

PLENARY SPEAKERS

Pam Cook

University of Delaware, Department of Mathematical Sciences, Newark, DE 19716, cook@math.udel.edu

Mesoscale Modeling and Simulation of Transient (liquid gel) Networks

Many polydisperse entangled materials, such as physically cross-linked gels and biopolymer networks, exhibit "slow" (power-law-like rather than exponential) relaxation. One such class of materials includes concentrated wormlike micellar dispersions. For a range of the ratio of counter ion salt concentration to surfactant concentration the linear response of the materials exhibits Maxwellian, exponential, stress decay. As the counter ion concentration decreases the decay is better described by a stretched exponential at long times, a power law decay at short times. Such power-law-like viscoelastic responses can be captured at the macroscale, by a "fractional" Maxwell model. In order to understand the dynamics of these (fluidic) gels, and to avoid inaccurate closure relationships when constructing continuum-scale models, we model and simulate stochastically at the transient network (mesoscale) level. Model predictions are compared with experimental results and with the predictions of related macroscopic/mesoscale models. Joint work with Yun Zeng (University of Delaware), Lin Zhou (New York City College of Technology), and Gareth McKinley (Massachusetts Institute of Technology).

Daniel F. Heitjan

University of Pennsylvania, Department of Biostatistics, Philadelphia, PA 19104, dheitjan@mail.med.upenn.edu

What They Say and What They Mean: Modeling Misreported Counts

Self-reported count data are subject to a variety of types of measurement error. One distinctive form of error is what we call "heaping", or the tendency of subjects to report round numbers in place of true values. Heaping appears in many types of data—from ages, to numbers of cigarettes smoked, to numbers of sexual partners, to church attendance.

Heaping differs fundamentally from other types of measurement error, and therefore is not amenable to treatment with standard statistical methods for measurement error. Statisticians have made progress on analyzing heaped data by considering it a form of missing or incomplete data. But such methods rely on specification of a "coarsening mechanism", meaning a stochastic model describing how one gets from the true underlying data value ("what they mean") to the observed value ("what they say"). Model parameter estimates can be sensitive to this specification, however; thus when the true mechanism is not known, answers from putative models are unreliable.

In this talk I will describe a unique data set that includes both true and reported values of daily cigarette counts, enabling precise estimation of the coarsening mechanism. Results suggest that cigarette count data are perhaps less accurate than we had believed.

Yvon Maday

Jacques-Luis Lions Laboratory, Pierre and Marie Curie University, 75252 Paris Cedex 05, France ,
maday@ann.jussieu.fr

Some Results on Numerical Analysis (a priori and a posteriori) for Electronic Structure Calculations and Applications

Abstract TBA.

Esteban Tabak

Courant Institute of Mathematical Sciences, NYU, 251 Mercer Street, New York, NY 10012, tabak@cims.nyu.edu

Biological Data through Mathematical Eyes

The statement that we live in a data-rich era holds particularly true in the biological sciences, with the potential to revolutionize both basic science and applications. This talk explores some new ways in which mathematics can help find structure in data and address questions of biological significance. Topics include:

- * Deciding if two populations are significantly distinct and characterizing their difference, with an application to the study of the relation between neurons and behavior in drosophila.
- * Maximum conditional likelihood, applied to the reverse engineering of neuronal signals and biological pathways.
- * Medical diagnosis through fluid-like flows in feature space.
- * Determination of the effect of medical treatment through optimal transport.

MINISYMPOSIUM SPEAKERS

Alejandro Aceves

Southern Methodist University, Department of Mathematics, Dallas, TX 75275, aaceves@smu.edu

Nonlinear Localized Modes in Binary Waveguide Arrays

Since the experimental demonstration in the late 90's by Silberberg and collaborators of light localization in uniform nonlinear waveguide arrays, there has been a long list of theoretical and experimental studies that have followed. Examples include light trapping on defects, Anderson localization and spatio-temporal light bullets generation. The interest in nonlinear photonic systems continues both because of the applications in all optical circuits, but also because of the emergence of new designs based on novel materials. Here, we report the existence and stability properties of a new class of discrete localized modes in nonlinear binary waveguide arrays with alternate positive and negative nearest neighbor coupling. The non-uniformity makes the model depart from the well-known discrete nonlinear Schroedinger equation and instead a discrete coupled mode equation system arises from which localized modes are obtained by numerical and asymptotic methods. For comparison, we also derive a long-wave continuous approximation and characterize the nonlinear continuum bright-dark soliton-like solutions and compare them with the discrete modes.

This work was done in collaboration with Aldo Auditore, Matteo Conforti and Costantino De Angelis from the Dipartimento di Ingegneria della Informazione, Universita' degli Studi di Brescia, Italy.

Nathan Albin

Kansas State University, Department of Mathematics, 234 Cardwell Hall, Manhattan, KS 66506, albin@math.ksu.edu

Advances in Fourier Continuation

The Fourier Continuation (FC) method utilizes an efficient one-dimensional periodic extension to enable the use of Fourier space methods in non-periodic settings while avoiding the Gibbs phenomenon. Due to their accuracy, these methods are especially well-suited to long-range wave propagation and transport problems. This talk will present recent advances in the construction and theory of FC-based solvers and summarize some of the most interesting properties of these solvers, including exceptionally accurate dispersion curves, efficient parallelization, and optimal CFL scaling. Additionally, several example applications to which FC solvers have been successfully applied, including models for ultrasound cancer therapies, scattering of chirped radar signals, and complex fluid flows, will be presented.

Asohan Amarasingham

City College of New York, Department of Mathematics, Convent Avenue at 138th Street, New York, NY 10031, aamarasingham@ccny.cuny.edu

Statistical Repeatability and Timing in Electrophysiology

TBA

Dhammika Amaratunga

Janssen Research & Development, Senior Director and Janssen Fellow in Nonclinical Biostatistics, 920 Route 202, Raritan, NJ 08869, damaratung@yahoo.com

Enriched Ensemble Methods for Classification of High-dimensional Data

A spate of technological advances has led to an explosion of high-dimensional data. One of the challenges of modern statistics is how to deal with this type of data. We will consider data from biomedical research that are characterized by the fact that they are comprised of a large number of variables measured on relatively few subjects. Classification and regression techniques are often used for analyzing this data, both for prediction as well as for identifying combinations of variables associated with response. However, standard methods do not work well in this setting, due to the small sample size and surfeit of variables, a problem sometimes also exacerbated by the presence of non-specific signals. Enriched methods are a way of circumventing these difficulties. We will describe enriched methods, particularly enriched ensemble methods, that work well with this type of data. Real examples will be used to illustrate the methodology. Joint work with Javier Cabrera and others.

Yuriy Antipov

Louisiana State University, Department of Mathematics, Baton Rouge, LA 70803, antipov@math.lsu.edu

Scattering of an Obliquely Incident Electromagnetic Wave by an Impedance Right-angled Wedge

Scattering of a plane electromagnetic wave by an anisotropic impedance concave wedge at skew incidence is analyzed. In the case of a right-angled wedge, by splitting the incident wave into two waves, the one that strikes the vertical wall and the other that impinges upon the horizontal face of the wedge, the two Helmholtz equations coupled by the boundary conditions are reduced to two symmetric order-2 vector Riemann-Hilbert problems (RHPs). The problem of matrix factorization leads to a scalar RHP on a genus-3 hyperelliptic surface. Its closed-form solution is derived by the Weierstrass integrals. Because of the problem symmetry the associated Jacobi inversion problem is solved in terms of elliptic integrals, and the use of the genus-3 Riemann theta function is bypassed. It is shown that the solvability of the physical problem is governed by the number of zeros in the upper half-plane of the product of two quadratic polynomials associated with the two vector RHPs. The coefficients of these polynomials are expressed through the wave number, the impedance parameters and the angle of incidence. A relation between the solution to the vector RHPs and the Sommerfeld integrals is established. In the case when the solution is unique, the reflected, surface and diffracted waves are recovered.

Arvind Baskaran

University of California-Irvine, Department of Mathematics, Irvine, CA 92697, baskaran@math.uci.edu

Kinetic Density Functional Theory: A Mesoscale Model to Study the Effect of Flow on the Freezing of a Pair Potential Fluid

The Classical Density Functional Theory (CDFT) and the Phase Field Crystal (PFC) models have proven to be good approaches to model crystal growth from a fluid phase. These models capture atomic level details including defects and grain boundaries. However these approaches usually involve a phenomenological gradient descent based time evolution and do not take the convection of the fluid phase into consideration. In this talk, we coarse-grain the microscopic equations to obtain a classical kinetic theory governing the freezing of a pair potential fluid. Using the techniques of classical density functional theory, we use a functional expansion about an equilibrium fluid to derive a new, nonlocal model of hydrodynamics that incorporates phase transitions and fluid flow. Using a numerical method for which the discrete energy is non-increasing in time (energy-stable), we perform numerical simulations demonstrating that the model captures the freezing process. Using a simplified PFC-like version of the model, we then investigate how the flow strength affects the phase diagram and influences the maximally stable crystal size. This is joint work with John Lowengrub and Aparna Baskaran.

Andrew Belmonte

Penn State University, Department of Mathematics, University Park, State College, PA 16802, alb18@psu.edu

Non-diffusive Spatial Patterns in Evolutionary Games

Evolutionary games involve the introduction of time into game theory, in the context of populations playing against each other and changing strategies. Spatial degrees of freedom are typically included into the rate equations for strategy evolution (such as the replicator equation) by adding diffusion terms for each strategy. I will discuss a more recent development, with roots in ecological modeling: the inclusion of non-diffusive flux effects, with terms dependent on the payoff matrix itself. Numerical and analytic studies of pattern dynamics will be presented, focusing on 1D travelling wave solutions in the prisoner's dilemma game, and 2D spiral waves in the rock-paper-scissors game. This is joint work with Russ deForest.

Jerzy Blawdziewicz

Texas Tech University, Department of Mechanical Engineering, Box 41021, Lubbock, TX 79409, jerzy.blawdziewicz@ttu.edu

Locomotion of C. elegans: Evolutionary Adaptation and Neuromuscular Control

A millimeter-size nematode *Caenorhabditis elegans* is one of the most important model organisms used for investigations ranging from cellular development to genetics to neurobiology. Since the topology of neural connections of this nematode has been fully mapped out, one can envision a complete reverse engineering of the function of its nervous system. However, this great challenge cannot be met without systematic studies of biophysics of nematode locomotion in complex environments to quantify the interplay of sensing processes, control mechanisms, and mechanical interactions that include frictional, capillary, and hydrodynamic forces. In this talk we will analyze the kinematics of nematode motion, demonstrate that the worms choose optimal gait for crawling and swimming, and describe how they navigate diverse environments ranging from smooth agar surfaces to arrays of

microfabricated pillars. Simple models of neuro-muscular control of nematode body will be presented and used to elucidate chemotaxis mechanisms. We will also analyze gait transition observed in fluids of different viscosities. Such studies have not only a fundamental value, but are also necessary for applications, for example to screen genes associated with neuromuscular diseases. This vast knowledge base will eventually be harnessed to design smart artificial crawlers.

Nicolas Brunel

University of Chicago, Department of Neurobiology, Chicago, IL 60637, nbrunel@uchicago.edu

Collective Oscillations in Networks of Spiking Neurons: Mechanisms and Input Dependence

Collective synchronized oscillations are observed in many brain areas, at a wide range of frequencies and spatial scales. In this talk, I will first review theoretical studies that shed light on possible circuit mechanisms for such oscillations. I will then show how external inputs can switch networks of neurons from asynchronous to synchronous oscillatory states, and compare theoretical results to experimental data from primary visual cortex of monkeys during presentation of a movie.

