments for two problem involving such a flow are presented to drive the motion of a viscous non-conducting oil, in a micron scale geometries, called a Hele-Shaw cell that is a model for flow in porous media. The first problem involves a radial flow and the second a vertical flow where the displacement opposes gravity. The theoretical results yield a parameter, called the electrostatic Reynolds number, that will be used to distinguish between convective dominated and viscous dominated flow. Experiments are performed using silicone and castor oil at gap spacing less than the capillary length. The experimental results for the interface displacement as a function of elapsed time are compared with the theoretical predictions for the average propagating front position as a function of time with knowledge of the needed physical parameters.

CONTRIBUTED TALKS

Sunil Ahuja
Princeton University

Stabilization of Unstable Steady States in Low-Reynolds Number Flows Past Airfoils

Design of micro air vehicles (MAVs) has recently been inspired by bio-fliers in which a leading edge vortex (LEV) is found to be stably attached even at post-stall angles of attack, providing high lift. Current efforts in designing MAVs focus on designing controllers that can keep the LEVs attached in steady flights with stationary wings. From a dynamical systems perspective, as the angle of attack of an airfoil in steady flow is gradually increased, the flow transitions to periodic vortex shedding via a Hopf bifurcation. Our approach is to stabilize the co-existing branch of unstable steady states to achieve high-lift flow fields. In this presentation, we focus on a model problem of 2D flow past a flat plate at a high angle of attack ( ) and a low Reynolds number (Re) of around 100. We perform numerical simulations using an immersed boundary method, and perform a continuation study in the parameter space of Re and, using a time-stepper based Newton-GMRES method. We derive reduced order models of the flow linearized about the unstable steady states using a technique from control theory called balanced truncation, recently made computationally tractable by Rowley [1] for large-dimensional systems such as encountered in fluid flows. The existing method is valid only for stable systems and we present an extension to unstable systems. The actuation is modeled as a localized body force close to the leading edge of the flat plate. We first assume full-state feedback and use the reduced order models along with linear control techniques to derive feedback laws that stabilize the unstable steady state. The resulting controller has a large-enough basin of attraction to suppress the periodic vortex shedding. Since it is not practical to implement a full-state feedback controller, we develop reduced-order observers based on a few velocity measurements in the near-wake of the flow. The observers accurately reconstruct the entire flow-field and, along with the controllers, stabilize the unstable steady states. [1] Rowley, C. W., "Model reduction for fluids using balanced proper orthogonal decomposition," Int. J. Bifurcation Chaos, 15 (3), 997–1013, 2005.

Jeffrey Aristoff
Massachusetts Institute of Technology

Water Entry of Small Hydrophobic Spheres

We present the results of a combined experimental and theoretical investigation of the water entry of hydrophobic spheres. Particular attention is given to characterizing the shape of the resulting air cavity in the low Bond number limit, where cavity collapse is driven principally by surface tension rather than gravity. A parameter study reveals the dependence of the cavity structure on the governing dimensionless groups. A theoretical model is developed to describe the evolution of the cavity shape, and is found to compare favorably with our experimental observations. Finally, we present a theoretical model for the evolution of the splash curtain formed at high Weber number, and couple it to the underlying cavity dynamics.

Maria Cameron
Courant Institute of Mathematical Sciences

Seismic Velocity Estimation from Time Migration

We address the problem of the estimation of the sound speed inside the Earth from time migration. The velocities chosen in the process of time migration, known as time migration velocities, are used as the input.We have derived theoretical relationships between the time migration velocities and the true seismic velocities in 2D and 3D.These relationships revealed that the conventional estimate of the seismic velocity from the time migration velocity, the Dix velocity, is the ratio of the true seismic velocities and the geometrical spreading of the image rays. We have formulated an inverse problem of estimation of the true seismic velocities from the Dix velocities and developed a numerical procedure for solving it. This procedure consists of two steps: (1) computation of the geometrical spreading of the image rays from the Dix velocities and find the true seismic velocities in the time-domain coordinates; (2) conversion of the true seismic velocities from the time-domain coordinates to the depth-domain coordinates and computation of the transition matrices from the time-domain to depth-domain coordinates.

For step 1, we derived a PDE relating the Dix velocity and the geometrical spreading of the image rays. This is a nonlinear elliptic PDE. The physical setting allows us to pose a Cauchy problem for it. This problem is ill-posed. However we were able to solve it numerically in two ways on the required interval of time. One way is a finite difference scheme inspired by the Lax-Friedrichs method. The second way is a Spectral Chebyshev method. We have shown that this is possible due to (i) the special input corresponding to a positive finite seismic velocity, (ii) the special initial conditions corresponding to the image rays, (iii) damping or truncation of the high harmonics by our numerical schemes, (iv) the need to compute the solution only a short interval of time, so that the growing low harmonics fail to develop significantly.

For step 2, we have developed an efficient Dijkstra-like solver motivated by Sethian's Fast Marching Method. We have tested our numerical procedure on a collection of 2D and 3D synthetic examples and applied it to field data.We have shown that our algorithms provide significantly and qualitatively more accurate velocity estimates than the conventional Dix inversion.

Linlin Chen
University of Rochester

Balancing Type One and Two Errors in Multiple Testing for Differential Expression of Genes

Microarray technology has become an indispensable tool for measuring expression levels of thousands of genes simultaneously and has been widely used to find genes that are differentially expressed between two (e.g., treatment versus control) or more phenotypes. The most basic issue to be addressed in this setting is that of multiple hypothesis testing. Correlation structure is a central fact of microarray data, and that it may have sources that are not related to specific gene function, therefore, statistical procedures for which control are needed. In this talk, a new procedure is proposed to balance type I and II errors in significance testing for differential expression of individual genes. Suppose that a collection, F_k, of k lists of selected genes is available, each of them approximating by their content the true set of differentially expressed genes. For example, such sets can be generated by a sub-sampling counterpart of the delete-d-jackknife method controlling the per-comparison error rate for each sub-sample. A final list of candidate genes, denoted by S^*, is composed in such a way that its contents be closest in some sense to all the sets thus generated. To measure "closeness" of gene lists, we introduce an asymmetric distance between sets with its asymmetry arising from a generally unequal assignment of the relative costs of type I and type II errors committed in the course of gene selection. The optimal set S^* is defined as a minimizer of the average asymmetric distance from an arbitrary set S to all sets in the collection F_k. The minimization problem can be solved explicitly, leading to a frequency criterion for the inclusion of each gene in the final set. The proposed method is tested by re-sampling from real microarray gene expression data with artificially introduced shifts in expression levels of pre-defined genes, thereby mimicking their differential expression.

Yekaterina Epshteyn
Carnegie Mellon University

New Discontinuous Galerkin Methods for the Chemotaxis Model and Closely Related Biomedical Problems

In this work, first, we propose a family of interior penalty discontinuous Galerkin methods for the Keller-Segel chemotaxis model. This model is described by a system of two nonlinear PDEs: a convection-diffusion equation for the cell density coupled with a reaction-diffusion equation for the chemoattractant concentration. It has been recently shown that the convective part of this system is of a mixed hyperbolic-elliptic type, which may cause severe instabilities when the studied system is solved by straightforward numerical methods. Therefore, the first step in the derivation of the proposed methods is made by introducing the new variable for the gradient of the chemoattractant concentration and by reformulating the original Keller-Segel model in the form of a convection-diffusion-reaction system with a hyperbolic convective part. We then design interior penalty discontinuous Galerkin methods for the rewritten Keller-Segel system. Our methods employ the central-upwind numerical fluxes, originally developed in the context of finite-volume methods for hyperbolic systems of conservation laws. We prove error estimates for the proposed high-order discontinuous Galerkin methods. Our proof is valid for pre-blow-up times since we assume boundedness of the exact solution. We also show that the blow-up time of the exact solution is bounded from above by the blow-up time of our numerical solution. In the numerical tests that will be presented, we first compare three different discontinuous Galerkin schemes applied to the Keller-Segel model: 1) primal discontinuous Galerkin methods applied to the original formulation of the Keller-Segel model, 2) primal discontinuous Galerkin methods with the standard upwind numerical fluxes for the reformulated Keller-Segel model and, 3) the new discontinuous Galerkin methods. We show, that compare to the new discontinuous Galerkin methods, the first two schemes fail to give the accurate, oscillation free solutions for the classical Keller-Segel chemotaxis model.

Second, we consider application of the proposed discontinuous Galerkin schemes, to some biomedical problems.

Weihua Geng

Michigan State University

The Matched Interface and Boundary Method Based High-Order Possoin-Boltzmann Equation Solver and its Application on Computing Solvation Forces

A novel method is presented for solving the Poisson-Boltzmann (PB) equation based on a rigorous treatment of geometric singularities of the dielectric interface and a Green's function formulation of charge singularities. Geometric singularities, such as cusps and self-intersecting surfaces, in the dielectric interfaces are bottleneck in developing highly accurate PB solvers. Based on an advanced mathematical technique, the matched interface and boundary (MIB) method, we have recently developed an accurate PB solver, MIBPB-II by rigorously enforcing the flux continuity conditions at the dielectric interface where geometric singularities may occur. However, when mesh size approaches half of the van der Waals radius, MIBPB-II cannot maintain its accuracy because the grid points that carry the interface information overlap with points carrying distributed charges. In the present Green's function formalism, charge singularities are transformed into interface jump conditions, which are treated on an equal footing as the geometric singularities in our MIB framework. The resulting method, denoted as MIBPB-III, is able to provide highly accurate electrostatic potentials at a mesh as coarse as 1.2 angstrom for proteins. The MIBPB-III has been extensively validated by using analytically solvable problems and molecular surfaces of polyatomic systems, and proteins. An important and direct application of the solution of PBE is to calculate the solvation forces, which are the basis for molecular dynamics simulation. We provide MIB based solvation forces calculation schemes, taking advantage of the accurate potentials output from MIBPB solver and again the incorporation of interface jump conditions. As one of the important components of the solvation forces, the accuracy of dielectric boundary forces, which were traditionally calculated by using smoothed dielectric interface, is improved by resorting to a level set based 1st order surface integral. Several examples and comparisons are presented to validate the schemes.

Samiran Ghosh

Indiana University Purdue University Indianapolis

A Semiparametric Modeling Framework for the Development of Metabonomic Profile and Bio-Marker Discovery Mechanism

The discovery and validation of biomarkers is an important step towards the development of criteria for early diagnosis of disease status. Recently electrospray ionization (ESI) and matrix assisted laser desorption (MALDI) time-of-flight (TOF) mass spectrometry have been used to identify biomarkers both in proteomics and metabonomics studies. Data sets generated from such studies are generally very large in size and thus require the use of sophisticated statistical techniques to glean useful information. Most recent attempts to process these types of data model each compound's intensity either discretely by positional (mass to charge ratio) clustering or through each compounds' own intensity distribution. Traditionally data processing steps such as noise removal, background elimination and m/z alignment, are generally carried out separately resulting in unsatisfactory propagation of signals in the ¯nal model. It is more intuitive to develop models for patterns rather than discrete points following the basic principle of “borrowing strength" for such a scenario. In the present study a novel semi-parametric approach has been developed to distinguish urinary metabolic profiles in a group of traumatic patients from those of a control group consisting of normal individuals. Data sets obtained from the replicates of a single subject were used to develop a functional profile through Dirichlet mixture of beta distribution. This functional profile is flexible enough to accommodate variability of the instrument and the inherent variability of each individual, thus simultaneously addressing different sources of systematic error. To address instrument variability, all data sets were analyzed in replicate, an important issue ignored by most studies in the past. We used different choices of centering functions to capture non-standard profile shapes. Different model comparisons were performed to select the best model for each subject. The m/z values in the window of the irregular pattern are then further recommended for possible biomarker discovery.

Ian Griffiths
University of Oxford

Mathematical Modelling of Non-Axisymmetric Glass Tubing Production

We present a mathematical model for the industrial production of non-axisymmetric capillary tubing. Molten glass is fed through a die and drawn off, with its cross-sectional profile controlled by surface tension and internal pressurization. Asymptotic analysis is used to reduce the problem to a system of ordinary differential equations describing the flow along the tubing and the evolution of the cross-section shape. Exact, asymptotic and numerical solutions of these equations allow us to tackle the inverse problem of predicting the die shape required to produce a desired tubing geometry.

Anthony Kellems
Rice University

Radical Dimension Reduction of Morphologically Accurate Neuronal Models

Biophysically accurate neuronal models typically result in systems of thousands of nonlinear ordinary differential equations. Although these detailed models are useful for single-cell simulations, the computational cost associated with them prohibits their use in realistic, large-scale network simulations. Such simulations are often achieved by compromising the morphology of the neuron, namely simplifying the dendritic structure into just a few compartments. However, this ignores the intricate manner in which synaptic input is transmitted to the site of action potential initiation. We retain this rich input structure while radically reducing the internal dynamics by employing state-of-the-art model reduction techniques based on Balanced Truncation and on Krylov methods. We demonstrate that the subthreshold dynamics of a 10000 compartment quasi-active model, with a 60000 dimensional state space, may be captured with a 15 dimensional system--without sacrificing the position or timing of any of the 10000 original synapses. We show that our method dramatically accelerates investigations of dendritic democratization and resonance and we speculate on its applicability to investigations of large-scale network activity.