Ken Cheung

Columbia University, Department of Biostatistics, 722 West 168th Street, New York, NY 10032,

cheung@biostat.columbia.edu

Objective Calibration of the Bayesian Continual Reassessment Method

The continual reassessment method (CRM) is a Bayesian model-based design for percentile estimation in sequential dose finding trials. The main idea of the CRM is to treat the next incoming patient (or group of patients) at a recent posterior update of the target percentile. This approach is intuitive and ethically appealing on a conceptual level. However, the performance of the CRM can be sensitive to how the CRM model is specified. In addition, since the specified model directly affect the generation of the design points in the trial, sensitivity analysis may not be feasible after the data are collected.

As there are infinitely many ways to specify a CRM model, the process of model calibration, typically done by trial and error in practice, can be complicated and time-consuming. In my talk, I will first review the system of model parameters in the CRM, and then describe some semi-automated algorithms to specify these parameters based on existing dose finding theory. Simulation results will be given to illustrate this semi-automated calibration process in the context of some real trial examples.

Christopher Chong

University of Massachusetts, Department of Mathematics and Statistics, Amherst, MA 01003,

chong@math.umass.edu

Dark Breathers in Granular Crystals

We present a study of the existence, stability and bifurcation structure of families of dark breathers in a one-dimensional chain of granular crystals. We will discuss some fascinating features of the Hamiltonian model describing granular crystals, such as the relevance of the NLS approximation and the failure of spectral stability predictions. We will also discuss the damped-driven counterpart of the model and report on preliminary experimental observations of dark breathers in the lab.

Darren Crowdy

Imperial College London, Department of Mathematics, 180 Queen's Gate, London, SW7 2AZ, UK,

d.crowdy@imperial.ac.uk

Mixed Boundary Value Problems in Stokes Flows: Theory and Applications

This talk will describe theoretical investigations into a variety of mixed boundary value problems, involving boundaries that are both fixed and free, in Stokes flows. Motivating applications range from the study of so-called Janus particles in colloid science, the motion of swimmers at low Reynolds numbers, and surfactant effects in free surface flows.

Carina Curto

University of Nebraska-Lincoln, Department of Mathematics, Lincoln, NE 68588, ccurto2@math.unl.edu

Encoding Binary Neural Codes in Networks of Threshold-linear Neurons

Networks of neurons in the brain encode preferred patterns of neural activity via their synaptic connections. Despite receiving considerable attention, the precise relationship between network connectivity and encoded patterns is still

poorly understood. Here we consider this problem for networks of threshold-linear neurons whose computational function is to learn and store a set of binary patterns (e.g., a neural code) as "permitted sets" of the network. We introduce a simple Encoding Rule that selectively turns "on" synapses between neurons that co-appear in one or more patterns. Our main results precisely describe the stored patterns that result from the Encoding Rule – including unintended "spurious" states. In particular, we find that binary patterns are successfully stored in these networks when the excitatory connections between neurons are geometrically balanced -- i.e., they satisfy a set of geometric constraints. Furthermore, we find that certain types of neural codes are "natural" in the context of these networks, meaning that the full code can be accurately learned from a highly undersampled set of patterns. As an application, we construct networks that encode hippocampal place field codes nearly exactly, following presentation of only a small fraction of patterns. To obtain our results, we prove new theorems using classical ideas from convex and distance geometry, such as Cayley-Menger determinants, revealing a novel connection between these areas of mathematics and coding properties of neural networks.

Uri Eden

Boston University, Department of Mathematics and Statistics, 111 Cummington Street, Boston, MA 02215, tzvi@bu.edu

Estimating Neural Spiking Dynamics using Point Process Filters

Although it is well known that brain areas receive, process and transmit information via sequences of sudden, stereotyped electrical impulses, called action potentials or spikes, most analyses of neural data ignore the localized nature of these events. The theory of point processes offers a unified, principled approach to modeling the firing properties of spiking neural systems, and assessing goodness-of-fit between a neural model and observed spiking data. We develop a point process modeling framework and state space estimation algorithms to describe and track the evolution of dynamic representations from individual neurons and neural ensembles. This allows us to derive a toolbox of estimation algorithms and adaptive filters to address questions of static and dynamic encoding and decoding.

These methods will be illustrated through a couple of examples. First, we will model spatially specific spiking activity in the rat hippocampus and use a point process filter to reconstruct the animal's movement trajectory during a spatial navigation task. Next, we will develop a sequential importance sampling procedure for estimating biophysical parameters of conductance based neural models using only the resulting spike times. Issues of model identification and misspecification will also be discussed.

Malena Español

University of Akron, Department of Mathematics, Akron, OH 44325, mespanol@uakron.edu

Multilevel Methods for Image Deblurring

In this talk, we will introduce multilevel methods for discrete ill-posed problems arising from the discretization of Fredholm integral equations of the first kind. In particular, we will present wavelet-based multilevel methods for signal and image restoration problems. In these methods, orthogonal wavelet transforms are used to define restriction and prolongation operators within a multigrid-type iteration. The choice of the Haar wavelet operator has the advantage of preserving matrix structure, such as Toeplitz, between grids, which can be exploited to obtain faster solvers on each level where an edge-preserving Tikhonov regularization is applied. We will show results that indicate the promise of these approaches on restoration of signals and images with edges.

Edward Farnum

Kean University, NJ Center for Science & Tech Ed, 1000 Morris Avenue, Union, NJ 07083, efarnum@kean.edu

Short Pulse Perturbation Theory

A perturbation theory for the Short Pulse Equation is developed to investigate the effects of various perturbations to optical solitons propagating in nonlinear media in the few femtosecond regime. Because linear analysis about the exact solution is not possible, the theory is formulated using a variational approach. A variety of physically realizable perturbations are considered, especially those which result from short-pulse mode-locking. In each case, the analytic results are in agreement with full numerical simulations of the short-pulse theory. Given the success of soliton perturbation theory as applied optical solitons, this analysis attempts to provide the same theoretical framework for understanding physically realizable mechanisms that affect pulse evolution and stability when slow envelope approximation is no longer a realistic assumption.

Yang Feng

Columbia University, Department of Statistics, 1255 Amsterdam Avenue, New York, NY 10027, yangfeng@stat.columbia.edu

Consistent Cross-Validation for Tuning Parameter Selection in High-Dimensional Variable Selection

Asymptotic behavior of tuning parameter selection in the standard cross-validation methods is investigated for the high-dimensional variable selection. It is shown that the shrinkage problem with LASSO penalty is not always the true reason for the over-selection phenomenon in cross-validation based tuning parameter selection. After identifying the potential problems with the standard cross-validation methods, we propose a new procedure, Consistent Cross-Validation (CCV), for selecting the optimal tuning parameter. CCV is shown to enjoy the model selection consistency. Extensive simulations and real data analysis support the theoretical results and demonstrate that CCV also works well in terms of prediction.

Simon Garnier

New Jersey Institute of Technology, Department of Biological Sciences, University Heights, Newark, NJ 07102, simon.j.garnier@njit.edu

TBA

Michael Graham

University of Wisconsin-Madison, Department of Chemical and Biological Engineering, Madison, WI 53706, graham@engr.wisc.edu

Collide and Conquer: Flow-induced Segregation Phenomena in Blood and Other Multicomponent Suspensions

Blood is a suspension of particles of various shapes, sizes and mechanical properties, and the distribution of these particles during blood flow is important in many contexts. In flow, red blood cells (RBCs) migrate away from blood vessel walls, leaving a so-called cell-free layer, while white blood cells (WBCs) and platelets are preferentially found near the walls, a phenomenon called margination that is critical for the physiological responses of inflammation and hemostasis. Furthermore, drug delivery particles in the bloodstream also undergo segregation, whose influence on the efficacy of such particles is unknown.

This talk describes efforts to gain a systematic understanding of flow-induced segregation in blood and other complex mixtures. We study this problem numerically using boundary integral simulations of model cells in flow as well as theoretically with a master equation model that incorporates two key sources of wall-normal particle transport: wall-induced migration and hydrodynamic pair collisions. Additionally, a non-local drift-diffusion equation of the Fokker-Planck form is developed from the master equation model, which provides further insights into the segregation behavior in terms of the drift and diffusion of various species.

Ian Griffiths

University of Oxford, Mathematical Institute, 24-29 St. Giles', Oxford OX1 3LB, UK, Ian.Griffiths@maths.ox.ac.uk

The Control of Solute Transport in a Permeable Pipe: the Optimal Growth of Tissue in a Hollow Fibre Bioreactor

Tissue engineering involves the development of biological substitutes that restore, maintain, or improve tissue function or a whole organ. In a hollow fibre bioreactor, cells are seeded on the outside of a thin permeable fibre, through which a nutrient-fluid mixture is injected. The nutrient then flows out through the fibre walls and feeds the cells. If the wall permeability is spatially uniform then cells closer to the inlet will inevitably receive a greater proportion of nutrient than those further down the fibre. This will lead to undesirable heterogeneities in the tissue growth. In this talk we show how to choose the spatial dependence of the wall permeability so that the nutrient is distributed uniformly to all cells. To address this question we develop a mathematical model that describes the nutrient transport and dispersion within a permeable-walled tube. The resulting model provides an interesting generalization of classical Taylor dispersion for a permeable tube and allows for simplified analysis to understand how to control the nutrient transport within the system. The resulting predictions extend to a wide range of other applications, including field flow fractionation and targeted drug delivery to tumours.

Subharup Guha

University of Missouri, Department of Statistics, Columbia, MO 65211, guhasu@missouri.edu

Survival Predictor Detection by Dirichlet Processes

The selection of useful predictors is an essential part of regression analysis for survival outcomes. The importance of choosing a parsimonious model for achieving reliable results becomes even greater in high-dimensional problems

with complex structures where the number of covariates, p , overwhelms the number of responses, n . This talk proposes a novel variable selection method for small n , large p problems called Predictor Detection by Dirichlet Processes (PDDP). The sparsity of Dirichlet processes is utilized to group the large number of covariates into a smaller number of latent clusters containing correlated covariates. The "large p , small n " problem is essentially reduced to a "small n , small q " problem, where q is the unknown number of latent clusters induced by the Dirichlet Process. The clusters themselves are modeled by Dirichlet processes that capture the across-individual pattern of the covariate members. Assuming an indicator prior for the cluster effects, we perform an efficient stochastic variable search for the clusters associated with the responses. Simulation studies compare PDDP to other high-dimensional variable selection methods for survival data. PDDP is applied to relate disease survival times to gene expression profiles for the individuals. The results are validated against random-split test samples to demonstrate the value of the methodology. This work is joint with Veera Baladandayuthapani.

David Hu

Georgia Institute of Technology, School of Biology, 310 Ferst Drive, Atlanta, GA 30332, david.hu@me.gatech.edu

Ants Cooperate to Build Rafts and Towers

We present experiments and theory on the ability of fire ants to both flow like a fluid and aggregate like a solid. During floods, fire ants link their bodies together to weave hydrophobic rafts in the manner of Gore-Tex. Upon returning to land, they construct towers that are shaped such that each ant supports an equal load throughout construction. Particular attention is paid to rationalizing construction rates based upon individual behaviors and constraints of the ants.

Sunghwan Jung

Virginia Tech, Department of Engineering Science and Mechanics, Blacksburg, VA 24061, sunnyjsh@vt.edu

Dynamics of Paramecium Swimming in a Viscous Fluid

Interaction of swimmers with complicated mazes of solid boundaries is ubiquitous in natural situations. For example, while foraging in nature, microscopic swimmers often change their body shapes and swimming strategies. In experiments, we used Paramecium Multicellulose Nucleatum which is a unicellular organism and swims by synchronous beating of thousands of cilia around the body surface. Paramecium swims in three different ways; Helical ballistic, meandering, and circling. In natural situations, the helical ballistic swimming mode is predominant. However, in 2D films of decreasing thickness, we observe the probabilistic transition of swimming tracks from helical ballistic to meandering with frequent turns. Furthermore, while swimming in a channel; this unicellular eukaryote self-bends its cell-body and reverses its swimming direction. The self-bending represents an unexpected behavior in locomotion of Paramecium within the geometric confinements. Using a simple analogue to an elastic beam model, we attempt to understand the mechanical process of bending.

Mohan Kadalbajoo

IIT Kanpur, Department of Mathematics and Statistics, Kanpur, 208016, India, kadal@iitk.ac.in

Non-Uniform B-Spline Collocation Method for Solving Generalized Burger-Fisher and Burger-Huxley Equations

In this paper, we shall present a numerical method for solving a generalized Burger-Fisher and Burger-Huxley equation with high Reynolds number. Due to the presence of high Reynolds number, the problem exhibits layer behaviour. Due to the multiscale behaviour of the solution, the problem becomes quite difficult and challenging to approximate its solution. We present an approach which is based on linearization using generalized Newton's method and then describe the horizontal method of lines for its approximate solution. A B-spline collocation method in space and Crank-Nicholson method in time are used. The convergence and stability analysis of the proposed method is given. Numerical simulation is carried out on some benchmark problems to validate the theoretical results.

Hakmook Kang

Vanderbilt University School of Medicine, Department of Biostatistics, 1161 21st Avenue South, Nashville, TN 37232, hakmook.kang@vanderbilt.edu

Spatio-spectral Mixed-Effects Model for fMRI Data Analysis

In this talk, we demonstrate that in order to accurately estimate the activation patterns in functional magnetic resonance imaging (fMRI) data, it is important to properly take into account the intrinsic spatial and temporal correlation. Standard approaches to fMRI analyses avoid specifying the spatio-temporal correlation because of the

computational demand. One clever way to reduce the computational complexity is to transform the time series data into the frequency domain because the Fourier coefficients are approximately uncorrelated. The resulting spatio-spectral data has a block diagonal structure which is considerably simpler than the spatio-temporal data. Hence, we propose a spatio-spectral mixed effects model which (1.) accounts for variation in activation between voxels within a region of interest (ROI); (2.) gives a multi-scale spatial correlation structure that disentangles local correlation (between voxels in an ROI) and global correlation (between ROIs); and (3.) gives a covariance structure that greatly reduces computational burden. Building on existing theory on linear mixed effect models to conduct estimation and inference, we applied our model to fMRI data collected to estimate activation in pre-specified regions in the prefrontal cortex and to estimate the correlation structure in the brain network. The result is consistent with known neuroanatomy and supports the existence of a functional network among those regions associated with the experimental task.

Zachary P. Kilpatrick

University of Houston, Department of Mathematics, 4800 Calhoun Road, Houston, TX 77004,
zpkilpat@math.uh.edu

Noise and Multistability in Spatially Organized Neural Fields

Neural field models can describe spatially organized activity in large populations of neurons. These models are integrodifferential equations where the kernel of the integral term describes the strength of synaptic connections between neurons. Typical analyses of these equations assume: (i) effects of noise can be ignored and (ii) connections between neurons only depend upon the distance between them (spatially homogeneous). Recent studies show noise causes traveling front (Bressloff and Webber 2012) and stationary bump (Kilpatrick and Ermentrout 2013) solutions to wander diffusively about their mean position. Pure diffusion of solutions relies on the translation symmetry of the system, which only occurs in neural fields if synaptic connections are spatially homogeneous. We show that a variety of rich behaviors arise when one considers more realistic spatially heterogeneous synaptic connections. Namely, spatial heterogeneity establishes a multistable potential landscape in space that can then be traversed by solutions with the aid of noise. The dynamics then evolves as a particle kicked between multiple wells. Stationary bumps and traveling waves become pinned to stationary attractors in the deterministic system, but noise leads to rare events where their position moves between attractors, recovering diffusion and/or propagation. Aperiodic spatial heterogeneity leads to a spatial bias in the rate of these transitions which must then be calculated for each well.

Tsampikos Kottos

Wesleyan University, Department of Physics, Middletown, CT 06459, tkottos@wesleyan.edu

Taming the Flow of Light via Parity-Time Symmetry

We will introduce the notion of Parity-Time (PT) symmetry and present its implications in classical wave propagation. Using photonics as a playfield we show how one can construct new circuitry designs that allow for asymmetric light transport due to interplay of the novel properties of PT-symmetry and non-linearity or gyrotropic elements.

Brenton LeMesurier

College of Charleston, Department of Mathematics, Charleston, SC 29424, lemesurierb@cofc.edu

Energetic Pulses in Exciton-Phonon Chains, and Conservative Numerical Methods for Quasi-linear Hamiltonian Systems

The phenomenon of coherent energetic pulse propagation in exciton-phonon molecular chains such as alpha-helix protein is studied using a Davydov-Scott type model, with both numerical studies using a new unconditionally stable fourth order accurate energy-momentum conserving time discretization, and with analytical explanation of the main numerical observations.

It is shown that for physically natural impulsive initial data associated with the energy released by ATP hydrolysis, coherent traveling pulses are seen that have a form related to the Airy function, with slowly varying amplitude but rapid variation of phase along the chain.

This can be explained in terms of a new long wave approximation by the third derivative nonlinear Schroedinger equation, which differs from the previous continuum limit approximations related to the standard NLS equation.

A convenient method is described for construction the highly stable, accurate conservative time discretizations used, with proof of its desirable properties for a large class of Hamiltonian systems, including a variety of molecular models.

Peijun Li

Purdue University, Department of Mathematics, 150 North University Street, West Lafayette, IN 47907, lipeijun@purdue.edu

Inverse Surface Scattering in Near-Field Imaging

This talk is concerned with an inverse surface scattering problem in near-field optical imaging, which is to reconstruct the scattering surface with a resolution beyond the diffraction limit. The surface is assumed to be a small and smooth deformation of a plane surface. Based on a transformed field expansion, the boundary value problem with complex scattering surface is converted into a successive sequence of a two-point boundary value problems in the frequency domain, where an analytic solution for the direct scattering problem is derived from the method of integrated solution. By neglecting the high order terms in the asymptotic expansion, the nonlinear inverse problem is linearized and an explicit inversion formula is obtained. The method works for sound soft, sound hard, and impedance surfaces, and requires only a single illumination at a fixed frequency and is realized efficiently by the fast Fourier transform. Numerical results show that the method is simple, stable, and effective to reconstruct scattering surfaces with subwavelength resolution.

Ruosha Li

University of Pittsburgh, Department of Biostatistics, 130 DeSoto Street, Pittsburgh, PA 15261, rul12@pitt.edu

Assessing Quantile Prediction with Censored Quantile Regression Models

In biomedical studies, quantiles of survival outcomes are often of interest and provide comprehensive insights into disease progression. Quantile regression model serves a flexible tool for modeling the survival outcomes, and facilitates straightforward prediction of the quantile survival times. In this work, we propose a meaningful measure that summarizes the model performances in terms of quantile prediction. The proposed measure extends the absolute error to account for censoring and different quantiles. We construct an estimator of the proposed measure without assuming that the model is correctly specified, and establish its asymptotic properties via empirical process theory. In addition, we develop consistent variance estimators that properly account for the non-smoothness of the estimating equations. Extensive numerical studies demonstrate satisfactory performances of the proposed methods under realistic sample sizes. Joint work with Limin Peng.

Xiaodong Lin

Rutgers University, School of Business, Piscataway, NJ 08854, lin@business.rutgers.edu

Alternating Linearization for Structured Regularization

We adapt the alternating linearization method for proximal decomposition to structured regularization problems, in particular, to the generalized lasso problems. The method is related to two well-known operator splitting methods, the Douglas-Rachford and the Peaceman-Rachford method, but it has descent properties with respect to the objective function. Each iteration of the procedure consists of solving two relatively simple subproblems, and a block coordinate descend algorithm is developed to facilitate faster convergence. We present implementation for large problems with the use of specialized algorithms and sparse data structures. Extensions to regularization problems with non-convex penalties will also be discussed. Finally, we present numerical results for several synthetic and real-world examples including a three-dimensional fused lasso problem, which illustrate the efficacy and accuracy of the method.

Yufeng Liu

University of North Carolina at Chapel Hill, Department of Biostatistics, CB 3260, Chapel Hill, NC 27599, yfliu@email.unc.edu

Joint Estimation of Multiple Dependent Gaussian Graphical Models

Gaussian graphical models are widely used to represent conditional dependence among random variables. In this talk, we propose a new estimator for such models appropriate for data arising from several dependent networks. Existing methods that assume independence among graphs are not applicable in this setting. To estimate multiple dependent graphs, we decompose the graphical models into two layers: the systemic layer, which is the network shared among graphs, and the category-specific layer, which represents the graph-specific variation. We propose a new graphical EM technique that jointly estimates the two layers of graphs. Applications to mouse genetic data will be presented. This is based on joint work with Yuying Xie and William Valdar at UNC-CH.

Mark Lyon

University of New Hampshire, Department of Mathematics, 105 Main Street, Durham, NH 03824,
mark.lyon@unh.edu

Fourier Continuation Algorithms, Fast Transforms, and Techniques for PDE Solution

Fourier Continuation methods, which have been successfully applied to the solution of a variety of Partial Differential Equations (PDEs), allow for highly-accurate approximation and convergence in a PDE solver by allowing Fourier series to be applied to non-periodic functions. FFT speed algorithms have been developed and additionally exhibit minimal pollution for wave propagation problems (i.e. growth in the global error with the scale of the problem) with spectral error decay away from the boundaries and, at minimum, high-order polynomial interpolation based error near the boundaries. Various methods for applying the FC methodology will be discussed along with demonstrations.

Shreyas Mandre

Brown University, School of Engineering, 184 Hope Street Box D, Providence, RI 02912,
Shreyas_Mandre@brown.edu

The Effect of Size and Shape on the Capillary Attraction between Nearby Floating Objects

Attraction between floating objects is caused by capillary effects. The attraction is dubbed the Cheerios effect referring to the common observation of breakfast cereal clumping in a bowl of milk. When the objects are far from each other, multipole expansion of the meniscus deformation provides a framework for understanding the interaction. However, when the objects come close to each other the ensuing dynamics also cause the objects to rotate, but no framework exists to address them.

We derive an alternative framework in the limit of small distance between the objects using an asymptotic expansion in the distance. This framework allows us to investigate the effect of size and shape of the object on the attractive force. Through asymptotic analysis and simple-table-top experiments, we find that the curvature of the contact line governs the interaction. Before the objects touch, the capillary interaction rotates the objects to minimize the distance between the points of highest curvature on the contact line. After contact, the capillary interaction brings closer the points of lowest curvature on the contact line.

Sashi Marella

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, sashi.k.marella@njit.edu

Asynchronous Inhibition and Small Neuronal Network Dynamics

In cortical neuronal network models, basket cells are assumed to mediate a fast phasic inhibitory signal via GABA-A synapses due to the synchronous release of neurotransmitter vesicles which is tightly linked to the spike-time in the interneuron. Recent experimental studies however, have highlighted a class of basket cells that provide inhibitory inputs whose action on the postsynaptic neuron is mediated predominantly by asynchronous release of neurotransmitter that is not tightly linked to the time of spike in the interneuron. Since basket cells can exert significant control over the timing and rate of action potentials in the postsynaptic neuron, it is important to understand the contribution of such asynchronously releasing inhibitory basket cells to the overall dynamics of the cortical network. In this study we investigate the effects of asynchronous synaptic release on single pyramidal neuron activity and small networks. We also study the temporal evolution and modulation of spiking activity in a small neuronal network with excitatory, fast-spiking inhibitory neurons and a novel class of inhibitory neurons that can release neurotransmitter vesicles asynchronously.