Shilpa Khatri
Courant Institute of Mathematical Sciences

A Numerical Method for Soluble Surfactants on Moving Interfaces

In many real world multiphase flow problems, there are surfactants present. These are surface reacting agents that modify the strength of the surface tension. The concentration of the surfactant on the interface separating the fluids can be modeled with a time-dependent differential equation defined on the time-dependent and deforming interface. For soluble surfactants, this is also coupled to a PDE for the concentration of surfactants in the bulk. We present a second order method based on an explicit but yet Eulerian discretization of the interface. We use standard finite difference schemes on the discretization of the interface to solve the PDE for the surface concentration. The PDE for the concentration in the bulk will, in the spirit of interface tracking methods, be solved on a fixed uniform grid. The interface arbitrarily cuts through the uniform grid so the boundary flux condition for the bulk surfactant needs a special treatment. We will discuss the details of this implementation and show results in two dimensions.

Charles Kiyanda
University of Illinois at Urbana-Champaign

Reduced Detonation Models for Insensitive High Explosives

The combustion of energetic materials can occur in a very rapid and violent fashion, called a detonation. In the detonation process, the material first undergoes adiabatic compression through a shock wave, raising the material pressure and temperature to high levels. In this compressed state, rapid chemical reactions occur, liberating energy which, in turns, supports the shock wave from decaying. The coupled exothermic chemical reactions and shock wave form the detonation wave. Because of the high pressure and temperature variations within the wave, the modelling of detonation waves requires a knowledge of the chemical kinetic characteristics of the material as well as the response of materials to various thermodynamic processes such as shock compression. The modelling of detonation waves in solid high explosives has traditionally been done through the use of

empirically developed equations of state, which present great flexibility in modelling various materials, but with free parameters which bear little connection to physical parameters, rendering the analysis of such models difficult. In this talk, we explore the level of modeling complexity required to describe the propagation of detonations in insensitive high explosives (IHE), specifically PBX 9502. We examine models with sufficient complexity to capture the main properties of detonations in IHE, yet simple enough to remain, to a large extent, analytically tractable. Examples include mixture models based on Stiffened-Gas, Birch and Birch-Murnaghan equations of state. We compare such models some of to the standard models used to describe such materials.

Harper Langston
New York University

Fast Elliptic PDE Solver for Non-homogeneous Force Distributions in Complex Geometries

Many problems in scientific computing call for a fast and efficient solution to elliptic partial differential equations. Three particular problems of this sort are the Poisson equation, the Modified Helmholtz equation, and the Stokes equations, where solutions are often required inside or outside of a complex domain subject to Dirichlet boundary conditions. For simple rectangular, circular or spherical domains, well-established fast methods for solving such problems exist. For more complex domain discretizations, many solvers rely on adaptive meshes, domain decomposition strategies and multigrid acceleration, yet when geometries become complex, grid-generation methods can become unstructured and computationally expensive. Another approach is to incorporate fast direct solvers, which are efficient, scalable, and do not require a hierarchy of grids. Fast-Multipole-Method based solvers in particular allow for the handling of very non-uniform force distributions, allow for complex geometries and provide a high degree of accuracy. We propose an embedded boundary solver approach, decoupling an inhomogeneous interior/exterior Dirichlet elliptic PDE into a problem involving a simple domain with distributed forces and another problem absent forces with complex geometry. For the first problem, we introduce a kernel-independent FMM-based volume solver, which can handle highly irregular source distributions. For the second problem, a pre-existing boundary-integral solver is utilized. Examples of the volume solvers and coupled embedded boundary solvers will be discussed.

Caroline Muller
Courant Institute of Mathematical Sciences

Instability and Dissipation of Internal Tides

The presence of celestial bodies induces a barotropic current in the ocean, known as the barotropic tide. Without topography, this flow represents the usual solution to the tidal equation. With topography, this barotropic tide interacts with the seafloor resulting in the radiation of internal waves known as the internal tides. These waves are the subject of active research since their dissipation through wave breaking and concomitant three-dimensional turbulence contributes to vertical mixing in the deep ocean, and hence could play an important role in the large-scale ocean circulation. As part of an ongoing effort to develop a theory for the vertical distribution of wave breaking over seafloor topography, we investigate the instability of internal tides in a very simple linear model that allows us to relate the formation of unstable regions to simple features in the seafloor topography. We will see that the distribution of unstable wave breaking regions can be highly non-uniform even for very simple idealized topography shapes. Interestingly, for three-dimensional tides over two-dimensional topography, there can be geometric focusing of wave energy into localized regions of high wave amplitude, and we will investigate this focusing effect in simple examples. Our next step is to quantify how much wave energy is lost in unstable regions. We develop a parametrization that models nonlinear wave breaking and energy dissipation, and we find vertical profiles of mixing consistent with oceanic measurements using realistic random topography. An interesting finding is that the wave-induced mixing could be much more confined to the bottom than previously assumed. This vertical variability in the mixing could imply a radically different interior circulation in the models than that with uniform mixing schemes.

Megan Othus
Harvard University

A Class of Semiparametric Mixture Cure Survival Models with Dependent Censoring

Modern cancer treatments have substantially improved cure rates and have generated a great interest in and need for proper statistical tools to analyze survival data with nonnegligible cure fractions. Data with cure fractions are often complicated by dependent censoring, and the analysis of this type of data typically involves untestable parametric assumptions about the dependence of the censoring mechanism and the true survival times. Motivated by the analysis of the National Cancer Institute (NCI) Surveillance Epidemiology and End Results (SEER) prostate cancer data, we propose a class of general semiparametric transformation cure models that allows for dependent censoring without making parametric assumptions on the dependent relationship. An inverse-censoring-probability re-weighting scheme is used to derive unbiased estimating equations that account for dependent censoring. The proposed class of models is general and encompasses a number of common models for the latency survival function, including the proportional hazards model and the proportional odds model, and also allows for time-dependent covariates. To properly evaluate the variability of the parameter estimates we employ a novel application of the weighted bootstrap and verify its utility via simulations. We apply the proposed methods to the NCI SEER prostate cancer dataset to investigate racial differences in prostate cancer cures.

Xaq Pitkow

Center for Theoretical Neuroscience, Columbia University

Benchmarks for Vision: Calculation of Arbitrary Statistics for Naturalistic Images

The natural visual environment has considerable structure, but to date the characterization of this structure has been restricted to fairly simple statistical regularities. Here I describe a method to calculate the joint statistics of complex image features exactly, for a generative model of images known as the Dead Leaves model. The world described by this model is composed of independent, textured objects which occlude each other. This simple structure allows us to calculate the joint probability distribution of image values sampled at many arbitrarily located points, in some cases without approximation. By choosing the samples appropriately, one can then convert this result into joint probabilities of edges, T-junctions, and other image features thought to be important for object recognition. I will conclude by briefly describing how some of these regularities may explain aspects of visual perception such as contour facilitation, phantom edges, and amodal completion.

Asya Shpiro

New York University, Center for Neural Science

Balance Between Noise and Adaptation in Competition Models of Perceptual Bistability

Perceptual bistability occurs when a physical stimulus gives rise to two distinct interpretations that alternate irregularly. Noise and adaptation processes are two possible mechanisms for switching in neuronal competition models that describe the alternating behaviors. Either of these processes, if strong enough, could alone cause the alternations in dominance. It is difficult to disentangle the effects of noise and adaptation in experiment alone, because we have no methods to control the magnitude of noise and/or adaptation independently. Mathematical models can provide insight into this question by allowing to vary these parameters at will. We examine the relative role of noise and adaptation in producing alternations by studying models where by smoothly varying the parameters, one can change the rhythmogenesis mechanism from being adaptation-driven (that is, noise is not necessary to produce alternations) to noise-driven (no alternations can occur in the absence of noise). Two idealized firing rate models that describe bistable perception are considered. In one, neuronal competition is implemented by a simple reciprocal inhibition architecture (Shpiro et. al., J Neurophys 2007). The other model characterizes a different, global excitation-local inhibition architecture (Moreno-Bote et. al., J Neurophys 2007). We focus on four statistical measures of bistable perception: the mean dominance duration of a percept (typically of the order of a few seconds), the CV (the ratio between the standard deviation and the mean; typically about 0.5), the shape of distribution of dominance durations (typically, fit by gamma or lognormal functions), and the correlations between the successive dominance durations (weak, but finite). We seek to find regions in the noise-adaptation parameter space where computed alternation statistics are similar to those observed experimentally, and ask whether we can rule out one of the rhythmogenesis mechanisms. In both models, alternations are possible over large regions of parameter space but the experimental constraints are satisfied in only a restricted domain. This region lies primarily in the noise-driven alternations regime. However, the gamma-like distribution of dominance durations, as well as finite correlations between the successive durations require some adaptation mechanism as well. We conclude that in order to comply with the observed statistics of bistable perception, the models must operate within a balance between the noise and adaptation strength – both mechanisms are involved in producing alternations, in such a way that the system operates near the boundary between being adaptation-driven and noise-driven. This work is done in collaboration with Ruben Moreno-Bote, John Rinzel, and Nava Rubin.

Rajat Singhania
Virginia Tech

Cell Cycle Modeling Using a Hybrid Approach

It is well known that there is a direct relationship between cancer and the mammalian cell cycle. Therefore, it is important to develop models that accurately and comprehensively mimic the molecular regulatory networks governing the cell cycle. Current techniques in vogue that are used to model cell cycle regulatory networks mostly rely on continuous Ordinary Differential Equations (ODEs) that use a large number of kinetic parameters as an essential ingredient in their set-up. However, most of these kinetic parameters are hard to estimate and/or there is lack of experimental data to quantify them authoritatively. In that context, we have developed, in collaboration with Dr. James W. Jacobberger at Case Western Reserve University, a "hybrid model" of mammalian cell cycle regulation. We build the hybrid model by first separating the protein species involved in cell cycle regulation into two classes: the cyclins (proteins that are the primary drivers of cell cycle progression), and the cyclin regulators (such as transcription factors and cyclin degradation pathway initiators). The activity or inactivity of the cyclin level regulators is represented by discrete (Boolean) variables that are essential components of the continuous (ordinary differential) equations used to model the synthesis and degradation of the cyclins. This is how our model is hybrid in the continuous-discrete sense. Our model proceeds through the various stages of the cell cycle by dividing up the cell cycle into distinct "states" in which each state comprises of a specific combination of the values of the Boolean-modeled cyclin regulators. Furthermore, while this sequence of Boolean states is deterministic, the residence time in each state is modeled stochastically, using an exponential distribution centered around the average residence time of each state, which is guesstimated from experimental data. This is how our model is hybrid in the deterministic-stochastic sense. This hybrid model needs a minimal number of kinetic parameters compared to full-blown ODE models, and is much easier to construct. By successfully using this hybrid approach to simulate flow cytometry experimental data from colon carcinoma (RKO) cells, we have demonstrated that this is indeed a valid and viable approach for modeling complex cell cycle data from cancerous cell lines in the future.

Svetlana Tlupova
New Jersey Institute of Technology

Domain Decomposition Methods for Solving Stokes-Darcy Systems Based on Boundary Integrals

We consider a coupled problem of Stokes and Darcy equations. This involves solving PDEs of different orders simultaneously. To overcome this difficulty, we apply a non-overlapping domain decomposition method based on a Robin boundary condition obtained by combining the velocity and pressure interface conditions. The coupled system is then reduced to solving each problem separately by an iterative procedure using a Krylov subspace method. The numerical solution in each subdomain is based on the boundary integral formulation, where the kernels are regularized and the leading term in the regularization error is eliminated for higher order accuracy.

Solmaz Torabi
University of California-Irvine

Effect of Elastic Energy on Epitaxial Quantum Dots Formation and Growth

Self-assembly semiconductor nanostructures such as quantum- dots are a promising inexpensive and effective approach to manufacture novel nanoscale electronic devices. Producing such quantum-dot-based devices, however, is still challenging. The main goal is the production of large numbers of spatially ordered nanostructures with narrow size distribution via a controlled self- assembly process. Consequently, we need to have a fundamental understanding of the self-organization process (nucleation, growth and coarsening) during epitaxial growth to achieve spatially ordered quantum scale structures. For this reason we study the influence of strain, surface energies and kinetics on heteroepitaxial thin film growth. Modeling and numerical studies are presented that complement experimental investigations. Here, we present a new approach for modeling strongly anisotropic crystal and epitaxial growth using regularized, anisotropic Cahn-Hilliard-type equations as a model for the growth and coarsening of thin films. When the surface anisotropy is sufficiently strong, sharp corners form and unregularized anisotropic Cahn-Hilliard equations become ill-posed. Our models contain a high order Willmore regularization to remove the ill posedness at the corners. A key feature of our approach is the development of a new formulation in which the interface thickness is independent of crystallographic orientation. We provide matched asymptotic analysis to show the convergence of our diffuse interface model to the analytical sharp interface model. In previous models there was no such convergence to sharp interface model when the Willmore energy was considered. We present 2D and 3D numerical results using an adaptive, nonlinear multigrid finite-difference method. In particular, we find excellent agreement between the computed shapes using the Cahn-Hilliard approach, with a finite but small Willmore regularization, with dynamical numerical simulations of a sharp interface model. The equilibrium shapes from our diffuse model are compared with an analytical sharpinterface theory recently developed by Spencer (2004) at the corners, and there is an excellent match. Away from the corners there is an excellent agreement between the diffuse model with the classical Wulff shape. Finally, in order to model the misfit and displacement strains, we add the elastic energy to our diffuse model. We analyze numerically the effect of elastic stress on the corner regularization in terms of two parameters: one parameter that describes the relative strength of the elastic energy to surface energy and the second that characterizes the strength of the surface energy anisotropy. Adding elastic energy modifies the equilibrium shape and in particular affects the shape of the corners. We can predict different Qdot shapes, such as pyramids and domes, based on the strength of the elastic interactions.