Scott McCue

Queensland University of Technology, Australia, Department of Mathematics, Brisbane QLD 4001, Australia,
scott.mccue@qut.edu.au

Bubbles Contracting, Expanding and Translating in Hele-Shaw Cells

The authors are Scott W. McCue and Michael C. Dallaston (Queensland University of Technology, Brisbane, Australia)

We first treat radial Hele-Shaw flows in which a doubly-connected annular region of viscous fluid surrounds an inviscid bubble that is either expanding or contracting. The zero-surface-tension problem is unusual in that it is ill-posed for both bubble expansion and contraction, as both scenarios involve viscous fluid displacing inviscid fluid. By applying a conformal mapping to an annulus and deriving an appropriate Polubarinova-Galin equation, we present exact solutions that start with cusps on one interface and end with cusps on the other, as well as solutions

that have the bubble contracting to a point. Next, we simplify the geometry to treat an inviscid bubble either expanding or contracting in an infinite body of viscous fluid. By applying a combination of formal asymptotics and complex variable theory, we can classify the surprisingly interesting possible solution behaviours when the physical effects of surface tension and/or kinetic undercooling are included on the bubble interface. In a certain small bubble regime, these flows represent a generalisation of a well-known class of curve-shortening flows. We finish by presenting results for the selection problem for an evolving finger in a Saffman-Taylor channel geometry with kinetic undercooling instead of surface tension. This is joint work with my PhD student Michael Dallaston.

N. Robb McDonald

University College, London, Department of Mathematics, Gower Street, London WC1E 6BT, UK,
n.r.mcdonald@ucl.ac.uk

Poisson Growth and the Geometry of Valleys

The two-dimensional free boundary problem in which the field variable is governed by Poisson's equation and for which the velocity of the free boundary is given by its gradient--Poisson growth--is considered. The problem can be considered a generalisation of classic Hele-Shaw free boundary flow or Laplacian growth problem. In the case when the right hand side of Poisson's equation is constant, a formulation is obtained in terms of the Schwarz function of the free boundary. Examples of exact solutions are given.

The formulation is used to find an explicit solution for the shape of the valley or ravine formed by groundwater seepage. This is a flow in porous media problem which is modelled as a Poisson growth free boundary problem. The resulting geometry compares favourably to alternative theories of valley shape.

Paul Miller

Brandeis University, Department of Biology, 415 South Street, Waltham, MA 02453, pmiller@brandeis.edu

Optimal Decision Making under Biological Constraints: Linear Perfect Integrators versus Nonlinear Attractor-based Neural Circuits

Analysis of cortical activity by Hidden Markov modeling, an approach which incorporates trial-to-trial variability of the data, suggests that the slow ramps of neural firing rates sometimes seen in trial-averaged data, could in fact be produced by more abrupt transitions between discrete states. This observation motivated us to analyze whether behavioral choices could be produced by noise-induced transitions from an "undecided" state to another attractor state, rather than by the established optimal method of perfect integration of evidence. We solved the diffusion model in a system with parametric variation, via a nonlinearity term in the neural response curve, which when set to zero produced a perfect integrator, but otherwise (depending on sign) could produce a stable or unstable fixed point for the initial neural activity after stimulus onset. We find that with incorporation of biological constraints, including limited time for decision making, finite neural thresholds and intrinsic noise within the neural decision-making circuit, that the system with a stable fixed point could outperform the perfect integrator. Our results suggest a computational role for attractor-based systems, which can benefit from both inherent and external noise.

Jeffrey F. Morris

CCNY, Levich Institute and Department of Chemical Engineering, 140th Street & Convent Avenue, New York, NY 10031, morris@ccny.cuny.edu

Microstructural Analysis and Rheology of Concentrated Colloidal Dispersions

A theoretical framework will be presented for analytical prediction of structure and rheology of sheared colloidal hard-sphere suspensions, based on work of E. Nazockdast [1]. The theory computes the steady pair distribution function, $g(\mathbf{r})$, as a solution to the pair Smoluchowski equation (SE) where \mathbf{r} is the pair separation vector. The interactions of the surrounding bath particles on the pair dynamics are modeled through third particle integrals; as a result the theory is formulated based on an integro-differential form of the SE and is able to give predictions of pair microstructure over a wide range of particle volume fractions and Peclet numbers, Pe . Here Pe is the ratio of hydrodynamic to Brownian forces at the particle length scale. The predicted $g(\mathbf{r})$ is used to compute the steady simple shear rheology, namely viscosity and first and second normal stress differences. The predictions of microstructure and rheology are compared against Accelerated Stokesian Dynamics (ASD) simulations.

Emphasis will be placed in the discussion on unresolved mathematical issues, one related to the large- Pe behavior and infinite- Pe limit, and another to the manner in which hydrodynamic diffusion is handled in developing the Smoluchowski equation from a general Fokker-Planck type of formalism.

[1] E. Nazockdast & J. F. Morris 2012 Microstructural theory and rheological analysis for concentrated colloidal dispersions. J. Fluid Mech. 713, 420-452.

Sebastien Motsch

University of Maryland, Center for Scientific Computation and Mathematical Modeling (CSCAMM), College Park, MD 20742, smotsch@cscamm.umd.edu

Trail Formation Based on Directed Pheromone Deposition

Ants are able to build trail networks on a very large scale using chemical markers. To understand this pattern formation, we have developed an Agent-Based Model aiming at reproducing this network formation. The novelty of the model is to consider the chemical marker, also called pheromone, as a small piece of trail. As such, the pheromones indicate a direction that can be used by other ants to orientate. This assumption of the model has been motivated by experimental observations.

The numerical simulations reveal that the model does create large and flexible networks. We analyze how the trail patterns depend on the strength of the ant-pheromone interaction and show the existence of a phase transition. Finally, we introduce a kinetic and macroscopic limit of the dynamics to apprehend the large scale behavior of the model.

Giovanni Motta

Columbia University, Department of Statistics, 1255 Amsterdam Avenue, New York, NY 10027, g.motta@stat.columbia.edu

Spatial Identification of Epilepsy Regions

The surgical outcomes of patients suffering from neocortical epilepsy are not always successful. The main difficulty in the treatment of neocortical epilepsy is that current technology has limited accuracy in mapping neocortical epileptogenic tissue (see Haglund and Hochman 2004). It is known that the optical spectroscopic properties of brain tissue are correlated with changes in neuronal activity. The method of mapping these activity-evoked optical changes is known as imaging of intrinsic optical signals (ImIOS). Activity-evoked optical changes measured in neocortex are generated by changes in cerebral hemodynamics (i.e., changes in blood oxygenation and blood volume).

ImIOS has the potential to be useful for both clinical and experimental investigations of the human neocortex. However, its usefulness for human studies is currently limited because intra-operatively acquired ImIOS data is noisy. To improve the reliability and usefulness of ImIOS for human studies, it is desirable to find appropriate statistical appropriate methods for the removal of noise artifacts and its statistical analysis (see Lavine et al. 2011).

In this paper we introduce a novel flexible tool, based on spatial statistical representation of ImIOS, that allows for source localization of the epilepsy regions. In particular, our model incorporates spatial correlation between the location of the epileptic region(s) and the neighboring regions, non-stationarity of the observed time series, and heartbeat/respiration cyclical components. The final goal is clustering (dimension reduction) of the pixels in regions, in order to localize the epilepsy regions for the craniectomy.

The advantage of our approach compared with previous approaches is twofold. Firstly, we use a *non-parametric* specification, rather than the (more restrictive) parametric or polynomial-based specification. Secondly, we provide a statistical method --based on the spatial information-- that is able to identify the clusters in a *data-driven* way, rather than the (sometimes arbitrary) ad-hoc currently used approaches.

To demonstrate how our method might be used for intra-operative neuro-surgical mapping, we provide an application of the technique to optical data acquired from a single human subject during direct electrical stimulation of the cortex.

Sean Nixon

University of Vermont, Department of Mathematics and Statistics, Burlington, VT 05405, sean.nixon@uvm.edu

Nonlinear Dynamics of Wave Packets in \mathcal{PT} -symmetric Optical Lattices

Nonlinear dynamics of wave packets in \mathcal{PT} -symmetric optical lattices near the phase-transition point are analytically studied in one- and two- dimensional systems. We show analytically that when the strength of the gain-loss component in the \mathcal{PT} lattice rises above the phase-transition point, an infinite number of linear Bloch bands turn complex simultaneously. For the 1D case, a nonlinear Klein-Gordon equation is derived for the envelope of wave packets. A variety of novel phenomena known to exist in this envelope equation are shown to also exist in the full equation including wave blowup, periodic bound states and solitary wave solutions. In 2D a novel equation is derived for the envelope dynamics, and wave packets exhibit pyramidal diffraction.

Duane Nykamp

University of Minnesota, School of Mathematics, Minneapolis, MN 55455, nykamp@umn.edu

Capturing Effective Neuronal Dynamics in Random Networks with Complex Topologies

We derive effective equations for the activity of recurrent spiking neuron models coupled via networks in which different motifs (patterns of connections) are overrepresented. We present an analysis of network dynamics that shed lights on how network structure influences mean behavior as well as leads to the initiation and propagation of variability and covariability. One key result is that network topology can increase the dimension of the effective dynamics and allow for a larger repertoire of behavior. We demonstrate this behavior through simulations of spiking neuronal networks.

Reuben O'Dea

University of Nottingham, School of Mathematical Sciences, University Park, Nottingham NG7 2RD, UK,

Reuben.o'dea@nottingham.ac.uk

A Multiscale Analysis of Solid Tissue Growth in vitro

The derivation of continuum models which represent underlying discrete or microscale phenomena is emerging as an important part of mathematical biology: integration between subcellular, cellular and tissue-level behaviour is crucial to understanding tissue growth and mechanics. For this reason, various multiscale (or homogenisation) techniques have been employed to derive continuum models directly from underlying microscale systems. Such methods have been widely used to study (e.g.) porous and poroelastic materials; however, a distinguishing feature of biological tissue is its ability continuously to remodel in response to local environmental cues. Here, a new macroscale formulation is presented, coupling tissue growth, fluid flow, and nutrient transport. The model is appropriate to describe cell growth and extracellular matrix (ECM) deposition within tissue engineering scaffolds, such as those employed in perfusion bioreactors. Illustrative numerical solutions are presented to indicate the influence of microscale growth on model dynamics and, via the incorporation of muCT data from an experimentally-relevant scaffold, the influence of scaffold geometry in determining micro- and macroscale flow dynamics, and its importance in nutrient delivery to cells seeded in such structures.

Sarah Olson

Worcester Polytechnic Institute, Department of Mathematical Sciences, Worcester, MA 01609, sdolson@wpi.edu

Hydrodynamic Interactions of Sperm

Sperm have been observed to form sperm trains and self organize into vortices. What is the relative role of biochemistry, flagellar waveform, and hydrodynamics in these interactions? In this talk, we will present recent computational results on attraction, synchronization, and the formation of sperm trains in 2-d and 3-d using the method of regularized Stokeslets. These results will be studied for planar waveforms that are symmetrical and asymmetrical (varying amplitude). Time permitting, a new regularized Stokes formulation for a Kirchhoff rod will be presented and motivated to capture nonplanar motility of flagella.

Daniel Onofrei

University of Houston, Department of Mathematics, 4800 Calhoun Road, Houston, TX 77004,

onofrei@math.uh.edu

Active Control of Acoustic and Electromagnetic Fields

The problem of controlling acoustic or electromagnetic fields is at the core of many important applications such as, energy focusing, shielding and cloaking or the design of super-directive antennas. The current state of the art in this field suggests the existence of two main approaches for such problems: passive controls, where one uses suitable material designs to control the fields (e.g., material coatings of certain regions of interest), and active control techniques, where one employs active sources (antennas) to manipulate the fields in regions of interest. In this talk I will first briefly describe the main mathematical question and its applications and then focus on the active control technique for the scalar Helmholtz equation in a homogeneous environment. The problem can be understood from two points of view, as a control question or as an inverse source problem (ISP). This type of ISP questions are severely ill posed and I will describe our results about the existence of a unique minimal energy solution. Stability of the solution and extensions of the results to the case of nonhomogeneous environment and to the Maxwell system are part of current work and will be described accordingly.