Dmitri Tseluiko

University of East Anglia, Norwich

Steady Electrified Film Flow Down an Indented Wall

We investigate the effect of an electric field on a liquid film flowing down an inclined, corrugated wall at zero Reynolds number. The film is taken to be either a perfect conductor or a perfect dielectric. The region above the film is assumed to be a perfect dielectric. Using a long-wave asymptotic analysis, we derive a nonlinear, non-local equation for the thickness of the liquid film and compute steady solutions over rectangular downward and upward steps and into rectangular trenches and over rectangular mounds. In the absence of an electric field, the film develops a capillary ridge above a downward step and a depression in front of an upward step. For a perfect-conductor film, the results show that as the electric field strength increases, there appear short-wave oscillations upstream of a downward step, the height of the capillary ridge decreases, and a depression right downstream of the step is introduced. At an upward step, imposing an electric field leads to the creation of a free-surface ridge downstream of the step and introduces short-wave oscillations upstream of the step. Solutions for a perfect-dielectric film are similar to those for a perfect-conductor film, although the height of the capillary ridge varies non-monotonically with the electric field strength. Using a small-step-height asymptotic analysis for the long-wave model and for the full Stokes flow problem, we obtain some insight into the mechanisms responsible for the flow features. This analysis not only provides a qualitative explanation of such features as the appearance of short-wave oscillations upstream of a downward/upward step when an electric field is introduced but also gives analytical estimates for the quantitative characteristics of these features, e.g. for the wavelength and the amplitude of the oscillation. The results are corroborated by fully nonlinear boundary-element calculations for Stokes flow.

POSTERS

Shuchi Agrawal
New Jersey Institute of Technology

Stability and Bifurcation Analyses of Microwave Heated Ceramic Cylinders and Slabs

One and two-dimensional reaction diffusion equations, which contain a functional and an inhomogeneous source term, are good models for describing microwave heating of thin ceramic cylinders and slabs in a single mode, highly resonant cavity. We apply numerical methods to accurately approximate the steady state solutions of these equations and to determine their stability. In addition we use numerical and analytic techniques to approximate local bifurcation structure of their steady state.

David Albers
Columbia University

On a Statistical Mechanics-Like Formulation for Real Electronic Medical Records

Using an analogy with statistical mechanics and ergodic theory, a framework for utilizing electronic health records (EHR) to formulate and interact with constructive, dynamic models of disease and patient populations is proposed. By importing the respective technology, language and interpretive structure of the abstract theory of statistical mechanics, it is hoped that a multitude of partial solutions will eventually be attainable, including: multi-scale analysis; establishment of a model coordinate system; a means of coping with incomplete data; a means of quantifying information present in various representations of data; and interaction with deterministic modeling techniques. The talk will focus on two components of this program: i.) the practical form of the raw EHR, and thus the real-world limitations and constraints of EHR data; and ii.) a language for mapping the raw electronic medical records into a matrix-like form that can interact with the more abstract tools and analysis.

Puneet Arora
Indian Institute of Technology, Kanpur, India

B-Spline Collocation Method for the Singular Perturbation Problem using Artificial Viscosity

In this paper, we develop a B-spline collocation method using artificial viscosity for solving singularly perturbed equations given by

$$\varepsilon u''(x)+a(x)u'(x)+b(x)u(x)=f(x),$$
$$a(x)\geq a^{*}>0,\ b(x)\geq b^{*}>0,$$
$$u(0)=\alpha,\ u(1)=\beta.$$

We use the artificial viscosity to capture the exponential features of exact solution on a uniform mesh and use B-spline collocation method which leads to a tridiagonal linear system. The convergence analysis is given and the method is shown to have uniform convergence of second order. The design of artificial viscosity parameter is confirmed to be a crucial ingredient for simulating the solution of the problem. Known test problems have been studied to demonstrate the accuracy of the method. Numerical results show the behaviour of the method with emphasis on treatment of boundary conditions. Results shown by the method are found to be in good agreement with the exact solution.

Lyudmyla Barannyk
University of Idaho

Numerical Simulations of Shear Instability in Strongly Nonlinear Solitary Waves in a Channel

We apply boundary integral methods to simulate dynamics of large amplitude internal solitary wave solutions of Euler equations in a channel. The initial conditions are taken to be traveling solitary wave solutions of a strongly nonlinear long-wave model studied by Jo and Choi [Stud. Appl. Math. 109 (2002) 205--227]. We compare our numerical results using the vortex sheet model to those obtained using the long-wave model cited above. Joint work with Wooyoung Choi (NJIT) and Robert Krasny (University of Michigan).

Alexander Barnett

Dartmouth College

Solving Helmholtz Problems with a Basis of Fundamental Solutions: The Role of Singularities in the Analytic Continuation

The method of fundamental solutions (MFS) has been successfully used for solving wave problems: Greens function sources are placed outside the domain of interest and their coefficients adjusted to match desired boundary conditions. For example, in conjuction with the scaling method, one can use it to compute high-frequency eigenmodes with unprecedented efficiency (A. H. Barnett, Comm. Pure Appl. Math, 59, 1457 (2006)), with applications including quantum chaos. However, there is currently little understanding of how to choose the source locations, and poor choices lead to an unusable method. We analyse this in analytic domains, proving spectral convergence in the disc, and showing numerically similar behavior in non-convex analytic domains. We demonstrate that it is singularities in the analytic continuation of the solution field that control stability, in particular the coefficient sizes, in the algorithm. This enables us to develop a method for source location which adapts to the singularities induced by the so-called Schwarz function of the domain. We also show that MFS is highly competitive with boundary integral methods while possessing the advantage that the field may be accurately evaluated up to the boundary. (Authors contributing to the work presented: A. H. Barnett and T. Betcke)

Andrea Barreiro

University of Illinois at Urbana-Champaign

Bifurcation Theory for a Model of the Oculomotor Neural Integrator

In order to control the movement of the eyes, the brain must convert sensory signals proportional to desired eye velocity into eye position commands. The neural network that accomplishes this is the oculomotor neural integrator. This network produces integration through positive feedback and maintains a time constant of about 20 seconds in humans. In order to ensure that the integrator produces effective eye position commands under changing circumstances, it is regulated by the cerebellum. The cerebellar control mechanism is capable of independent adjustment of time constant and gain. We analyze neural network models of the coupled integrator-cerebellar system. Our analysis, which uses ideas from the perturbation theory of operators and classical differential geometry, shows that, in order to function normally, the system must operate in a narrow region where small perturbations can push it into regions of instability or oscillations. Our model will also simulate a class of eye movement disorders known as "congenital nystagmus". Both normal and abnormal behavior depend crucially on the non-normality of the system.

Ernest Barreto

George Mason University

Ion Concentration Dynamics: Novel Mechanisms for Bursting and Seizing

We develop a conductance-based model neuron that includes intra- and extra-cellular ion concentration dynamics. We further formulate a reduction of this model to identify the bifurcation structure. Using these models, we describe a novel mechanism for bursting and seizing that results in behavior that is strikingly similar to that seen in experiments.

Ricardo Barros and Wooyoung Choi

New Jersey Institute of Technology

Effects of the Free Surface on Nonlinear Internal Waves

In this work, we study the propagation of large amplitude internal waves in two-layer flows by considering strongly nonlinear long wave models. Both rigid-lid and free-surface are considered for the upper boundary and internal solitary-wave solutions are compared in both configurations. Shear instability at the interface is also examined with and without the hydrostatic assumption and, in particular, free surface effects are discussed in detail.

M.C. Bhattacharjee[1] and S. Balaji[2]

[1] New Jersey Institute of Technology, [2] George Washington University

On the Shape Duality of Failure Rate and Mean Remaining Life Functions

We investigate when the shape of the failure rate (FR) function translates to a corresponding dual shape of the mean residual life (MRL). The converse problem of MRL to FR shape duality is also explored. Our results (i) consolidates and generalizes earlier results which are more restricted in scope, and corrects an incorrect illustration in the literature.

Denis Blackmore, Aminur Rahman, and Jigar Shah

New Jersey Institute of Technology

Discrete Dynamical Modeling and Analysis of the R-S Flip-Flop Circuit

A simple discrete planar dynamical model for the ideal (logical) R-S} flip-flop circuit is developed with an eye toward mimicking the dynamical behavior observed for actual physical realizations of this circuit. It is shown that the model exhibits most of the qualitative features ascribed to the R-S flip-flop circuit, such as an intrinsic instability associated with unit set and reset inputs, manifested in a chaotic sequence of output states that tend to oscillate among all possible output states, and the existence of periodic orbits of arbitrarily high period that depend on the various intrinsic system parameters. The investigation involves a combination of analytical methods from the modern theory of discrete dynamical systems, and numerical simulations that illustrate the dazzling array of dynamics that can be generated by the model. Validation of the discrete model is accomplished by comparison with certain Poincaré maps corresponding to three-dimensional differential equation models of electrical circuits that produce R-S flip-flop behavior.

Michael Booty and Michael Siegel

New Jersey Institute of Technology

The Influence of Surfactant and Surfactant Solubility on Drops and Bubbles

We present recent results on the influence of surfactant on stretched drops and bubbles.

Asymptotic results, found by slender body theory, are given for a drop of arbitrary viscosity that is stretched in a cylindrically axisymmetric uniaxial extension flow. The surfactant is insoluble in the bulk flow but can diffuse on the drop interface. A variety of drop shapes are found for drops that are completely coated in surfactant or are partly surfactant-free but have surfactant end-caps. The drop shape depends mainly on a single dimensionless grouping of the drop to suspending fluid viscosity ratio and the surfactant's surface Peclet number.

Numerical results, using a hybrid asymptotic-numerical method that is designed to resolve narrow transition layers of a surfactant that is soluble in the bulk flow but has large bulk Peclet number, are presented. The geometry is 2D Cartesian, the drop is inviscid, and the imposed flow that stretches the bubble is an arbitrary linear strain or shear. The accuracy and speed of the hybrid method are compared to a more traditional finite-difference scheme for surfactant solubility.

Joshua Bostwick

Cornell University

Capillary Oscillations of Coupled Spherical Cap Droplets

Fluid droplets tend to spherical shapes under surface tension in order to minimize their surface energy. As a function of the total volume of the system, it has been shown that coupling two droplets gives rise to symmetric/asymmetric steady state solution

branches. The linear, inviscid, volume-preserving oscillations of coupled spherical cap droplets constrained by pinning along a latitude is solved here. The formulation for oscillations about each steady state branch generates an integro-differential boundary value problem on the free surface deformation. A spectral method, using properly chosen basis functions, delivers a truncated solution to the eigenvalue problem. Along the asymmetric branch, it is shown that the effect of the pinned constraint is to introduce a new low frequency eigenmode, which is important for applications.

Temitope Brotherson[1], Karina Aliaga[1], and Gareth Russell[1,2]

[1] New Jersey Institute of Technology, [2] Rutgers University

Island Biogeography with Active Dispersal

Macarthur and Wilson's theory of island biogeography models the effect of distance and area of an island on the immigration and extinction rates of species, and therefore on equilibrium species richness. Like many classic spatial models in ecology, it assumes 'passive' dispersal and population dynamics. Here, we introduce the concept of emigration as a choice-based disappearance mechanism whereby species play an active role in deciding whether to leave, or remain on, an island. We link the emigration rate to both the area and distance of an island, using a variety of functional forms, and demonstrate how this function alters traditional species-area and species-distance relationships. We show how our modified model explains some otherwise puzzling patterns found in real data.

Michael Buice

National Institutes of Health

Correlations, Fluctuations, and Stability of a Finite-Size Network of Coupled Oscillators

The Kuramoto model is a widely used model for biological systems which describes a system of coupled oscillators. The incoherent state of the Kuramoto model of coupled oscillators exhibits marginal modes in mean field theory. We demonstrate that corrections due to finite size effects render these modes stable in the subcritical case, i.e., when the population is not synchronous. This demonstration is facilitated by the construction of a nonequilibrium statistical field theoretic formulation of a generic model of coupled oscillators. This theory is consistent with previous results. In the all-to-all case, the fluctuations in this theory are due completely to finite size corrections, which can be calculated in an expansion in $1/N$, where N is the number of oscillators. The $N \to \infty$ limit of this theory is what is traditionally called mean field theory for the Kuramoto model.

Mariana Cassimiro, Brian Emmanuel, Michael Lam, and David J. Horntrop

New Jersey Institute of Technology

Aliasing and Convolutions in Fourier Series

The goal of this project was to study the aliasing errors involved in performing convolutions in the stochastic setting using Fourier series, as well as some of the different methods to reduce this error. Since spectral methods for solving differential equations can be very sensitive to perturbations, the reduction of error using dealiasing techniques is extremely important. The two particular dealiasing techniques used here were the padding and the phase shift method. These two techniques were first applied in a deterministic setting. In many cases the aliasing error was quite noticeable and was greatly reduced through the use of these dealiasing techniques. The next step in studying the effects of aliasing in a probabilistic setting was the generation of Gaussian random fields. Finally, the above techniques were used to study the effect of aliasing in the stochastic setting, which is work currently in progress. This project was part of the NSF CSUMS program at NJIT for undergraduate research in computational mathematics.