Panagotis Panayotaros

Universidad Nacional Autónoma de México, Department of Mathematics, Mexico City, Mexico,
panos@mym.iimas.unam.mx

Solitary waves in nematic liquid crystals

We present some new results on properties of energy minimizing solitary wave solutions in a 2-D nonlinear Schrödinger equation with a nonlocal Hartree-type nonlinearity used to model light propagation in nematic liquid crystals. Solitons obtained through optimization are smooth, radial, and monotonic (up to symmetries), and we also provide theoretical evidence that they can only exist above a power threshold. We also compare the theory with some numerical results, and discuss differences between finite and infinite planar domains. This is joint work with T. Marchant, U. Wollongong, Australia.

Jose L. Pena

Albert Einstein College of Medicine, Rose F. Kennedy Center, 1410 Pelham Parkway South, Bronx, NY 10461,
jose.pena@einstein.yu.edu

'The biased owl'

Although owls can accurately localize sounds near the center of gaze, they systematically underestimate direction of sound sources in the periphery. Other species including humans also underestimate peripheral sound directions. This behavior and the underlying neural implementation can be predicted by statistical inference. We found evidence of how statistics of the input could be encoded in the owl's brain. In the presence of noise, owls would assume that the sound source lies toward the front. Paradoxically, this error may improve the owl's performance in frontal space. We have followed this work investigating mechanisms of population-wide biases in the owl's map of auditory space that could lead to optimal performance.

Zhen Peng

Ohio State University, The ElectroScience Laboratory, 1330 Kinnear Road, Columbus, OH 43212,
peng.98@osu.edu

Recent Advances in Surface Integral Equation Methods for Time-Harmonic Maxwell Equations

Surface integral equation (SIE) methods have shown to be effective in solving electromagnetic wave scattering and radiation problems. It is mainly due to the fact both the analysis and unknowns reside only on the boundary surfaces of the targets. However, applications of the SIE methods often lead to dense and ill-conditioned matrix equations. The efficient and robust solution of the SIE matrix equation poses an immense challenge. This talk shall present some recent advances in surface integral equation methods for solving time-harmonic Maxwell's equations.

The first topic is domain decomposition for surface integral equations via multi-trace formulations. The entire computational domain is decomposed into a number of non-overlapping sub-regions. Each local sub-region is homogeneous with constant material properties and described by a closed surface. Through this decomposition, we have introduced at least two pairs of trace data as unknowns on interfaces between sub-regions (multi-trace formulation). This multi-trace feature admits two major benefits: the localized surface integral equation for the homogeneous sub-region problem is amenable to operator preconditioning; the resulting linear systems of equations readily lend themselves to optimized Schwarz methods.

A discontinuous Galerkin surface integral equation, herein referred to as IEDG, is proposed for the numerical solution of sub-regions. The main objective of this work is to allow the solution of combined field integral equation using discontinuous trial and test functions without any considerations of continuity requirements across element's boundaries. It enables the possibility to mix different types of elements and employ different order of basis functions within the same discretization.

Adrien Peyrache

New York University Medical Center, 450 East 29th Street, 9th Floor, New York, NY 10016,
adrien.peyrache@gmail.com

Inferring Cell Assembly Organization from Neuronal Correlations

In vivo recordings of large ensembles of neurons reveal unique insights into network processing spanning the time-scale from single spikes to global fluctuation. It has been hypothesized that neurons would dynamically self-organize in subgroups of coactivated elements referred to as cell assemblies. Cross-correlation between the output spike trains of neurons is a simple yet powerful method to quantify their functional interaction. Based on data from various brain structures and animal species, it will be shown how correlation patterns depend on the complexity of the inputs and of the local circuitry. We will then present recent advances in data analysis for the assessment of the

significance of cell assembly organization based on a null hypothesis directly inspired by random matrix theory. Cell assembly formation and dynamics were strongly correlated to change in animal's behavior and thus, presumably, to the associated memory traces.

Sridhar Raghavachari

Duke University Medical Center, Department of Neurobiology, Durham, NC 27710, sri@neuro.duke.edu
TBA

Luis Rivero

Universidad Nacional Autónoma de México, Department of Mathematics, Mexico City, Mexico,
lfeliperiverog@gmail.com

Pullback Attractors and Nonlinear Wave Equations

The aim of this talk is to describe some basic notions of the theory of pullback attractors, and to give examples of possible applications to nonlinear evolution equations, especially nonlinear waves and lattices. Pullback attractors are analogues of global attractors of dynamical systems, defined for nonautonomous dynamical systems and more general evolution processes that include systems with noise or time dependent coefficients. We present some results on forced and damped nonlinear wave equations, which were made in collaboration with T. Caraballo and J.A. Langa from the Universidad de Sevilla (Spain) and A.N. Carvalho from the Universidade de São Paulo (Brazil). We talk about the gradient structure of the pullback attractor and show how, under certain conditions, the attractor behaves continuously under some perturbation. Our recent work in discrete nonlinear Schrödinger equations will also be presented.

Michael Rubenstein

Harvard University, School of Engineering and Applied Sciences, 33 Oxford Street, Room 236, Cambridge, MA 02138, mrubenst@seas.harvard.edu

Kilobot: A 1024 Robot Platform for Implementing Collective Behaviors

In current robotics research there is a vast body of work on algorithms and control methods for groups of decentralized cooperating robots, called a swarm or collective. These algorithms are generally meant to control collectives of hundreds or even thousands of robots; however, for reasons of cost, time, or complexity, they are generally validated in simulation only, or on a group of a few tens of robots. When using a simulation to validate an algorithm for a collective of robots, it is difficult to accurately model the system. This modeling difficulty can lead to disparities in algorithm behavior when operating on a simulated collective versus a real robotic collective. Additionally, operating an algorithm designed for a large collective of robots on just a few may hide scaling issues within the algorithm that can only be uncovered in a much larger collective. To address these issues, I designed a robot called Kilobot, and produced a collective of 1024 of these robots. To the best of my knowledge, this group of 1024 robots is by far the largest cooperating group of distributed robots ever built.

In this talk, I will first discuss the challenges of building a large group of robots and why past efforts in building large groups have been limited to around 100 robots. I will then describe the Kilobot design and how it overcomes the challenges associated with building large robot groups. Next, I will describe my work on three collective algorithms and show their implementation on the Kilobot collective. The first algorithm describes the formation of coordinate systems on a group of simple distributed robots. This coordinate system gives the robots a location within the collective similar to GPS, but uses only local communication in a decentralized system. The second algorithm I will describe uses the coordinate system formed by the robots to control the shape of a collective. This algorithm allows for the group to form any desired solid connected shape. Finally I will talk about an algorithm that allows a large group of simple robots to work together to move an object that is too large for any of the individuals to move. This algorithm provides guarantees about successful transport of the object, and is agnostic to the shape of the object as well as where the robots carry the object.

Kausik Sarkar

George Washington University, Department of Mechanical and Aerospace Engineering, Newark, DE, 19716,
sarkar@gwu.edu

Effects of Viscoelasticity on Drop Dynamics and Emulsion Rheology

Over the past decade, we have been simulating the dynamics of single and multiple viscous and viscoelastic drops using a front tracking finite difference method. A novel finite-analytic time integration scheme for rate-type constitutive equations has been developed that automatically obtains an elastic-viscous stress-splitting alleviating

some of the numerical difficulties at high Weissenberg numbers. Unlike viscous cases, our intuition and understanding of viscoelasticity for multiphase flows are severely limited; there were widespread disagreement and contradictory experimental findings as to the effects of viscoelasticity, e.g. whether it increases or decreases drop deformation in shear. I will discuss how we were able to resolve some of these issues using simulation and detailed investigation of the stress field. We show that viscoelastic effects often give rise to competing forces resulting in nonmonotonic behaviors with increasing viscoelasticity. I will also discuss the cases of retraction of a sheared drop, a viscoelastic drop falling in a viscous medium and migration of a viscous drop in a wall bounded viscoelastic sheared flow. Wherever possible, I will explain the numerical results using simple ordinary differential equation models. I will also discuss the effects of drop phase viscoelasticity. Finally, I will discuss our discovery that small amount of inertia can give rise to qualitatively new effects in emulsion rheology such as change of signs of normal stress differences explaining the underlying physics.

Peter Smereka

University of Michigan, Department of Mathematics, 530 Church Street, Ann Arbor, MI 48109, psmereka@umich.edu

The Gaussian Wave Packet Transform: Efficient Computation of the Semi-classical Limit of the Schroedinger Equation

An efficient method for simulating the propagation of a localized solution of the Schroedinger equation near the semiclassical limit is presented. The method is based on a time dependent transformation closely related to Gaussian wave packets and yields a Schroedinger type equation that is very amenable to numerical solution in the semiclassical limit. The wavefunction can be reconstructed from the transformed wavefunction whereas expectation values can easily be evaluated directly from the transformed wavefunction. The number of grid points needed per degree of freedom is small enough that computations in dimensions of up to 4 or 5 are feasible without the use of any basis thinning procedures. This is joint work with Giovanni Russo.

Michael Sobel

Columbia University, Department of Statistics, 1255 Amsterdam Avenue, New York, NY 10027, michael@stat.columbia.edu

Compliance Mixture Modelling with a Zero-Effect Complier Class and Missing Data

Michael E. Sobel^{1,*} and Bengt Muthén²

¹ Department of Statistics, Columbia University New York, New York 10027, U.S.A.

² Professor Emeritus, University of California, Los Angeles, California, U.S.A.

Randomized experiments are the gold standard for evaluating proposed treatments. The intent to treat estimand measures the effect of treatment assignment, but not the effect of treatment if subjects take treatments to which they are not assigned. The desire to estimate the efficacy of the treatment in this case has been the impetus for a substantial literature on compliance over the last 15 years. In papers dealing with this issue, it is typically assumed there are different types of subjects, for example, those who will follow treatment assignment (compliers), and those who will always take a particular treatment irrespective of treatment assignment. The estimands of primary interest are the complier proportion and the complier average treatment effect (CACE). To estimate CACE, researchers have used various methods, for example, instrumental variables and parametric mixture models, treating compliers as a single class. However, it is often unreasonable to believe all compliers will be affected. This article therefore treats compliers as a mixture of two types, those belonging to a zero-effect class, others to an effect class. Second, in most experiments, some subjects drop out or simply do not report the value of the outcome variable, and the failure to take into account missing data can lead to biased estimates of treatment effects. Recent work on compliance in randomized experiments has addressed this issue by assuming missing data are missing at random or latently ignorable. We extend this work to the case where compliers are a mixture of types and also examine alternative types of nonignorable missing data assumptions.

Key words: Causal inference; Compliance; Latent ignorability; Missing data; Mixture distributions.

Eric Sobie

Mount Sinai School of Medicine, Icahn Medical Institute, 1425 Madison Avenue, New York, NY 10029, eric.sobie@mssm.edu

Leveraging Mathematical Models to Understand Population Variability in Cardiac Physiology

Mathematical models of heart cells and tissues are sufficiently advanced that the models can recapitulate normal physiology, and can predict, for example, mechanisms underlying pro-arrhythmic or anti-arrhythmic drug effects.

At present, however, these models are not adequate for understanding variability across a population, i.e. why a drug may be effective in one patient but ineffective in another patient. I will describe novel computational approaches my laboratory has developed to quantify and predict differences between individuals.

Hans Peter Stimming

Wolfgang Pauli Institute Vienna, Nodbergstrasse 15, 1090 Wien, Austria, hans.peter.stimming@univie.ac.at

Modeling and Simulation of Bose-Einstein Condensates (BEC) by Nonlinear Schroedinger equations: Quantification of Dephasing

The modeling of a Double-Well experiment for Bose-Einstein-Condensate condensates is described and discussed from a numerical simulation point of view. The experiment consists of the creation of a BEC in a double-well trapping potential, which splits a single condensate into two parts. The interference patterns observed after opening the trap in the experiment can be reproduced by simulations. Exact quantization of dephasing between the two condensate parts of the experiment in the time evolution of the GPE can be simulated and connected to state-of-the-art theory for coherence decay in Quasi-condensates. This work results from an interdisciplinary cooperation with experimentalists from Vienna U. of Technology.

Daisuke Takagi

University of Hawaii at Manoa, Department of Mathematics, 2565 McCarthy Mall, Honolulu, HI 96822, dtakagi@math.hawaii.edu

How Synthetic Microswimmers Move, Turn, Flip, and Spread

Microscopic swimmers are envisioned to perform medical and technological tasks, but predicting their motion and dispersion is challenging. I will show how chemically propelled bimetallic rods move in large circles and flip over spontaneously on a surface. In a suspension of solid spheres, the rods orbit closely around the spheres. These movements can be understood using simplified analytical models. They demonstrate that confining boundaries have major effects on the long-term dispersion of swimmers.

Colin Torney

Princeton University, Ecology & Evolutionary Biology Department, Princeton, NJ 08544, ctorney@princeton.edu

Information Use and Collective Behaviour in Animal Groups

Collective behavior is pervasive throughout the natural world, ranging from hydrodynamically interacting bacteria to the acoustic communication of migrating whales. Studying these systems is not only ecologically important but also represents a significant mathematical challenge, as simple interactions between individuals lead to complex emergent behavior at the collective level. In this talk I will outline some empirical results relating to information use in schooling fish that demonstrate how groups can outperform individuals due to emergent effects. I will then present some reduced models based around simple coordination games, that capture the same qualitative features as the real systems, such as localized interaction, social influence, and rapid transitions to ordered states, but which allow some analytical treatment.

David Trubatch

Montclair State University, Mathematical Sciences Department, 1 Normal Avenue, Montclair, NJ 07043, david.trubatch@montclair.edu

Recurrence in Discretizations of the KdV Equation

Like the Fermi-Pasta-Ulam lattice from which it was ultimately derived, the Zabusky-Kruskal (ZK) lattice exhibits near-recurrence of its initial state at regular time intervals in simulations. The recurrence observed in simulations of the ZK lattice has generally been attributed to the solitons or, less specifically, the integrability of the continuum limit of the lattice, namely the Korteweg-de Vries equation (KdV). This line of reasoning leads to the hypotheses that: (i) simulations on smaller grid separations (ii) more-accurate (e.g., higher-order) discretizations and/or (ii) discretizations that are integrable as spatially discrete systems should all exhibit stronger recurrences than those observed in the original simulations of ZK. However, systematic simulations of (i) ZK, (ii) a spectral (Galerkin) discretization of KdV and (iii) an integrable discretization of KdV, all over a wide range of grid scales, are not consistent with these hypotheses. Instead, recurrence of a low-mode initial state is observed to be strongest and most persistent at a middle scale. As grid scales shorten, simulations with all three discretizations show common convergence (presumably to KdV), but recurrence intensity and persistence weaken in this limit. On the other hand, for grid scales over a threshold value, no recurrence is observed. Instead, for grid sizes beyond a threshold, energy is rapidly distributed across the spatial Fourier spectrum. Equipartition, the equal distribution of energy among the

spatial Fourier modes of the solution (over some time-averaged window), precludes recurrence. However, unequal distribution of energy among the modes does not itself imply recurrence. Indeed, lattice simulations show a characteristic unequal partition of energy on a range of grid scales over which the persistence and strength of recurrences vary significantly, while simulations on sufficiently coarse grids show a relatively rapid transition to equipartition.

Antai Wang

Columbia University, Mailman School of Public Health, 1130 Saint Nicholas Avenue, New York, NY 10032, aw2644@columbia.edu

The Analysis of Bivariate Truncated Data Using the Clayton Copula Model

In individuals infected with human immunodeficiency virus (HIV), distributions of quantitative HIV RNA measurements may be highly left-censored due to values falling below assay detection limits (DL). It is of the interest to find the relationship between plasma and semen viral loads. To address this type of problem, we developed an empirical goodness-of-fit test to check the Clayton model assumption for bivariate truncated data. We also used truncated tau to estimate the dependence parameter in the Clayton model for this type of data. It turns out that the proposed methodology works for both truncated and fixed left censored bivariate data. The proposed test procedure is demonstrated using an HIV data set, and statistical inference is drawn based on corresponding test result.

Huixia Judy Wang

North Carolina State University, Department of Statistics, Raleigh, NC 27695, hwang3@ncsu.edu

Local Buckley-James Estimator for the Heteroscedastic Accelerated Failure Time Model

In survival analysis, the accelerated failure time model is a useful alternative to the popular Cox proportional hazards model due to its easy interpretation. Current estimation methods for the accelerated failure time model mostly assume independent and identically distributed random errors. However, as shown in our two motivating examples, the conditional variance of log survival times may often depend on covariates exhibiting some form of heteroscedasticity. We develop a local Buckley-James estimator for the accelerated failure time model with heteroscedastic errors. We establish the consistency and asymptotic normality of the proposed estimator and propose a resampling approach for inference. Simulation study demonstrates that the proposed method is flexible and leads to more efficient estimation when heteroscedasticity is present. The value of the proposed method is further assessed by the analysis of the two motivating survival data sets. This is a joint work with Drs. Lei Pang from Merck and Wenbin Lu from North Carolina State University.

Martin Wechselberger

University of Sydney, School of Mathematics and Statistics, NSW 2006, Australia, wm@maths.usyd.edu.au

Neuronal Excitability and Canards

The notion of excitability was first introduced in an attempt to understand firing properties of neurons. It was Alan Hodgkin who identified three basic types (classes) of excitable axons (integrator, resonator and differentiator) distinguished by their different responses to injected steps of currents of various amplitudes.

Pioneered by Rinzel and Ermentrout, bifurcation theory explains repetitive (tonic) firing patterns for adequate steady inputs in integrator (type I) and resonator (type II) neuronal models. In contrast, the dynamic behavior of differentiator (type III) neurons cannot be explained by standard dynamical systems theory. This third type of excitable neuron encodes a dynamic change in the input and leads naturally to a transient response of the neuron. In this talk, I will show that "canards" - peculiar mathematical creatures - are well suited to explain the nature of transient responses of neurons due to dynamic (smooth) inputs.

This is joint work with John Mitry (University of Sydney) and John Rinzel (Courant Institute, NYU).

Aihua W. Wood

Air Force Institute of Technology, Department of Mathematics and Statistics, AFIT/ENC, 2950 Hobson Way, WPAFB, OH 45433-7765, aihua.wood@afit.edu

Topics on Electromagnetic Scattering from Cavities

The analysis of the electromagnetic scattering phenomenon induced by cavities embedded in an infinite ground plane is of high interest to the engineering community. Applications include the design of cavity-backed conformal antennas for civil and military use, the characterization of radar cross section (RCS) of vehicles with grooves, and

the advancement of automatic target recognition. Due to the wide range of applications and the challenge of solutions, the problem has been the focus of much mathematical research in recent years.

This talk will provide a survey of mathematical research in this area. In addition I will describe the underlining mathematical formulation for this framework. Specifically, one seeks to determine the fields scattered by a cavity upon a given incident wave. The general way of approach involves decomposing the entire solution domain to two sub-domains via an artificial boundary enclosing the cavity: the infinite upper half plane over the infinite ground plane exterior to the boundary, and the cavity plus the interior region. The problem is solved exactly in the infinite sub-domain, while the other is solved numerically. The two regions are then coupled over the artificial boundary via the introduction of a boundary operator exploiting the field continuity over material interfaces. We will touch on both the Perfect Electric Conducting and Impedance ground planes. Results of numerical implementations will be presented.

Cun-Hui Zhang

Rutgers University, Department of Statistics, Piscataway, NJ 08854, czhang@stat.rutgers.edu

Statistical Inference with High-Dimensional Data

We propose a semi low-dimensional (LD) approach for statistical analysis of certain types of high-dimensional (HD) data. The proposed approach is best described with the following model statement:

$$\text{model} = \text{LD component} + \text{HD component}.$$

The main objective of this semi-LD approach is to develop statistical inference procedures for the LD component, including p-values and confidence regions. This semi-LD approach is very much inspired by the semiparametric approach in which a statistical model is decomposed as follows:

$$\text{model} = \text{parametric component} + \text{nonparametric component}.$$

Just as in the semiparametric approach, the worst LD submodel gives the minimum Fisher information for the LD component, along with an efficient score function. The efficient score function, or an estimate of it, can be used to derive an efficient estimator for the LD component. The efficient estimator is asymptotically normal with the inverse of the minimum Fisher information as its asymptotic covariance matrix. This asymptotic covariance matrix may be consistently estimated in a natural way. Consequently, approximate confidence intervals and p-values can be constructed.

Zhiwei Zhang

Food and Drug Administration, Division of Biostatistics, Office of Surveillance and Biometrics, Center for Devices and Radiological Health, Silver Spring, MD 20993, Zhiwei.Zhang@fda.hhs.gov

Blinding Assessment and the Placebo Effect: A Causal Inference Perspective

Evaluation of medical treatments is frequently complicated by the presence of substantial placebo effects, especially on relatively subjective endpoints, and the standard solution to this problem is a randomized, double-blinded, placebo-controlled clinical trial. However, effective blinding does not guarantee that all patients have the same mentality with regard to the treatment received (or treatmentality, for brevity), making it difficult to interpret the usual treatment comparison as a causal effect. We discuss the causal relationships among treatment, treatmentality and the clinical outcome of interest, and propose a causal model for joint evaluation of placebo and treatment-specific effects. The model highlights the importance of measuring and incorporating patient treatmentality and suggests that each treatment group should be considered a separate observational study with a patient's treatmentality playing the role of an uncontrolled exposure. This perspective allows us to adapt existing methods for dealing with confounding to joint estimation of placebo and treatment-specific effects using measured treatmentality data, commonly known as blinding assessment data. We first apply this approach to the most common type of blinding assessment data, which is categorical, and illustrate the methods using an example from asthma. We then propose that blinding assessment data can be collected as a continuous variable, specifically when a patient's treatmentality is measured as a subjective probability, and describe analytic methods for that case.

Lin Zhou

New York City College of Technology, Mathematics Department, 300 Jay Street, Brooklyn, NY 11201,
lzhou@citytech.cuny.edu

Shear Responses of the VCM model for Wormlike Micellar Mixtures

The VCM (Vasquez, Cook and McKinley) model is a simple two-species kinetic model that was developed to study the rheology of wormlike micellar mixtures. Wormlike micelles are known as *living polymers* due to their continuous breakage and reforming even in equilibrium. The VCM model incorporates this key feature of the fluids and has been studied in a number of different flow conditions including elongational flow, pressure driven flow and Large Amplitude Oscillatory Shear (LAOS).

In this talk, numerical simulations of the VCM model, a set of coupled nonlinear partial differential equations, will be presented and compared with experimental results. The competing effects of elasticity, inertia, and diffusivity in the transient and steady state responses of the fluids will be discussed. Spatio-temporal results include the damped elastic shear waves, waves that can interfere with the creation of shear bands. The resultant multi-banded shear flow persists for long times when diffusive effects are small. Experimental confirmation of these predictions will be presented. Joint work with Pam Cook and Gareth H. McKinley.

Jun Zhu

University of Wisconsin-Madison, Department of Statistics and Department of Entomology, 1300 University Avenue, Madison, WI 53706, jzhu@stat.wisc.edu

Autologistic Regression Models for Spatial Binary Data

Autologistic regression models are suitable for relating spatial binary responses on a lattice to covariates. Model parameters can be estimated via maximum likelihood or Bayesian methods, although they often involve Monte Carlo simulation and tend to be computationally intensive. For large data samples, pseudolikelihood estimation is appealing due to its ease of computation, but several challenges remain. In this talk, I describe an approach to dealing with some of these challenges and illustrate the idea by numerical examples.