Lakshmi Chandrasekaran

New Jersey Institute of Technology

Role of Plasticity in Coincidence Detection in the Avian Auditory Brainstem

Interaural time difference (ITD) is the difference in the time of arrival of sounds to both the ears, used by birds and mammals as cues for locating the sound source. Nucleus magnocellularis (NM), one of the major neurons in the cochlear nucleus of the auditory brainstem, sends depressing excitatory synapses onto the NL neuron which acts as a coincidence detector. Coincidence detection means a NL neuron has a higher firing rate, when it receives simultaneous inputs from the NM neurons of both the left and right ear. Another factor which affects coincidence detection is the inhibition from SON (superior olivary nucleus) onto the NM neurons. SON is another group of neurons in the auditory brainstem. The SON has been shown to play a vital role in controlling the dynamics of the NM neurons when there is an input bias to either of the ears, which causes ambiguity among the NL neurons in being able to discriminate between strong monaural excitation and binaural coincidence detection.

Here we develop mathematical models to show how both NM depression and SON inhibition contribute towards enhancing coincidence detection. We make use of a firing rate model for the NL neurons and show that NM depression makes NL firing rate more phase dependent and less input frequency dependent. We verify these results using a spiking model namely, the integrate and fire neuron. We also model the SON with a facilitating inhibition onto the NM neuron to show that SON plays a role in eliminating ambiguity among the NL neurons during input bias to the NM cells.

Chung Chang
Columbia University

A Bootstrap Resampling Approach: Tests of Significance on Functional Data

In many areas of application, data are of functional nature, such as 1-dimensional spectral data and 2- or 3-dimensional imaging data. It is often of interest to test for the significance of some set of factors in the functional observations (e.g., test for mean differences between two groups). One important motivating example involves testing for changes in neuroimaging data among subjects in two groups (depressed vs. normal control), although proposed procedures are applicable to a wide variety of functional data. Testing hypotheses voxel-by-voxel in such a framework results in a severe multiple comparisons problem because the number of measurements made per observation is typically much larger than the number of observations ("large p, small n" problem). Good solutions to this problem must take into account the spatial correlation inherent in the imaging. Statistical Parametric Mapping (SPM) and the permutation test have become popular in this setting but they rely on parametric and exchangeability assumptions, respectively, which are not always satisfied in practice. We propose two bootstrap-based methods (L1 and L2) that takes the spatial correlation structure into account. These methods are free of the parametric assumptions made by SPM and are more flexible than the permutation test. We propose a bootstrap approach (L1) that is free of the parametric assumptions made by SPM and also are more flexible than the permutation test. We compare the performance of the L1 method with that of SPM, the permutation test, and another bootstrap approach (L2). For the L2 method, we present sufficient conditions that ensure asymptotic control of the family-wise error rate.

Laura Cimponeriu
Universität Potsdam, Germany

Uncovering Interaction of Coupled Biological Oscillators from Data

Oscillations and their interaction play an important role in the dynamics of biological systems at all levels of organization. Mathematical models of coupled oscillators have become important tools in the study of coupled oscillations, providing a useful framework for understanding the temporal coordination of biological processes. My talk focuses on the usage of phase dynamics models in the study of interaction among observed oscillator systems. A novel approach for reconstructing an observable independent, invariant representation of the dynamics of coupled oscillators will be presented. The main issues addressed are: (1) reconciling theoretical phase dynamics models with observational data, (2) reconstructing invariant phase models from time series, and (3) inferring interaction properties (e.g., strength, directionality). I further illustrate how this novel approach can be used to uncover the interaction of coupled oscillators from experimental data. The analysis of neural oscillators and a version of the classical Huygens' pendulum clocks experiment are used for demonstration.

Federico E. Contiggiani[1], Fernando Tohme[1], and Horacio G. Rotstein[2]
[1] Universidad Nacional del Sur and CONICET, Argentina, [2] New Jersey Institute of Technology

Dynamic Aspects of a Decision-Making Process in a Hot/Cool System

This presentation concerns the interaction between a cognitive ("cool", slow, reflective) and an emotional ("hot", fast, reflexive) systems in decision making processes. Based on theoretical (static) frameworks presented by other authors, most notably Metcalfe and Mischel (1999), we construct a minimal mathematical model that describes both the internal dynamics of each system and the dynamics of their interactions. Each system has two nodes, excitatory and inhibitory. The intrinsic connections are such that the resulting dynamics is monostable and bistable for the hot and cool systems respectively, representing different ways of processing information. Each option is represented by a stable fixed point. This model captures some important phenomenological aspects including individual's impulsive decisions contrary to an optimal (intended) plan of action, and it is simple enough to give some insight into the underlying dynamics. We use it as a first step in our investigation of a decision making process under intertemporal and uncertain contexts.

Ned Corron
U.S. Army RDECOM, AMSRD-AMR-WS-ST, Redstone Arsenal, AL 35898

High-Dimensional Chaos without Nonlinear Dynamics

A time-continuum limit for an iterated shift map reveals a linear filter driven backward in time. The limit is derived by factoring the shift iterate into an arbitrarily large number of identical fractional iterates. Application to a coupled map lattice (CML) of shift maps results in a set of coupled filters, revealing a linear decomposition of spatially extended chaos. A consequence is the capability to construct high-dimensional chaos via linear synthesis and convolution. This unnerving result undermines the usual assumption that deterministic chaos results only from the evolution of a nonlinear dynamical system.

Tanujit Dey
Case Western Reserve University

A Bimodal Spike and Slab Model for Model Space Exploration and Model Selection

Variable selection in linear regression models is an important aspect of many scientific analyses. We have developed a simple spike and slab model for model space exploration and variable selection in linear regression models. Model selection using our mathematical tool is based on final prediction error (FPE) approach. Classical examples of FPE's are AIC and BIC. The model chosen is the best model with minimum FPE values among all the models. However, model selection based on FPE criteria can be doubtful as FPE criteria can be sensitive to perturbations in the data. More stable model selection is accomplished by using a bootstrap wrapper. The heart of the method is the notion of model averaging for stable variable selection. Out-of-bagging is used to estimate the prediction error and the predictor with the smallest prediction error is determined. Optimal model of size k is determined by ordering first k variables based on an averaged Bayesian model averaged (BMA) predictor formed by averaging the BMA estimator over the bootstrap draws. We have developed an R package (modelSampler) to implement this unique model selection technique. This R package is very simple to implement. The returned objects from the package contain numerous information related to the model selection procedure. Several graphical wrappers interpret the returned objects allowing study of stability of variables over the entire model space, which is very useful in high dimensional situations.

Sunil K. Dhar and Soumi Lahiri
New Jersey Institute of Technology

A Log-Linear Model under the Generalized Inverse Sampling Scheme

This research discusses the log-linear model for multi-way contingency table, where the cell values represent the frequency counts that follow an extended negative multinomial distribution. This model represents an extension of negative multinomial log-linear model. The parameters of the new model are estimated by maximum likelihood method. The likelihood ratio test for the general log-linear hypothesis is derived. An application of the log-linear model under the generalized inverse sampling scheme is

demonstrated by an example.

Oleksandr Dybenko, Anthony D. Rosato, and David J. Horntrop
New Jersey Institute of Technology

Self-Organization in Density Relaxation by Tapping

Density relaxation describes the phenomenon in which granular solids undergo an increase in bulk density as a result of a properly applied external load. Density relation is modeled here using both Monte Carlo and dissipative molecular dynamics simulations to investigate the effect of regular taps applied to a vessel having a planar floor filled with identical spheres. Results suggest the existence of a critical tap intensity which produces a maximum bulk solids fraction. A striking observation is a mechanism that appears to be responsible for the relaxation phenomenon itself in which an evolving quasi-ordered packing structure propagates upward from the planar floor.

Fatima Elgammal, Matthew Peragine, and Roy Goodman
New Jersey Institute of Technology

Algorithms for Recursively Rendering Parametric Curves

Nonlinear dynamical systems are typically regulated by invariant manifolds, stable and unstable, that exhibit regions of erratic trajectories and very high curvature. Parametric functions are a way of representing curves where we define the independent and dependent variables, respectively x and y, in terms of a third term, t. Our goal is to make an adaptive recursive scheme for subdivision- adaptive because we want to add points where needed based on a local condition and generate as few function calls as possible. Previous attempts have been made with linear interpolation, namely those of R. Chandler and L. Figueriedo, though we are extending our algorithm to higher order interpolation.

Leonardo Espin and Demetrios T. Papageorgiou
New Jersey Institute of Technology

Effect of Inlet Boundary Conditions in Self-Similar Solutions of the Navier-Stokes Equations in Bounded Domains

We investigate the effects that different inlet boundary conditions have in the development of the solutions of the Navier-Stokes equations in a two-dimensional, finite channel with accelerating walls. When the channel is infinite, the Navier-Stokes equations admit solutions of the similarity form, which as previous studies have shown, may or may not be recovered depending on the form of the inlet conditions. We find that even in the case when the inlet profiles are of the similarity form, the Navier-Stokes equations admit solutions which present a behavior which differs considerably from the one expected from the similarity solutions. As an example we show an unstable branch of solutions of the simpler, similarity model, which emerges as a stable branch for the Navier-Stokes equations.

Edward D. Farnum[1], Brandon G. Bale[2], and J. Nathan Kutz[2]
[1] Kean University, [2] University of Washington

Variational Reduction for Multi-frequency Frequency Laser Mode-Locking Equations

A variational method is applied to various model of single-, dual- and multi-frequency mode-locked lasers. This reduction provides a simple but surprisingly accurate characterization of stable and unstable solutions to the full partial differential equation model, in terms of saddle points, stable nodes, and stable spirals. In particular, it fully captures the role that inhomogeneous gain saturation plays in the formation of stable mode-locked pulse solutions in the dual-frequency case. Furthermore, it accurately predicts the narrow region of parameter space in which simultaneous mode-locked pulses of different shapes can be formed and stabilized.

Sarosh Fatakia
NIH/NIDDK

Identification of a Common Binding Cavity for G Protein-Coupled Receptors using Mutual Information and Graph Theory

G protein-coupled receptors (GPCRs) are proteins with seven transmembrane domains (TMs) that are involved in a wide array of physiological functions and are the most common targets of pharmaceuticals. Here, we show that residues within the ligand-binding pocket can be identified with an algorithm involving mutual information and graph theory. Using a multi-sequence alignment of the 7-TMs, we calculate the mutual information between all inter-TM pairs of alignment positions and ranked the pairs according to mutual information. Invoking the top ranking pairs, a graph with positions at the vertices and edges weighted by the mutual information was constructed in abstract information space. Positions with high degree (i.e. had significant mutual information with a large number of other positions) with respect to a null hypothesis of an ensemble of random graphs, were found to reside in the binding cavity of class A and C GPCRs. These key TM positions, which form a clique, are identified solely on the basis of sequence analysis. No prior hypothesis involving the specificity or importance of TM positions is involved in the algorithm. This novel algorithm may serve as a tool for systematic identification of sets of coevolving residues in families of evolutionary related proteins.

Bernard Fendler
Florida State University

Synchronization of Insulin Secretion Through Intrapancreatic Ganglia

β-cells are cells located in the human pancreas and are known to produce electrical activity. When these cells are electrically active, they secrete a hormone necessary for maintaining glucose homeostasis in the blood called insulin. The β-cells are located in the pancreas in small micro-organs called islets of Langerhans. There are thousands of islets in the pancreas which are known to produce oscillatory insulin secretion. Measurements of insulin have shown that oscillatory secretion also occurs in the blood. Since plasma insulin reflects the secretion from the entire islet population, oscillations in plasma insulin levels suggest that islet oscillations must be largely synchronized. Bertram et al. "Bio. Phys. Jour., 92, 1544-1555, 2007" has developed a mathematical model of the β-cell which reproduces many of the measured electrical and calcium properties of the β-cell. We use this model to investigate methods of synchronization of the islet population. The islet is known to be innervated by neurons, in ganglia, interspersed throughout the pancreas. We investigate the viability of islet synchronization by coordinated action of the intrapancreatic ganglia.

Anna Ghazaryan
University of North Carolina-Chapel Hill

Traveling Waves in the High Lewis Number Combustion Model

I consider combustion wavefronts arising in the model for high Lewis number combustion processes such as combustion of high density liquid fuels. An efficient method for the proof of the existence and uniqueness of the combustion front is provided by geometric singular perturbation theory. The fronts supported by the model with very large Lewis numbers are small perturbations of the front supported by the model with the infinite Lewis number. The question of stability of the fronts is more complicated. I will discuss issues and recent results on the stability analysis that arises at both the linear and nonlinear level.

Dror Givon
Princeton University

On Extracting the Virtual Slow Manifold

In many applications, the primary objective of numerical simulation of time-evolving systems is the prediction of coarse-grained, or macroscopic, quantities. Multiscale schemes based on singular perturbation theory and the averaging principle have been successfully applied to systems where both the fast and the slow variables can be observed. Often a "coarse" evolution law for (a reduction of) the original system can be explicitly determined from short simulations of its full detailed, "fine scale" description.