Zhengyuan Zhu

Iowa State University, Department of Statistics, Ames, IA 50011, zhuz@iastate.edu

Non-stationary Variance Estimation and Kriging Prediction

We study the estimation and plug-in kriging prediction of a non-stationary spatial process. We assume the process has smoothly varying variance function with an additive independent measurement error to account for the heteroskedasticity in the data. A difference-based kernel estimator of the variance function and a modified likelihood estimator of the measurement variance are used for parameter estimation. Asymptotic properties of these estimators and the plug-in kriging predictor are established. A limited simulation study is presented to test our estimation-prediction procedure and the performance of kriging predictor is compared with the spatial adaptive local polynomial regression estimator proposed by Fan and Gijbels (1995).

CONTRIBUTED TALKS

Peter Buchak

Imperial College London, Mathematics Department, Room 746, 180 Queen's Gate, London SW7 2AZ, UK, peter.buchak@gmail.com

Modeling of Viscous Flow in Fibers for Fabrication of MOF's Peter Buchak, Darren Crowdy, Yvonne Stokes

Cummings & Howell (JFM, 1999) showed that the drawing of a slender viscous fiber with simply connected cross section decouples into a 1D problem for stretching and a classical 2D free-boundary Stokes flow problem for sintering. Griffiths & Howell (JFM, 2008) extended this to fibers with annular cross section and found explicit solutions when such fibers are characterized by thin walls. We consider fibers with a cross section of general shape, not necessarily characterized by a small length scale, and of arbitrary connectivity. When the imposed pressure is the same on all boundaries, explicit formulas relate the evolution of a cross section to the 3D problem and give parameter values for realizing a desired configuration experimentally. We illustrate with several examples motivated by the manufacture of fibers whose cross sections are multiply connected. Our methods will be used to address problems in the fabrication of microstructured optical fibers (MOF's), for which the deformation of the channels during the drawing process is inadequately understood.

Carlos Colosqui

Levich Institute, City College of New York, 140th Street and Convent Avenue, New York, NY 10031, ccolosqui@ccny.cuny.edu

C.E. Colosqui, J.F. Morris, and H.A. Stone

Computational Modeling of Colloidal Assembly in Dip Coating

Dip coating from a particle suspension is a promising technique for the synthesis of colloidal crystals and nanostructured materials. The spontaneous formation of highly organized crystals have been observed experimentally when the withdrawn coating film is comparable to or smaller than the particle size. We have developed a computational approach that is suitable for the study of colloidal assembly in thin coating films. The developed mesoscopic approach has successfully simulated the spontaneous formation of regular arrays of particles, revealing the role of nontrivial hydrodynamic interactions coupled with capillary forces. I will present recent theoretical and numerical results (Colosqui et al. Phys. Rev. Lett. 2013) demonstrating a “hydrodynamically-driven” assembly that can lead to spontaneous pattern formation and highly ordered colloidal crystals. These findings indicate possible new directions for the flow-driven assembly of functional nanostructured materials.

Casey Diekman

The Ohio State University, Mathematical Biosciences Institute, Columbus, OH 43210, cdiekman@mbi.osu.edu

Derived Patterns in Binocular Rivalry Networks

Binocular rivalry is the alternation in visual perception that can occur when the two eyes are presented with different images. Hugh Wilson proposed a class of neuronal network models that generalize rivalry to multiple competing patterns. The networks are assumed to have learned several patterns, and rivalry is identified with time periodic states that have periods of dominance of different patterns. Here we show that these networks can also support patterns that were not learned, which we call derived. This is important because there is evidence for perception of derived patterns in the binocular rivalry experiments of Kovacs, Papathomas, Yang, and Feher. We construct Wilson networks for these experiments and use symmetry breaking to make predictions regarding states that a subject might perceive. The network models make expected the surprising outcomes observed in these experiments.

Longfei Li

University of Delaware, Mathematical Sciences Department, 501 Ewing Hall, Newark, DE 19716, longfei@math.udel.edu

Modeling Tear Film Dynamics with Time Dependent Flux Boundary Conditions on a 2D Eye-Shaped Domain

We explore the human tear film dynamics on a 2D eye-shaped domain. We used the Overture computational framework developed at LLNL, which employs overlapping grids and curvilinear finite difference methods, to conduct the numerical simulations using some modifications added at UD. By including evaporation and wetting forces, we are able to reproduce results from in vivo experiments and from previous 1D models that included evaporation. Time dependent flux boundary conditions were used to model the tear supply from the lacrimal gland and tear drainage via the puncta. Results show our model captures the hydraulic connectivity and other key physics of human tear film observed in vivo.

Gavin Lynch

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, gl32@njit.edu

On Procedures Controlling the False Discovery Rate for Testing Hierarchically Ordered Hypotheses

Complex large-scale studies, such as those related to microarray and quantitative trait loci, often involve testing multiple hierarchically ordered hypotheses. However, most existing false discovery rate (FDR) controlling procedures do not exploit the inherent hierarchical structure among the tested hypotheses. In this poster, I present key developments toward controlling the FDR when testing the hierarchically ordered hypotheses. First, I offer a general framework under which hierarchical testing procedures can be developed. Then, I present hierarchical testing procedures which control the FDR under various forms of dependence. Simulation studies show that these proposed methods can be more powerful than alternative methods.

Paola Malerba

University of Utah, Brain Institute, 36 S. Wasatch Drive, Salt Lake City, UT 84112, paola.malerba@utah.edu

Sub- and Supra- threshold Dynamics Determine Firing Rate Sensitivity to Additive Noise

Most firing rate models of neural coding postulate a smoothing effect of additive noise on the firing rate - mean current relationship (f-I curve). The change in f-I curves induced by input noise is considered a measure of sensitivity to noise, which can be functional in gain control. However, electrophysiological data collected by our group show different cell types with similar deterministic f-I curves that do not maintain similar f-I relationships when noise of comparable variance is added.

In this study, we focus on a relatively simple (3D) single neuron model that, with different parameter sets, reproduces the differential sensitivity to noise seen across cell types. The models match realistic values of gain, sub-threshold voltage fluctuations, and the mean voltage-current relationship. Our study shows that the I-v curves result from the balance between the ohmic properties of the model cell and its sodium current. Also, underlying the differential sensitivity to noise is the non-linear relation between mean voltage and instantaneous firing rate, which is affected by noise.

Most single-cell models have very steep f-I relationship at low rates, that result in extensive smoothing when fluctuations are introduced. Overall, we find in data and simulations less dramatic changes in f-I curves, and that cells with I-v curves that are relatively flat have a higher sensitivity to noise than cells with steeper I-v profiles.

Lisa Mayo

Queensland University of Technology, Mathematical Sciences School, GPO Box 2434, Brisbane QLD 4001, Australia, lisa.mayo@student.qut.edu.au

Lisa Mayo, Scott McCue, and Timothy Moroney

Queensland University of Technology, Mathematical Sciences School, GPO Box 2434, Brisbane QLD 4001, Australia, lisa.mayo@student.qut.edu.au

Numerical Solutions for Thin Film Flow Down the Outside and Inside of a Vertical Cylinder

A numerical study is presented to examine the fingering instability of a gravity-driven thin liquid film flowing down a vertical cylinder. The lubrication model which governs the evolution of the flow is dependent on two parameters; the first measures the dimensionless cylinder radius and determines the strength of substrate curvature on the

cylinder wall, and the second allows the user to switch between the regimes of flow on the inside and outside of the cylinder. The governing equation is found to be perfectly analogous to the well-studied equation for flow on an inclined, vertical or inverted plane, revealing an important relationship between substrate curvature and substrate inclination. Fully three-dimensional simulations depict a fingering pattern at the advancing contact line of the film on the cylinder wall. We find that curvature on the outer wall of the cylinder generally tends to increase the instability of the flow, while that on the inner wall has a stabilising effect.

Taoufik Meklachi

University of Houston, Department of Mathematics, 4800 Calhoun Road, Houston, TX 77004, tmeklachi@gmail.com

Anomalous Localized Resonance: A Summary of the Behavior of the Power Dissipation

In this paper we are studying the power dissipated inside a metamaterial slab of permittivity $\epsilon_s = -1 + i\delta$, exposed to a compactly supported charge distribution ρ , placed in a medium of permittivity $\epsilon_m = 1$. We investigate the sensitivity of the energy stored in the slab in terms of small changes in the permeability of the medium on the left hand side of the slab, $\epsilon_m = 1 + i(\delta + \delta^*)$. This allows to study the physical feasibility of the metamaterial in media with varying properties.

Kellen Petersen

Courant Institute of Mathematical Sciences, NYU, New York, NY 10012, kellen@cims.nyu.edu

Shape Optimization of Superhydrophobic Surfaces

Much of the interest in the superhydrophobic surface literature is focused on how surface structure affects superhydrophobicity and droplet hysteresis. Simple surface structures that have been studied include semicircular protrusions, circular protrusions, saw-tooth surfaces, semicircular grooves, and surfaces with parabolic pillars.

In collaboration with B. Wirth, I have formulated a constrained minimization problem where the objective functional that is to be minimized is a function of energy barriers depending on surface geometry. We use a gradient method to update the surface geometry. Through methods of adjoint minimization, the gradient of the objective is found to only depend on derivatives with respect to the surface, greatly simplifying the complexity of numerical implementation. With this method, we numerically solve the problem in the case of a simple network of metastable and saddle point states.

Eric Platt

University of Houston, Department of Mathematics, 4800 Calhoun Road, Houston, TX 77004, eplatt@math.uh.edu

Modeling Nonlinear Properties and Fracture Mechanics of Elasto-viscoplastic Materials by Use of an Integrity Property

Elastic materials can be modeled with the elasticity equation. However no real material is purely elastic. When under enough strain a material undergoes nonlinear behavior, plastic deformation and eventually fracture. By use of an additional variable called integrity and an additional coupled differential equation most of the properties can be described. With a numerical model stress-strain curves as well as the location and time of fracture can be determined.

Aleksandr Smirnov

Louisiana State University, Department of Mathematics, Baton Rouge, LA 70803, asmirn1@tigers.lsu.edu

A.V. Smirnov and Y.A. Antipov

Rapid Propagation of a Crack Parallel to the Boundary of a Half-plane

A two-dimensional dynamic problem on a half-plane with a semi-infinite crack parallel to the boundary is considered. The crack propagates with a constant speed, and the sub-Rayleigh regime is analyzed. Using the Wiener-Hopf technique, the problem is formulated as an order-2 vector Riemann–Hilbert problem whose matrix coefficient has the form $bI + cF$, where b and c are Hölder functions, and I and F are the unit and a meromorphic matrix with the zero trace respectively. Its solution is obtained for the steady-state case by two techniques. The first one approximates the meromorphic functions by finite products of rational functions and reduces the vector problem on a plane to a scalar problem on a compact Riemann surface (its genus depends on the number of the approximants).

used). The second technique formulates the Riemann-Hilbert problem as a system of singular integral equations on a semi-axis with respect to the derivatives of the displacement jumps. Its solutions is represented in terms of an orthonormal basis of the associated Hilbert space, the orthonormal Jacobi polynomials. The stress intensity factors and the weight functions are determined and computed. The second method is also generalized for the transient case. This generalization, in addition, requires the inversion of the Laplace transform with respect to time.