In the case where the full system is known to possess scale separation but the decoupling of the variables into slow and fast subsets is unknown, an extension of these schemes becomes necessary. In this talk I will describe some numerical schemes that exploit the existence of slow dynamics/slow manifolds even when decoupling of the variables is not known in advance. Joint work with C.W. Gear and I.G. Kevrekidis.

Peter Gordon
New Jersey Institute of Technology

Asymptotic Model of Flame-Flow Interaction in Forward Smoldering

Departing from the classical Burke-Schumann theory of diffusion flames, a geometrical model for flame-flow interaction in forward smoldering is formulated. The model is then applied for description of the fingering instability triggered by the mobility contrast. This is a joint work with I. Brailovsky and G. Sivashinsky.

Arnaud Goullet
New Jersey Institute of Technology

Numerical Studies on the Evolution of Nonlinear Water Waves and their Validation with Laboratory Experiments

Accurate modeling of surface wave dynamics in the ocean is a difficult task due to the complex nonlinear interaction between different wave components and a lack of understanding of various physical processes such as wave breaking and wind-wave interaction. Here we study a set of nonlinear evolution equations for the surface elevation and velocity potential fields derived using an asymptotic expansion technique and solve the system numerically using a pseudo-spectral method. Regular and irregular surface wave fields are both considered and our numerical solutions are validated with laboratory experimental measurements.

Edward Green
The Ohio State University, Mathematical Biosciences Institute

Modelling the mechanical behaviour of collagen gels

Motivated by the aim of modelling the mechanical behaviour of biological gels (such as collagen gels) which have a fibrous microstructure, we consider the flow of a two-dimensional film of incompressible, transversely isotropic viscous fluid. Two regimes are considered: extensional flow, and squeezing flow of the fluid between two rigid plates. Neglecting inertia, gravity and surface tension, in each regime leading-order equations are derived from the full flow problem using a thin-film approximation. Special cases in which the solution may be determined explicitly are considered and the physical interpretation of the results is discussed.

Joon Ha, Amitabha Bose, Farzan Nadim, and Jorge Golowasch
New Jersey Institute of Technology

Network Activity Coupled By Gap Junctions

We study the network activity of excitable cells coupled by gap junctions. We investigate how the voltage response of two gap junctionally coupled cables depends on cable diameter. Specifically, we show that there exists an optimal diameter for which the signal can be transmitted most effectively and the propagation time also can be minimized at the optimal diameter. We find that diameter regulation allows neurons to selectively transmit action potentials in gap junctionally connected networks.

Baris Hancioglu
Virginia Tech

Ensemble Models for Human Immune Response to Influenza A Virus Infection

In our study, we construct ensembles of models that vary in parameter values and are ranked according to their likelihood to capture existing data or clinically available observations. The results obtained from an ensemble model are probabilistic predictions of the dynamics that accurately represents the variability of responses in individuals. Our main objective is to construct an ensemble model of the dynamics of influenza infection which makes probabilistic predictions on the course of disease, finds the likelihood of each model representing individual immune response and makes probabilistic estimates of the effectiveness of therapeutic interventions such as antiviral drug therapy. We develop methods to find the posterior distribution which contains all the information on the parameter space. Our main goal is to quantify uncertainty in model predictions due to parameter heterogeneity. Based on our published ODE model by Hancioglu et al.(JTB,2007), an ensemble model of human immune response to influenza infection consisting of multiple ODE models that are identical in form but differ in parameter values is developed. A probabilistic measure of goodness of fit of the ODE model is used to derive posteriori probability density of the space of parameter values. This probability density is sampled using Metropolis Monte Carlo method and sampling efficiency is enhanced using a parallel tempering algorithm. The ensemble model is employed to compute probabilistic estimates on trajectory of the immune response, duration of disease, maximum damage, likelihood of rebound in the disease and the probability of occurrence of superspreaders. The effectiveness of using an antiviral drug treating the infection is determined and optimal treatment scenarios are discussed. We generated an ensemble of 16,700 models with good fit to data and the probability density appeared to have reached asymptotic stability. The ensemble model predicts that 2% of the population will experience recurrence of the disease before eradication. A smaller proportion of models (78) are superspreaders, in these models display normal viral titers, but low interferon and low tissue damage, therefore apparent health. We also investigated the optimal starting time of antiviral drug therapy under a number of assumptions regarding pre-existing immunity and efficacy of antiviral drug. We found that optimal time to start treatment, in the case of virulent viruses, may not be right at infection, but rather after about 1 day. Availability of more clinical data and computational power would enhance the derivation of the posterior probability and give more reliable and accurate results.

Michael Higley
Pennsylvania State University

The Nonhomogeneous Single Fracture Poisson Process in One Dimension

We present a modeling framework for 1D fragmentation in brittle rods, in which the distribution of fragments is written explicitly in terms of the probability of breaks along the length of the rod. This work is motivated by the experimental observation of several preferred lengths in the fragment distribution of shattered brittle rods after dynamic buckling. The resulting relation qualitatively reproduces the experimentally observed fragment distribution, as well as some other common distributions such as a power law with a cutoff.

David J. Horntrop
New Jersey Institute of Technology

Mesoscopic Simulation of Ostwald Ripening

Self-organization of components of two phase mixtures through diffusion is known as Ostwald ripening. One class of models for Ostwald ripening consists of stochastic partial differential equations can be derived directly from the underlying microphysics. In order to study these models computationally, spectral schemes for stochastic partial differential equations have been developed and computationally verified. These schemes are then applied to this model and the simulation results are compared with theoretical results such as the Lifshitz-Slyozov growth law. Partially supported by NSF-DMS-0406633.

Zhengzheng Hu
University of California-Irvine

Phase-Field Modeling of Thin Film Growth: Applications to Step and Island Dynamics

We present a phase-field model to simulate the dynamics of step flow and a perturbed circular island during epitaxial growth. Asymmetric attachment/detachment kinetics, surface diffusion at the steps and a far-field flux are incorporated in the model. Moreover, a modified free energy function together with a correction to the initial phase variable profile is given to efficiently capture the morphological evolution when a large deposition flux is imposed. A block-structured adaptive mesh refinement

method and an efficient numerical method is developed using a second order accurate fully implicitly time discretization together with a second order accurate finite difference spatial discretization. Our results on step flow match with results presented by Frank Haußer et al., based on a front tracking method. In the long wavelength regime, we observe meandering with a wavelength being determined by the linear instability and endless growth of the amplitude. Whereas in the shorter wavelengths, we observe mushroom formation, subsequent pinch-off leading to the formation of a vacancy island. At later times, the vacancy island fills due to deposition and adatom diffusion. When we apply our model to the island dynamics, our simulations of the constant deposition flux confirm the linear stability results of Hu et al., and simulations of the variable deposition flux reveal the possibility of shape control in nanoscale.

Aridaman Jain[1], Francisco Artigas[2], Christine Hobble[2], and Ildiko Pechmann[2]

[1] New Jersey Institute of Technology, [2] Meadowlands Environmental Research Institute

Modeling of Sediment Chemistry and Biophysical Measurements Based on Remote-Sensor Images

The New Jersey Meadowlands Commission's Meadowlands Environmental Research Institute (MERI) has proposed to establish a long-term wetland-monitoring program in the New Jersey Meadowlands District based on new high-resolution remote sensing techniques. This new approach, which removes observer bias, is designed to capture information on the extent and health of large areas of urban fragmented wetland over time, without the need to make these measurements at the wetland locations. This approach requires the development of statistical models for estimating biophysical measurements (height, stem density, etc.) as well as sediment chemistry measurements (sulfide, salinity, orp, etc.) as a function of images obtained by remote sensors.

This paper describes the development of the linear regression models for estimating the three most important sediment chemistry measurements - sulfide, salinity and orp – collected during May/June, August, and October 2007 as a function of several image measurements made during June 2007 and October 2004. These models turn out to be good fits to the sediment chemistry measurements, since the lack of fit of these models are quite small. Similarly, linear regression models have been developed for estimating 5 biophysical measurements - height, elevation, length of inflorescences, stem density, inter-node length - as a function of the same image measurements obtained by remote sensors. These models also turn out to be good fits.

Rashi Jain and Zoi-Heleni Michalopoulou

New Jersey Institute of Technology

Particle Filtering for Arrival Time Estimation from Sound Signals in the Ocean

Locating and tracking a source in an ocean environment as well as estimating environmental parameters of a sound propagation medium is of utmost importance in underwater acoustics. Matched field processing is often the method of choice for the estimation of such parameters. This approach, based on full field calculations, is very computationally intensive and sensitive to assumptions on the structure of the environment. As an alternative, methods that use only select features of the acoustic field for source localization and environmental inversion have been proposed. The focus here is on inversion using arrival times of identified paths within recorded time-series at an array of vertically separated hydrophones. After a short study of a linearization techniques employing such features and numerical issues on their implementation, we turn our attention to the need for accurate extraction of arrival times for accurate estimation. We develop a particle filtering approach that treats arrival times as ``targets'', dynamically modeling their ``location'' at arrays of spatially separated receivers. Using Monte Carlo simulations, we perform an evaluation of our method and compare it to conventional Maximum Likelihood estimation. The comparison demonstrates an advantage in using the proposed approach, which can be employed as a pre-inversion tool for minimization of uncertainty in arrival time estimation.

M. Janjua[1], S. Nudurupati[1], P. Singh[1], I. Fischer[1], and Nadine Aubry[2]

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An Efficient Direct Numerical Simulation (DNS) Approach for Suspensions Subjected to Spatially Varying electric Fields

We have developed a numerical scheme to simulate the motion of dielectric particles in uniform and nonuniform electric fields of a micro fluidic device. The particles are moved using a direct simulation scheme in which the fundamental equations of motion of fluid and solid particles are solved without the use of models. The motion of particles is tracked using a distributed Lagrange multiplier method (DLM) and the electric force acting on the particles is calculated by integrating the Maxwell stress tensor (MST) over the particle surfaces. One of the key features of the DLM method is that the fluid-particle system is treated implicitly by using a combined weak formulation where the forces and moments between the particles and fluid cancel, as they are internal to the combined system. The MST is obtained from the electric potential, which, in turn, is obtained by solving the electrostatic problem. In our numerical scheme the Marchuk-Yanenko operator-splitting technique is used to decouple the difficulties associated with the incompressibility constraint, the nonlinear convection term, the rigid-body motion constraint and the electric force term. A comparison of the DNS results with those from the point-dipole approximation shows that the accuracy of the latter diminishes when the distance between the particles becomes comparable to the particle diameter, the domain size is comparable to the diameter, and also when the dielectric mismatch between the fluid and particles is relatively large.

M. Janjua[1], S. Nudurupati[1], P. Singh[1], and Nadine Aubry[2]

[1] New Jersey Institute of Technology, [2] Carnegie Mellon University

Micro- and Nano-Particles Self-Assembly for Virtually Defect-Free, Adjustable Monolayers

As chips further shrink toward smaller scales, fabrication processes based on the self-assembly of individual particles into patterns or structures are often sought. One of the most popular techniques for two-dimensional assembly (self-assembled monolayers) is based on capillary forces acting on particles placed at a liquid interface. Capillarity-induced clustering, however, has several limitations: it applies to relatively large (radius greater than ~10 m) particles only, the clustering is usually non-defect free and lacks long range order, and the lattice spacing cannot be adjusted. The goal of the present paper is to show that these shortcomings can be addressed by utilizing an external electric field normal to the interface. The resulting self-assembly is capable of controlling the lattice spacing statically or dynamically, forming virtually defect-free monolayers, and manipulating a broad range of particle sizes and types including nano-particles and electrically neutral particles.

Jun Jia

Oak Ridge National Laboratory

An Efficient, Stable and Spectrally Accurate Navier-Stokes Solver

In this talk, we present an accurate and efficient numerical method for the incompressible Navier-Stokes equations (NSE). The method is based on (1) an equivalent pressure Poisson equation formulation of NSE, which facilitates the design of high-order and stable numerical methods, and (2) the Krylov deferred correction (KDC) accelerated method of line transpose (MoLT), which is very efficient and of arbitrary order in time. Preliminary numerical experiments show that when combined with spectral spatial discretizations, the new method is fully spectrally accurate in space-time domain and very stable.

Shidong Jiang and Gregory A. Kriegsmann

New Jersey Institute of Technology

A Potential Problem Arising from Electromagnetic Homogenization in Doubly-Periodic Domains

A homogenization procedure has been recently employed to describe the propagation of electromagnetic waves in a dielectric structure, which is doubly-periodic in the X-Y plane and of arbitrary variation in the direction of propagation, Z. The fundamental cell is composed of an arbitrarily shaped pore filled with a dielectric and the host by another. This procedure describes the structure of the electromagnetic fields at the micro level and gives an effective medium equation at the macro level. The latter contains a simple arithmetic average of the dielectric constants and a correction term, which involves a line integral around the pore. The integrand of this integral depends upon the polarization of the wave and the solution to a canonical potential problem. In this paper we present a boundary integral method which produces an accurate approximation of the solution to this canonical potential problem. Our method depends upon a fast and accurate compilation of the periodic Green's function on a rectangular lattice. Although we only consider circular pores of arbitrary radius, more complicated geometries can be tackled. Finally, we compare our results with certain limiting cases and with a one-term variational approximation.

Yogesh Joshi
New Jersey Institute of Technology

Dynamics of Discrete Population Models: Higher Dimensional Pioneer-Climax Models

There are many population models in the literature for both continuous and discrete systems. We begin with a general discrete model that subsumes almost all of the discrete population models currently in use. Some results related to the existence of fixed points are proved. We then concentrate mainly on a 3-dimensional Pioneer-Climax model. Most of the previous studies of such models have been for 1-dimensional or 2-dimensional systems only. An extensive theoretical and computational investigation of the dynamics of discrete 3-dimension Pioneer-Climax models is conducted, including an analysis of fixed and periodic points, bifurcations and chaotic regimes.

Said Kas-Danouche
Universidad de Oriente, Cumaná, Sucre, Venezuela

A Mathematical Model for a Core-Annular Flow with a Moving Coaxial Rod

The nonlinear stability of core-annular flows with a moving coaxial rod is considered in the case when the two fluids are immiscibles and confined to an infinite cylinder of radius R. A full problem is derived carring out an asymptotic solution of the problem when the annulus is thin with respect to the core thickness. A nonlinear integro-differential equation which represents the evolution of the interface between the two fluids is obtained. It is interesting to note that such equation without the integral term is known as the Kuramoto-Sivashinsky equation.

Manmeet Kaur
New Jersey Institute of Technology

Acoustic and Fluid Flows on Perturbed Spherical Object

In this study, the time averaged acoustic radiation force and drag on a small, solid nearly spherical object suspended freely in a stationary sound wave field in a compressible, low viscosity fluid is to be calculated. This problem has been solved for a spherical object, and it has many important engineering applications related to segregation and separation processes for particles in fluids such as water. Small but significant errors have occurred in the predicted behavior of the particles using the existing approximate solutions based on perfect spheres. One of the main goals of this research is to extend the classical approach to objects that deviate slightly from spherical shape and to estimate the contributions to the acoustic and drag forces generated by the perturbations in shape.

Jin Sun Kim, Yu-Hau Tseng, Shuwang Li, and John Lowengrub
University of California-Irvine

Efficient and Accurate Numerical Algorithms for Simulating the Dynamics of Inextensible Vesicles in a Viscous Fluid

We investigate the nonlinear coupling between flow and vesicle morphology. Due to its highly flexible structure and forces involves in the system, a vesicle adopts a variety of morphologies. Here, we present efficient and accurate numerical methods for the evolution of inextensible vesicles in a Stokes flow. The dynamics of the interface is driven by bending force which involves not only the curvature but the second derivative of the curvature. This high-order term induces severe stability restriction to use explicit time discretization. However, there are many efficient methods have been developed for this issue in recent years. In this poster, we use the Small Scale Decomposition method proposed by [Hou, Lowengrub, and Shelley 1994] to remove the stiffness in the computation. First, the governing equations for this dynamical system are written in the tangent angle and arclength variables. Second, we use a boundary integral method (BIM) and an immersed boundary method (IBM) for the fluid to provide the normal velocity on the interface. The result of the BIM and IBM are compared and contrasted. Then by using the small scale decomposition of normal velocities in both approaches, we can obtain a non-stiff time-stepping method to simulate this system. In this poster, we also provide biological motivations and background, the mathematical formulation, a brief description of the numerical methods, some benchmark tests and interesting numerical results.

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Feedback to Descending Projection Neurons Can Override the Mechanisms Underlying Rhythmic Pattern Generation in the Target Network: A Modeling Study

Rhythmic motor networks are generally studied assuming a feed-forward architecture in which descending inputs from projection neurons initiate, terminate or modify the network output. Feedback from the target network to descending inputs is nonetheless pervasive in motor pattern generation, although its role is not well understood. We developed a mathematical model to understand how rhythmic feedback to a descending projection neuron shapes the output of the gastric mill (chewing) motor circuit in the stomatogastric ganglion (STG) of the crab C. borealis. Stimulating the projection neuron MCN1 elicits a gastric mill rhythm (GMR) in vitro, where the protractor LG neuron bursts in antiphase with the retractor neuron INT1 (Coleman et al, 1995 Nature). The half-center oscillation of the reciprocally inhibitory LG-INT1 pair underlies the MCN1-elicited GMR. Co-activation of MCN1 and the projection neuron CPN2 elicits a distinct GMR. The STG terminals of CPN2 are electrically coupled to the LG neuron, while the CPN2 soma is inhibited by a feedback synapse from INT1. Previous experiments indicated that the MCN1/CPN2-GMR persists without the inhibitory synapse from INT1 to LG, but the MCN1-GMR requires the presence of that synapse (Akay et al, 2004 SfN Abstract). We use a reduced mathematical model in parallel with a biophysically-detailed model to elucidate the mechanisms that enable the MCN1/CPN2-GMR (but not the MCN1-GMR) to persist without INT-LG reciprocal inhibition. First, we show that both GMRs are driven by modulatory input from MCN1 to LG. However, the MCN1/CPN2-GMR exhibits a slower frequency due to electrical coupling of the CPN2 axon terminals to LG. Next, we show that INT1 feedback to CPN2 causes the MCN/CPN2-GMR to persist without the INT1 to LG inhibitory synapse. In contrast, the MCN1-GMR, which does not involve feedback to CPN2, is disrupted without the INT1 to LG synapse. Interestingly, in the absence of reciprocal inhibition, the GMR cycle frequency is not regulated by the previously documented local input from the pyloric circuit (Bartos et al, 1999 J Neurosci). We conclude that network feedback to projection neurons can move the locus of pattern generation from a half-center oscillator to an excitation-feedback circuit, which in turn can alter inter-circuit interactions.

Martin Klein
University of Maryland, Baltimore County

Physiologically Based Pharmacokinetic Modeling: Overview and Statistical Issues

Physiologically based pharmacokinetic (PBPK) modeling provides a mathematical means to simulate the time courses of chemicals and their metabolites throughout the body. In this presentation I will first illustrate the basic principles behind this type of modeling by presenting one particular PBPK model in detail. Next I will show how one can use an appropriate PBPK model to carry out a statistical analysis of pharmacokinetic data. In general, pharmacokinetic data describe absorption, distribution, metabolism, and/or excretion of some chemical to which a subject is exposed. The PBPK model itself consists of a system of (nonlinear) ordinary differential equations (ODEs) and algebraic equations. These models are "physiologically based" because as we will see, the model consists of several inter-related compartments corresponding to bodily tissues such as fat, liver, blood, muscle, etc. To conclude the presentation, I will describe some of the statistical issues involved in the analysis of pharmacokinetic data using PBPK models.

Dong-Wook Lee
Texas Tech University

Traveling Wave Solutions in KdV Equation with a Higher-Degree Nonlinear Term

We first show exact analytical solution of single-degree-of-freedom (SDOF) oscillator whose spring force is quintic in displacement. When we consider multi-degree-of freedom oscillator with quintic nonlinearity, this problem is equivalent to new

Fermi-Pasta-Ulam (FPU) model which has quintic force. When we take the continuum limit of this FPU model, we obtain partial differential equation which models longitudinal vibration of rod. This equation is a new kind of Korteweg-de Vries (KdV) equation. Robert M. Miura suggests this equation as an open problem. We found some traveling wave solutions for this new KdV equation. These soliton solutions come from SDOF oscillator solutions.

Shenghua Li

Virginia Tech

Integrated Dynamics of Temporal Controls in the Cell Division Cycle of Caulobacter Crescentus

Caulobacter crescentus is an important model organism for studying the regulation of cell division cycle and cellular differentiation in prokaryotes. Caulobacter undergoes asymmetric division producing two progeny cells with identical genome but different developmental programs: the "swarmer" cell is flagellated and motile, and the "stalked" cell is sessile. Only stalked cells undergo chromosome replication and cell division. Swarmer cells must shed their flagellum and grow stalks before they can enter the replication-division cycle. Based on published experimental evidence, we propose a molecular mechanism for cell cycle control in this bacterium. Our mathematical model predicts detailed temporal dynamics of regulatory gene expression during the cell cycle and differentiation process of wild-type cells (both stalked cells and swarmer cells) as well as several mutant strains. The simulation presents a unified view of temporal regulation of protein activities during the asymmetric cell division cycle of Caulobacter. It helps to interpret phenotypes of known mutants and predict novel ones. The quantitative model can serve as a starting point for investigating the regulation of cell division and differentiation in other genera of alpha-proteobacteria, such as Brucella and Rhizobium, because recent experimental data suggest that these alpha-proteobacteria share similar genetic mechanisms for cell cycle control.

Changwon Lim

University of North Carolina-Chapel Hill

Robust Statistical Inference for Nonlinear Regression Models with Application to Toxicology Data

Often in toxicological studies, researchers are interested in investigating the dose-response relationship when rodents are exposed to varying doses of a chemical. Usually a non-linear regression model such as a Hill model is used to describe the relationship. However, toxicological studies are typically limited by the number of animals used at each dose. Furthermore, depending upon the design of the study and the end-point of interest, homoscedasticity across the dose levels may not hold. The ordinary least squares method is generally nonrobust for heteroscedastic models while iteratively weighted least squares methods are computationally cumbersome and may generally be less efficient when homoscedasticity prevails to a certain extent. As such, a preliminary test estimator (PTE) is proposed and its asymptotic properties are studied. Alternative robust (M-)estimators are also studied and bootstrap procedures are explored. The methodology is illustrated with a toxicology dataset.

Stefan Maehlmann

New Jersey Institute of Technology

Electric Field Effects on the Buoyancy-Driven Motion of a Gas Bubble through a Quiescent Liquid

The effects of an electric field on the buoyancy-driven motion of a single gas bubble through a quiescent liquid are numerically investigated. A system of two perfectly dielectric mediums with different dielectric constants is considered. The electric force acts only at the interface, and is zero is the bulk of the two fluids. The mathematical model to solve the free-boundary problem relies on the level-set technique coupled with a finite difference solution of the Navier-Stokes equations. Surface tension forces and electric forces are incorporated into the momentum equations by using the continuous surface force model. A multigrid approximation is applied to the Poisson equation for the pressure field and the Laplace equation governing the electric field potential. We describe the details of the method of solution and present the results of our numerical experiments on the effects of electric fields, inertia and surface tension on the dynamics of the bubble motion as function of Reynolds number, viscosity ratio, and electric Bond number.

Kamyar Malakuti, Michael Siegel, Alexandr Virodov, and Nan Pwint Maung
New Jersey Institute of Technology

The Numerical Analysis of Singular Solutions to Partial Differential Equations

Singularities often occur in solutions to partial differential equations; important examples include the formation of shock fronts in hyperbolic equations and self-focusing type blow up in nonlinear parabolic equations. Information about formation and structure of singularities can have significant theoretical importance. For example, the question of singularity formation for the 3D Euler equations of incompressible inviscid flow has important implications in turbulence, and has been an open problem for more than a century. In this paper, we present a new method for the numerical analysis of complex singularities in solutions to partial differential equations. In the method, we analyze the decay of Fourier coefficients using a numerical form fit to ascertain the nature of singularities in two and three-dimensional functions. Our results generalize a well known method for the analysis of singularities in one-dimensional functions to higher dimensions. As an example, we apply this method to analyze the complex singularities for the 2D inviscid Burger equations.

Vahagn Manukian
North Carolina State University

Traveling Wave for a Thin Liquid Film with Surfactant on an Inclined Plane

We show the existence of traveling wave solutions for a lubrication model of surfactant-driven flow of a thin liquid film down an inclined plane, in various parameter regimes by using geometric singular perturbation theory.

Judith R. Miller
Georgetown University

Inferring Selection on a Quantitative Trait in a Subdivided Population

Evolution by natural selection is a fundamental principle in biology, yet not all changes in plant or animal populations are due to selection. A major goal in evolutionary ecology is to be able to tell whether selection is responsible for differences between two populations of the same species in different locations. We discuss a currently popular statistical test for detecting the action of selection on a quantitative trait, that is, a trait like height or weight that can vary continuously and reflects contributions from many different genes. The theoretical basis of this test turns out to be questionable in a number of settings. We also propose a test that may improve power and accuracy by taking advantage of our rapidly increasing ability to collect detailed genetic information on large numbers of individuals. Joint work with M. Hamilton, B. Wood, and S. Leviyang (Rottenstreich).

Derek E. Moulton and John A. Pelesko
University of Delaware

Collapsing Bubble Systems and the Influence of an Electric Field

We explore the dynamics of bubbles deflating through tubes and subjected to an applied electric field. These systems have potential relevance in areas such as mushroom spore dispersal and optical microlens devices. The effect of added electrostatic pressure on a single bubble collapse is explored theoretically and experimentally. Differential equations describing the size of the bubble as a function of time are derived and analyzed. Systems of two bubbles connected via a common tube are also considered. Here, differences in surface tension and electrostatic forces between bubbles interact as bubbles compete for a fixed volume of air. The solution structure is fully characterized in the two bubble system for arbitrary surface tension and surface charge. Several examples demonstrate the drastic effect of parameters on system dynamics.

Nebojsa Murisic and Lou Kondic
New Jersey Institute of Technology

"Octopus"-shaped Instabilities of Evaporating Drops: Experiments and Theory

The motivation for this work stems from curious phenomena recorded in semiconductor industry. We report on instabilities during the spreading of volatile liquids, with emphasis on the novel instability observed when isopropyl alcohol (IPA) is deposited on a mono-crystalline Si wafer. The instability is characterized by emission of smaller drops ahead of the expanding front, with each smaller drop followed by a cloud of even smaller satellite droplets, forming structures which we nickname "octopi" due to their appearance. A less volatile liquid (DIW), or a solid having larger heat conductivity (Cu), are found to suppress this type of instability. We formulate a theoretical model, based on Navier-Stokes equations, and use lubrication approximation to obtain the equation for evolution of drop thickness. Linear stability analysis (LSA) of the full equation tells us that, indeed, IPA/Si set-up is most unstable. Finally, we compare our numerical results to experimental data. We find that our model reproduces the main features of the experiment, and relate them to evaporation induced Marangoni effects and thermal conductivity of both liquid and solid.

S. Nudurupati[1], M. Janjua[1], N. Aubry[2], and P. Singh[1]
[1] New Jersey Institute of Technology, [2] Carnegie Mellon University

Transport and Deformation of Droplets in a Micro-Device using Dielectrophoresis

In microfluidic devices fluid can be manipulated either as continuous streams or droplets. The latter is particularly attractive as individual droplets can not only move but also split and fuse, thus offering great flexibility for applications such as laboratory-on-a-chip. We consider the transport of liquid drops immersed in a surrounding liquid by means of the dielectrophoretic force generated by electrodes mounted at the bottom of a microdevice. The direct numerical simulation (DNS) approach is used to study the motion of droplets subjected to both hydrodynamic and electrostatic forces. Our technique is based on a finite element scheme using the fundamental equations of motion for both the droplets and surrounding fluid. The interface is tracked by the level set method and the electrostatic forces are computed using the Maxwell stress tensor. The DNS results show that the droplets move, and deform, under the action of non-uniform electric stresses on their surfaces. The deformation increases as the drop moves closer to the electrodes. The extent to which isolated drops deform depends on the electric Weber number. In the case of a small ratio, the drops remain spherical; otherwise, the drops stretch. Two droplets, however, that are sufficiently close to each other, can deform and coalesce, even if the electric Weber number is small. This phenomenon does not rely on the magnitude of the electric stresses generated by the bulk electric field, but instead is due to the attractive electrostatic drop-drop interaction overcoming the surface tension force. Experimental results are also presented.

Myongkeun Oh and Victor Matveev
New Jersey Institute of Technology

Alternating-Order Dynamics in Non-Weakly Coupled Two-Cell Inhibitory Networks

Inhibitory networks of weakly-coupled type-I model neurons can exhibit a transition from synchronous dynamics to alternating-order ("leap-frog") activity in response to an increase in synaptic coupling strength, whereby the spiking order of the coupled model cells changes in each cycle of the oscillation. This loss of synchrony is a result of a transient suppression of the post-synaptic cell below its excitability threshold, the saddle-node bifurcation, allowing the pre-synaptic cell to bypass it along the limit cycle trajectory. Here we describe the phase-space geometry of alternating-order activity, and examine the conditions for its existence and stability. We find that non-zero synaptic decay time is crucial for leap-frog firing in a network of limit cycle oscillators, and that the change in the firing order relies on the slow dynamics of each cell along the sub-threshold portion of the limit cycle. However, we show that order alternation can also be obtained in a purely pulse-coupled network of non-limit cycle oscillators such as quadratic integrate-and-fire model cells with asymmetric threshold and reset values. These results contribute to a better understanding of highly non-trivial synchronization properties of excitable cells, important for the study of neural circuit dynamics.

Andrew Oster

Mathematical Biosciences Institute, Ohio State University

Mitochondrial Excitability via the Permeability Transition Pore

In the study of calcium waves, the endoplasmic rheticulum (ER) and its IP3 mediated calcium induced calcium release (CICR) mechanism has dominated the spotlight. However, more than the ER can display this type of excitability. The oft-times overlooked (in regards to Ca2+ signaling) mitochondria also exhibit CICR via the permeability transition pore (PTP). In this paper, we extend the well-known Magnus-Fall-Keizer mathematical model for the Ca2+ dynamics between the ER, the cytosol, and the mitochrondria to include dynamics due to the PTP. Three key components come into play: non-steadystate mitochrondrial proton concentration, the permeability transition pore, and a weak-acid term that is essential for robust mitochondrial homeostasis. We show that, with these simple additions, the model exhibits mitochondrial CICR (mCICR). Furthermore, we extend the model from a single point to a spatially extended system and find traveling waves of both Ca2+ and potential, as found by Ichas et al. in 1997. In addition, the model also captures the pore "popping" event whereby the pore opens to and remains in a high-conductance state, which ultimately leads to apoptosis or necrosis due to calcium cytotoxicity.

Omar Padron, Christopher Costoso, and Edward Farnum

Kean University

Simulation of Nonlinear Mode-Locked Lasers in Fiber Optic Medium

Fiber optics has offered many improvements in telecommunications, especially with respect to the rate at which information is sent. Haus's Master Mode Locking Equation offers much insight into the existence and stability of light pulses in an optical fiber. We present a theoretical model based on the Haus's equation to describe the behavior of a laser source subject to wavelength division multiplexing. Depending upon values for system parameters describing gain saturation and nonlinear coupling between channels, the system may support a variety of solution types. These include simultaneously mode-locked pulse solutions and pulse splitting in one or more frequency channels. Of particular interest is how the stability of these mode-locked solutions depends upon various system parameters, including inhomogeneity in the gain saturation, gain bandwidth mismatch, and strength of inter-channel coupling terms due to cross-phase modulation. We explore these models primarily through numerical simulations in an effort to characterize these dependencies for a number of different frequency channels. Ultimately, these models may serve to guide the future engineering of super fast, mode-locked pulses of light to be used as optical bits, and further increase data transfer rates.

Anisha Panda and Robert M. Miura

New Jersey Institute of Technology

Mathematical Modeling of Spreading Depression

Leao first observed Spreading Depression (SD) in 1944. It is a slowly traveling wave phenomenon elicited in the cortex of various brain structures in many different animals. It is characterized by depression of electroencephalographic activity. The wave is accompanied by increased blood flow and is followed by a period of vasodilation. The wave propagates with a speed of 1-15 mm/min. SD has been shown to be the underlying physiological process that causes migraine with aura in some patients. The various factors affecting SD are ionic currents, pumps, neurotransmitters, spatial buffering, and osmosis. In our model we include different ionic currents, which are believed to have important effects on SD. We then introduce the phenomenon of spatial buffering. We consider a two-dimensional model of a circular cell and model spatial buffering using diffusion equations and the cable equation for describing the electrotonic spread of membrane potential. The aim of our model is to study how the excess K+ ions redistribute themselves in the ECS during spatial buffering. Finally, additional factors due to osmosis and glial cells are to be included in our model of SD.

F. Posta, S. Y. Shvartsman, and C. B. Muratov

New Jersey Institute of Technology

Compensated Optimal Grids for Elliptic Boundary-Value Problems

A method is proposed which allows to efficiently treat elliptic problems on unbounded domains in two and three spatial dimensions in which one is only interested in obtaining accurate solutions at the domain boundary. The method is an extension of the optimal grid approach for elliptic problems, based on optimal rational approximation of the associated Neumann-to-Dirichlet map in Fourier space. It is shown that, using certain types of boundary discretization, one can go from second-order accurate schemes to essentially spectrally accurate schemes in two-dimensional problems, and to fourth-order accurate schemes in three-dimensional problems without any increase in the computational complexity. The main idea of the method is to modify the impedance function being approximated to compensate for the numerical dispersion introduced by a small finite-difference stencil discretizing the differential operator on the boundary. We illustrate how the method can be efficiently applied to nonlinear problems arising in modeling of cell communication.

Juri Rappoport

Russian Academy of Sciences

Biostatistics of Cornea HumanTtransplants

The results of the total penetrating keratoplastics on human eyes are analyzed. The endothelium and morphology characteristics are considered in time and dynamics. The statistical prognosis for the patient's vision after the surgery is given.

Bo Ren, William J. Morokoff, and David J. Horntrop

New Jersey Institute of Technology

Multistep Simulation Methods for Collateralized Debt Obligations

Collateralized Debt Obligations (CDOs) are an important class of asset-backed securities. They offer investment opportunities with different risk-return profiles which are referred to as tranches. A key component of modeling of these securities is understanding the correlation and temporal dependence of defaults in order to capture the relationship between the performance of the tranches and the underlying risk of the portfolio. Here we review the fundamentals of CDO tranches and then describe a new multistep simulation approach which can accurately and efficiently track the dynamic properties of CDO cash flows.

Joseph Rhoads

Florida State University

Parallel Biological Simulations on the Graphics Processing Unit

Electrophysiological simulations and parameter estimation are areas where massively parallel simulations can have a profound impact. One method for massively parallel simulations is a network of computers. Here we describe an alternative method for massively parallel biological simulations using the Graphics Processing Unit (GPU). We are able to run Excitable cell systems with thousands of cells in parallel on the GPU at a fraction of the time required for serial simulations on a workstation. We will discuss applications of the GPU to areas such as parameter searching and simulations of networks of coupled neurons.

Ravinder Singh

Indian Institute of Technology, Kanpur, India

Linear Stability of Gyrotactic Plume

The problem considered here is that of linear stability of a gyrotactic infinitely long plume in cylindarical geometry. We have applied the linear stability theory, in which a typical disturbance is expressed as normal mode analysis. Both types of disturbances are considered: axisymmetric (or varicose) and asymmetric (meandering). It is has been found that these instabilities dominate one another depending on the wavelength and parameters of the problem. The linear stability analysis predicts that meandering instability dominates the varicose instability for long wavelengths but at short wavelengths varicose dominates the meandering. At sufficiently large wavenumbers plume is unconditionally stable. The effect of all the important parameters of the problem is also examined on stability of the plume in both cases.

Ana Maria Soane

University of Maryland, Baltimore County

Variational Problems in Weighted Sobolev Spaces with Applications to Computational Fluid Dynamics

We study variational formulations for the Poisson and Helmholtz problems in weighted Sobolev spaces, on bounded domains with corners. We prove existence and uniqueness of solutions in these spaces, establish the connection to classical theory, formulate a finite element approximation with C^1-compatible elements and prove convergence of these finite element approximations. The specific forms of our variational formulations are motivated by, and applied to, a finite element scheme for the time-dependent Navier-Stokes equations. Our goal is to extend the numerical scheme for the Navier-Stokes equations developed by Liu, Liu, and Pego (``Stability and convergence of efficient Navier-Stokes solvers via a commutator estimate'', CPAM 2007) to non-smooth domains. Their algorithm, which calls for solving a Poisson problem in H^1 for pressure and a Helmholtz problem in H^2 for velocity at each discretized time step, converges and is unconditionally stable on domains with sufficiently smooth boundaries. A naive application of the algorithm in non-convex polygonal domains (flow over a step, for example) produces incorrect solutions because the velocity field is not in H^2 near reentrant corners. We propose a modified version of the algorithm that applies appropriate weights near reentrant corners to compensate for singularities. Numerical results obtained this way show good agreement with those obtained by the usual H^1 methods.

Sundar Subramanian

New Jersey Institute of Technology

The Missing Censoring Indicator Model and the Smoothed Bootstrap

In survival studies, death certificate information can be missing, or incidental and fatal occurrences may be indistinguishable for some subjects, leading to missing censoring indicators. For the framework of right censored data with missing censoring indicators, sub-density function kernel estimators play a significant role in the estimation of a survival function. Data-driven bandwidths for computing these kernel estimators are proposed. The bandwidths are obtained as minimizers of certain estimates of the mean integrated squared error (MISE). It is shown that the smoothed bootstrap offers a motivation for choosing the proposed MISE estimates for minimization. The efficacy of the proposed procedures is investigated through several simulation studies. Two illustrations are provided.

Dmitri Tseluiko

University of East Anglia, Norwich, United Kingdom

Steady Electrified Film Flow Down an Indented Wall

We investigate the effect of an electric field on a liquid film flowing down an inclined, corrugated wall at zero Reynolds number. The film is taken to be either a perfect conductor or a perfect dielectric. The region above the film is assumed to be a perfect dielectric. Using a long-wave asymptotic analysis, we derive a nonlinear, non-local equation for the thickness of the liquid film and compute steady solutions over rectangular downward and upward steps and into rectangular trenches and over rectangular mounds. In the absence of an electric field, the film develops a capillary ridge above a downward step and a depression in front of an upward step. For a perfect-conductor film, the results show that as the electric field strength increases, there appear short-wave oscillations upstream of a downward step, the height of the capillary ridge decreases, and a depression right downstream of the step is introduced. At an upward step, imposing an electric field leads to the creation of a free-surface ridge downstream of the step and introduces short-wave oscillations upstream of the step. Solutions for a perfect-dielectric film are similar to those for a perfect-conductor film, although the height of the capillary ridge varies non-monotonically with the electric field strength. Using a small-step-height asymptotic analysis for the long-wave model and for the full Stokes flow problem, we obtain some insight into the mechanisms responsible for the flow features. This analysis not only provides a qualitative explanation of such features as the appearance of short-wave oscillations upstream of a downward/upward step when an electric field is introduced but also gives analytical estimates for the quantitative characteristics of these features, e.g. for the wavelength and the amplitude of the oscillation. The results are corroborated by fully nonlinear boundary-element calculations for Stokes flow.

Gisela Tunes-da-Silva
Medical College of Wisconsin

Regression Analysis of Mean Quality-Adjusted Survival Time Based on Pseudo-Observations

Regression models for the mean quality-adjusted survival time are specified from hazard functions of transitions between two states and the mean quality-adjusted survival time may be a complex function of covariates. We discuss a regression model for the quality-adjusted survival (QAS) time based on pseudo-observations, which has the advantage of directly modeling the effect of covariates in the QAS time. Both Monte Carlo simulations and a real data set are studied.

C. Arturo Vargas
Universidad Nacional Autonoma de Mexico

Evolution of Benjamin-Ono Solitons with a Weak Zakharov-Kutznetsov Lateral Dispersion

The effect of weak lateral dispersion of Zakharov-Kutznetsov type on a Benjamin-Ono solitary wave is studied asymptotically and numerically. The asymptotic solution is based on a approximate variational solution for the solitary wave, which is then modulated in time through the use of conservation equations. The effect of the dispersive radiation shed as the solitary wave evolves is also included in the modulation equations. It is found that the weak lateral dispersion produces a strongly anisotropic, stable solitary wave which decays algebraically in the direction of propagation, as for the Benjamin-Ono solitary wave, and exponentially in the transverse direction. It is found that the initial conditions with amplitude above a threshold evolve into a solitary wave while those with amplitude below the threshold evolve as lumps for a short time, then merge into radiation. The modulation equations are found to give a qualitatively accurate description of the evolution of an initial condition into an anisotropic solitary wave. Coauthors: J.C. Latorre, A.A. Minzoni, and N.F. Smyth.

Qiming Wang and Demetrios T. Papageorgiou
New Jersey Institute of Technology

Micro-Thread Formation in Conducting Viscous Liquid Threads under the Action of Radial Electric Fields

We study theoretically the stability of highly viscous conducting liquid jets or threads under the action of a radial electric field. The field is generated by a potential difference between the jet surface and a concentrically placed electrode of given radius. We develop a long-wave nonlinear model that is used to predict the dynamics of the system and in particular to address the effect of the radial electric field on jet breakup. Two canonical regimes are identified that depend on the size of the gap between the outer electrode and the unperturbed jet surface. For relatively large gap sizes, long waves are stabilized for sufficiently strong electric fields but remain unstable as in the non-electrified case for electric field strengths below a critical value. For relatively small gaps, an electric field of any strength enhances the instability of long waves as compared to the non-electrified case. We carry out numerical simulations based on our nonlinear models to describe the nonlinear evolution and terminal states in these two regimes. We find that jet pinching does not occur irrespective of the parameters. We identify regimes where capillary instability leads to the formation of stable quasi-static microthreads (connected to large main drops) whose radius decreases with the strength of the electric field. The generic ultimate singular event described by our models is the attraction of the jet surface towards the electrode and its contact with the electrode in finite time. A self-similar closed form solution is found that describes this event with the interface near touchdown having a cusp geometry locally. The theory is compared with the time-dependent simulations with excellent agreement.

Xinli Wang and Michael Siegel
New Jersey Institute of Technology

Simulation of Drops Rolling on an Inclined Super-Hydrophobic Plane

Recent improvements in the fabrication of extremely rough surfaces has led to the creation of super-hydrophobic surfaces. Experiments show that a drop resting on a super-hydrophobic surface has a very large contact angle (near 180 degrees). Also, viscous drops roll down a super-hydrophobic plane, in contrast to the usual sliding motion of drops on planar surfaces. The rolling motion has the ability to clean efficiently a dirty surface, which is very useful in engineering applications. We present a numerical study of rolling viscous drops by applying a boundary element method to the free boundary problem. Mathematically it is complicated because of the presence of a stress singularity at the contact line. There are several proposed ways to remove this singularity. One way commonly applied is a slip model; the other one, which has received much less attention, is to set the contact angle to be 180 degrees. We are interested in the second way. Numerical results are presented which agree with a simple scaling theory for drop motion and show that, for small drops, the drop velocity decreases as the drop size increases; the rolling velocity does not depend on the drop size for large drops. Also we present numerical evidence that there is no singularity at the contact line if the contact angle is 180 degrees.

Yunjiao Wang

University of Manchester, United Kingdom

Oscillations in the NF-kB Signaling Pathway

NF-*k*B oscillations were suggested by Hoffmann *et al* from electro-mobility shift assays (EMSA) in population studies of I*k*Bα-/- embryonic fibroblasts and simulated in a computational model. NF-*k*B oscillations were also observed by Nelson *et al* at the single cell level. The Hoffmann model gave a fairly good prediction of Nelson *et al* oscillatory experimental data using fluorescent proteins. It is commonly remarked that oscillatory behaviour can be accounted for by the existence of negative feedback loops. As a mathematical exercise, it is certainly possible to set up a simple system with a negative feedback loop that exhibits oscillatory behaviour resembling that observed in the experiments. However, different models with different structures can show similar dynamical behaviour. We argue that in order to understand the biological mechanism (of NF-*k*B signalling pathways in this case), it is necessary to work on models which are based on experimental data. Hoffmann's computational model consists of 24 coupled, nonlinear rate equations (with 64 parameters). We shall study the observed dynamical behaviour of this model using a combination computational and analytical methods. One outcome of this work will be a more detailed explanation of the source of the observed oscillations. We find that the computational model can be treated as a fast-slow system where the level of total I*k*B Kinase (IKK) is treated as a slow variable. If we consider the limit in which the level of total IKK does not change at all, then we can take the level of total IKK as a parameter. Since the total NF-*k*B is conserved in the model, we can also view the total NF-*k*B as a parameter. If the actual variation of IKK is suffciently slow, then orbits in the true system trace attractors in the reduced model. We find that for some range of the level of NF-*k*B, the reduced system experiences Hopf bifurcation twice while varying the level of total IKK. The damped oscillations observed in the computational system come from the existence of stable limit cycles and stable spirals in the reduced system family.

Tao Wu, X. Sheldon Wang, Hongya Ge, and Barry Cohen

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A Molecular Dynamics Modeling of Sickle-Cell Anemia

Sickle cell anemia is the first disease whose genetic cause was pinpointed at the DNA level. Sickle cell disease is caused by the switch of a single DNA base pair in the hemoglobin gene from A to T, which in turn changes an amino acid in the hemoglobin protein from glutamic acid to valine. Normal hemoglobin at this location is slightly hydrophilic and tends to form a protective layer of surrounding water molecules. Hemoglobin molecules, which are located in red blood cells and which play a role in oxygen transport, assume a globular, or beadlike, shape. Their protective water coating tends to keep them separate from other hemoglobin molecules. In the mutated hemoglobin molecule, one normally hydrophilic spot becomes slightly hydrophobic and, in a deoxygenated state, tends to lose its protective layer of water molecules. The hemoglobin molecules consequently stick together and form a chain of hemoglobin beads. Moreover, such chains form bundles, eventually causing the red blood cell membrane, which is normally flexible and fluid, to become stiff and sticky. In the end, sickle cells tend to block capillary vessels and cause sickle cell anemia. In this paper, we present a molecular dynamics model of the mutated hemoglobin molecule. Ultimately, we will use this red blood cell system (sickle or normal) to build a multi-scale and multi-physics modeling procedure ranging from molecular dynamics modeling of protein-protein interactions to immersed boundary/continuum methods for moving adhesive particles and soft fluid-solid continua.

Zhanghan Wu

Virginia Tech

Theoretical Modeling of the Mircrotubule Assembly Process

Microtubules, one of the three kinds of cytoskeleton components, play important roles in many eukaryotic cellular processes, including intracellular transporting, cell motility, meiosis and mitosis. It is widely accepted that the αβ-tublin dimers add onto the growing end of a microtubule one by one during the assembly process. However, recent experimental results suggest an alternative mechanism, where tublins first form a two-dimensional open sheet, which in turn closes into tubes (Wang & Nogales, 2005, Nature, 435:911-915). Cryo-EM studies show that within the two-dimensional sheet structure, two types of lateral interactions alternate between neighboring protofilaments. How is the sheet structure formed? Is this form physiologically relevant? Currently these are highly controversial and heatedly debated questions. We are addressing these problems using statistical thermodynamics analysis, coarse-grained stochastic dynamics simulations, and atomistic level energetic analysis. The results are consistent with observed experimental data in Nogales lab.

Arjun Singh Yadaw

Indian Institute of Technology, Kanpur

A parameter-uniform Ritz- Galerkin finite element method for singularly perturbed delay differential with delay in convection term

In this paper, we have presented a Ritz-Galerkin finite element method for solving a class of singularly perturbed delay differential equation with small delay in convection term. We have taken a piecewise-uniform fitted mesh (Shishkin mesh) to resolve the boundary layer and used hat functions as a basis function for the given method which leads to a tridigonal linear system. The convergence analysis is given and the method is shown to have almost second order parameter uniform convergence. Several numerical examples are solved using the presented method, compared the computed result with exact solution and plotted the graphs of the solution of the problems.

Ye Yang and Sheldon Wang

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A Three-Field Mixed Finite Element Formulation for Acoustoelastic/Slosh Fluid-Structure Interaction Systems

In this research, we employ a three-field mixed finite element formulation with displacement, pressure, and vorticity unknowns. This formulation is capable of handling complex fluid-solid systems with both immersed flexible structures and the free surface. The numerical examples will demonstrate that if primary slosh, structural, and acoustic modes are within separate frequency bands, this mixed formulation will be able to predict these frequencies and mode shapes. However, the key attribute of this formulation is to compute the coupled frequencies without the contamination of nonphysical spurious nonzero frequencies. Our numerical examples will also show that by imposing external forces with different coupled frequencies, predominant slosh, structural, and acoustic motions can be introduced to this fluid-solid system.

Yuan-nan Young

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Modeling of the Actin Filament Motion on Myosin Motility Assays

In motility assays, cytoskeletal actin filaments (actin filaments) glide over a surface coated with motor proteins, and the different modes of motion provide a simple measure of the force exerted by the motor proteins (Bourdieu, 1995). Motivated by these experiments, we consider the actin filament as a slender, elastic filament immersed in Stokesian flow, driven by a tangential forcing that mimics the force by the motor proteins. We find qualitative agreement on several points between our analysis and simulations and experimental observations. Furthermore, we study the correlation between filament transport and the characteristics of motion with the spatial pattern of motor protein density. This is joint work with Mike Shelley at Courant Institute.

HaijunYu
Purdue University

A Sparse Grid Method for Boltzmann Equation

The Boltzmann equation is among the most fundamental equations in mathematical physics. However, its numerical approximation is very challenging due to its high dimensionality. Traditional grid-based methods such as finite difference and finite elements are not suitable for high dimensional problems. Monte Carlo Methods are powerful tools for dealing with high dimensional problems but they suffer from low accuracy and noisy outputs. In this talk, we present a numerical method based on sparse grids for the Boltzmann equation. In particular, we develop an efficient sparse grid method for unbounded domains and apply it to the six-dimensional Boltzmann-BGK equation.

Qin Yu
University of Rochester Medical Center

Comparing Multiple Sensitivities and Specificities with Different Diagnostic Criteria: Applications to Sexual Abuse Research and Studies of High-Risk Sexual Behavior

When comparing sensitivities and specificities from multiple diagnostic tests particularly in biomedical research, the different test kits under study are applied to groups of subjects with the same disease status for a disease or medical condition under consideration. Although this process gives rise to clustered or correlated test outcomes, the associated inference issues have well been discussed in the literature. In mental health and psychosocial research, sensitivity and specificity have also been widely used to study the reliability of instrument for diagnosing mental health and psychiatric conditions and assessing certain behavioral patterns. However, unlike biomedical applications, outcomes are often obtained under varying reference standards or different diagnostic criteria, precluding applications of existing methods for comparing multiple diagnostic tests to such a research setting. We develop a new approach to address the problems including missing data by extending recent work on inference using inverse probability weighted estimates. The approach is illustrated with data from two studies in sexual abuse and health research as well as a limited simulation study, with the latter to study the performance of the proposed procedure.

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Using Recursive and Genetic Algorithms to Explore How Intrinsic Properties Affect Neurons' Activity Phase Following Inhibitory Input

Bursting oscillations occur in many neurons and other cell types and underlie rhythmic activity in many networks of the central nervous system. The transient potassium A-current is present in most neurons and plays an important role in determining the onset of rhythmic activity. The prototypes of our research are the follower pyloric constrictor (PY) neurons in the rhythmically active crustacean pyloric network. We build a 3-variable model to examine the role of the A-current on the activity phase of a follower neuron in a rhythmic feed-forward inhibitory network. The precise influence of the A-current in setting the activity of neurons depends on its interaction with the inhibitory synaptic inputs and with other intrinsic properties of the neuron. By deriving recursive equations, we can calculate the extent of the available A-current over cycles and predict the activity phase of both the model neuron and the real PY neurons. By implementing a Genetic Algorithm search, we have built a multi-compartmental realistic model to simulate the real PY neurons and to verify the predictions of our recursive formulation.

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