Jiannis Taxidis

Caltech, Division of Biology, 1200 E. California Blvd., Pasadena, CA 91125, jtaxidis@caltech.edu

Jiannis Taxidis¹, Kamran Diba², Costas A Anastassiou¹, György Buzsáki³, Christof Koch¹

¹Computation and Neural Systems, California Institute of Technology, Pasadena, CA 91125, USA

²Department of Psychology, University of Wisconsin at Milwaukee, Milwaukee, WI 53201, USA

³NYU Neuroscience Institute, New York University, New York, NY 10016, USA

Extracellular Field Signatures of CA1 Spiking Cell Assemblies

Although postsynaptic and transmembrane currents over local neuronal populations are considered the main factors for shaping local field potential (LFP) and current source density (CSD) fluctuations [1], high-frequency oscillatory LFPs can also be shaped by extracellular action potentials of pyramidal cell populations [2]. Sharp wave-ripple complexes (SWRs) are typical examples of such high-frequency oscillatory events, observed in hippocampal LFPs during deep sleep and awake immobility. They consist of an extensive depolarization in the CA1 dendritic layer (sharp wave) arising from population bursts in CA3, accompanied by a ~150-200 Hz LFP oscillation in the CA1 pyramidal layer (ripple). During SWRs, temporal firing patterns of correlated place cells, acquired during wakeful exploration, are replayed in fast-scale, providing a strong indication for the participation of SWRs in memory consolidation. Yet the particular effects of these pattern replays on the hippocampal extracellular field are largely unknown. How are the different ensembles of spiking cells encoded in the emerging ripple-LFPs? Here, we study this association through both a modeling and an experimental approach.

Firstly, we employ a spiking network model of the CA3 and CA1 hippocampal areas that reproduces key features of SWRs based on synchronous CA3 population bursts and strong, fast-decaying CA1 recurrent inhibition [3]. The synaptic input on CA1 pyramidal cells is implemented in a population of morphologically realistic, multi-compartmental models of CA1 pyramidal neurons, based on reconstructed cells [4]. The emerging extracellular fields accurately reproduce properties of SWR LFPs. By developing different spatial distributions of sets of CA1 cells that fire during ripples and others that remain silent, we explore in a systematic fashion the influence of spiking cell assemblies on the spatiotemporal characteristics of emerging extracellular fields during SWRs. In particular, we show how the different spatial arrangements of spiking cells give rise to differences in the depth-profile and CSD characteristics of raw and filtered LFPs.

Next, we apply our analysis to a set of LFPs and unit activity, recorded in vivo, from multiple locations in areas CA3 and CA1 of the rat hippocampus while animals run on a linear track with resting areas at both ends. The spiking activity of detected place cells, firing in sequence during the running sessions, is replayed in either forward or reverse order during SWRs occurring at the resting areas [5]. We trace the differences in the depth profile and CSDs of SWR LFPs between such forward and reverse replays. Based on our modeling results, we provide a link between systematic changes in the spatiotemporal features of the LFPs, with the corresponding ensembles that gave rise to each ripple episode.

This work provides a deeper understanding of the nature of extracellular fields and offers a new approach to the decoding of ongoing cell assemblies based on extracellular current flows. Differences in the emerging SWR field activity may play an important role in information processing during memory consolidation.

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Qiming Wang

University of British Columbia, Department of Mathematics, Vancouver, BC V6T 1Z4, Canada, qw6@math.ubc.ca

Breakup of a Poorly Conducting Liquid Thread in a Radial Electric Field

We study the breakup of an axisymmetric viscous liquid thread with finite conductivity immersed in another viscous fluid, which are confined to a concentrically placed cylindrical electrode that is held at a constant voltage potential. The annular fluid between the core thread and the electrode is assumed to be insulating. The flow then is driven by a radial electric field together with capillary and viscous forces. The nonlinear evolution and satellite drop formation near pinch-off are investigated by a combination of a long wave model and direct numerical simulation based on boundary integral method. The numerical results reveal that satellite formation as well as breakup time is affected significantly when the effect of charge convection is important compared with electric conduction. For large conduction, the evolutions of the thread are close to those obtained for a perfectly conducting core fluid. For relatively weak conduction, satellite structure becomes complex, depending on electric parameters and smaller satellite droplets are observed. Finally, we show that new scalings near breakup can be obtained from our long wave model, where thread is confined to a cylindrical tube that is initially placed close to the thread interface.

Jacek Wrobel

Tulane University, Department of Mathematics, 6823 St. Charles Avenue, New Orleans, LA 70118, jwrobel@tulane.edu

Surfactant Driven Tipstreaming in a Microfluidic Flow Focusing Device

We model a surfactant-mediated tipstreaming in a microfluidic flow focusing device. That microfluidic method for production of submicrometer and potentially nanoscale droplets and particles uses the elongational flow along with dissolved surfactant in one of the liquid phases to create strong surfaces tension gradient. The concentration of bulk soluble surfactant was found to significantly effect the mode of formation and size of the emitted droplets. By carefully controlling the surfactant concentration and other flow quantities, droplets can be created that are an order of magnitude or more smaller than the scale of both the device and droplets produced in the absence of surfactant.

Jiawei (Calvin) Zhang

University of California, Department of Mathematics, One Shields Avenue, Davis, CA 95616, jwzh@ucdavis.edu

Limb Coordination in Crayfish Swimming: the Neural Mechanisms and Mechanical Implications

A fundamental challenge in neuroscience is to connect behavior to the underlying neural mechanisms. Networks that produce rhythmic motor behaviors, such as locomotion, provide important model systems to address this problem. A particularly good model for this purpose is the neural circuit that coordinates limb movements in the crayfish swimmeret system. During forward swimming, rhythmic movements of limbs on different segments of the crayfish abdomen progress from back to front with the same period but neighboring limbs are phase-lagged by 25% of the period. This coordination of limb movements is maintained over a wide range of frequency. We examine different biologically plausible network topologies of the underlying neural circuit and show that phase constant rhythms of 0%, 25%, 50% or 75% phase-lags can be robustly produced. In doing so, we obtain necessary conditions on the network connectivity for the crayfish's natural stroke pattern with 25% phase-lags. We then construct a computational fluid dynamics model and show that the natural 25% back-to-front phase constant rhythm is the most efficient stroke pattern for swimming. Our results suggest that the particular network topology in the neural circuit of the crayfish swimmeret system is likely the result of evolution in favor of more effective and efficient swimming.

POSTERS

Zeynep Akcay

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, za25@njit.edu

Effects of Synaptic Plasticity on Phase and Period Locking of a Network of Two Oscillatory Neurons

We study the effects of synaptic plasticity on the determination of firing period and relative phase relations in a network of two oscillatory neurons coupled with reciprocal inhibition. We combine the phase response information of the neurons with the plasticity properties of the synapses to define Poincaré maps for the activity of an oscillatory network. The synaptic strength between the network neurons change dynamically with frequency according to the models we propose. On the other hand, these properties have an effect on determining the network frequency. We combine these two pieces of feed forward information to obtain feedback maps. These maps give the relative phases of the neurons and the network period as well as the dynamics of the synaptic strength from cycle to cycle. Fixed points of these maps correspond to the phase locked modes of the network. These maps allow us to analyze the dependence of the resulting network activity on the properties of network components. We do our analysis on a network of two Morris-Lecar neurons. We find conditions on the synaptic plasticity profiles and the phase response curves of the neurons for the network to be able to keep its firing period constant while varying its phasic relations or to keep a specific phasic relation fixed while varying its firing period.

Ali Allahverdi¹, Asiye Aydilek², and Harun Aydilek²

¹Department of Industrial and Management Systems Engineering, Kuwait University, P.O. Box 5969, Safat, Kuwait, Fax: +96524816137, e-mail: ali.allahverdi@ku.edu.kw

²Gulf University for Science and Technology, P.O. Box 7207, Hawally 32093, Kuwait, Fax: +96525307030, e-mail: aydilek.a@gust.edu.kw, e-mail: aydilek.h@gust.edu.kw

Minimizing the Number of Tardy Jobs on a Single Machine

Minimizing the number of tardy jobs is an important factor to consider while making scheduling decisions. This is because on-time shipments are vital for lowering cost and increasing customers' satisfaction. This paper addresses the single machine scheduling problem with the objective of minimizing the number of tardy jobs. The only known information is the lower and upper bounds for processing times, and deterministic job due dates. A dominance relation is established, and an algorithm is proposed. Several heuristics are generated from the proposed algorithm. Computational analysis indicates that the performance of one of the heuristics is very close to the optimal solution, i.e., on average, less than 1.5 % from the optimal solution. Keywords: Single machine scheduling, number of tardy jobs, heuristic.

Sonia Bandha

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, sb373@njit.edu

Sonia Bandha, Manish C. Bhattacharjee (deceased), and David Horntrop

Copula-based Modeling and Computational Solutions of Warranty Cost Management Problems

Much recent research on modeling and optimization of servicing costs for Non-Renewing Free Replacement Warranties (NR-FRW) assumes that a consumer's usage profile is constant and known. Such an assumption is unrealistic for moderately high value consumer durables. In such cases, it would be pragmatic to assume that the manufacturer/seller is uncertain about any customers fixed usage rate of the product; the usage rate is modeled by a probability distribution of the usage for target customers. This

research seeks to model and minimize the expected costs of pragmatic servicing strategies for NR- FRW warranties, using a Copula based approach to capture the adverse impact of increasing product usage rate on its time-to-failure. Since exact analytical solutions to these models are typically not obtainable, numerical methods using MATLAB and the Simulated Annealing algorithm for globally optimal cost minimization are used for computational solution. These methods and results are compared with those obtained from a well-known benchmark numerical example and then new results are derived.

Chenjing Cai

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, cc69@njit.edu

Bifurcation Properties of Nematic Liquid Crystals Exposed to an Electric Field: Switchability, Bistability and Multistability

Bistable Liquid Crystal Displays (LCDs) offer the potential for considerable power savings, compared with conventional (monostable) LCDs. The existence of two (or more) stable field-free states that are optically-distinct means that contrast can be maintained in a display without an externally-applied electric field. An applied field is required only to switch the device from one state to the other, as needed. In this paper we examine the basic physical principles involved in generating multiple stable states, and the switching between these states. We consider a two-dimensional geometry in which variable surface anchoring conditions are used to control the steady-state solutions and we explore how different anchoring conditions can influence the number and type of solutions, and whether or not switching is possible between the states. We find a wide range of possible behaviors, including bistability, tristability and tetrastability, and we investigate how the solution landscape changes as the boundary conditions are tuned.

Gabriel Chaves

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, gabriel.chaves@gmail.com

Energy Minimizers in Thin Ferromagnetic Nanorings with Four-Fold In-Plane Anisotropy

We present results obtained from micromagnetic simulations of thin ferromagnetic nanorings. We investigate annuli made of materials with non-negligible cubic anisotropy. In thin films the crystalline anisotropy favors magnetizations lying in the film plane along $\pm\hat{x}$ or $\pm\hat{y}$ directions. The magnetostatic energy separates into boundary and bulk terms. Our previous work provided a classification of remanent states based on the above contributions to the energy [1]. There are three regimes with distinct features of the remanent states depending on the dominant energy term. The magnetization configurations present four distinct domains. Different remanent states coexist in each of these regimes and they are characterized by the behavior of the domain walls spanning the annulus. Here, we compute the energies for these metastable states in a variety of ring dimensions and material parameters. In particular, we attempt to locate the ground state as a function of ring dimensions. This information is of importance for the design of magnetic storage devices based on configurations presenting 360° domain walls [2].

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Heejun Choi

Purdue University, Department of Mathematics, 150 N. University Street, West Lafayette, IN 47906, choi104@purdue.edu

A New Efficient Corrector of Spectral Deferred Correction for ODEs

We present a solver for ordinary differential equation which is based on spectral deferred correction (SDC). We use different kind of corrector whereas Euler's methods are applied as a corrector in SDC.

Our corrector is a high order method in the sense that order of accuracy increases by 2 at each correction while 1 in SDC. If the underlying problem is constant coefficient problem, the method is same as collocation method. Hence it is A-stable. The distribution of quadrature points can be arbitrary hence Gauss type points can be also used.

Carlo Fazioli

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, cfazzy@gmail.com

Overlapping Patches for Dynamic Problems

In this talk, we will briefly review the existing methods of "patches" for static surface problems. This method has been employed with considerable success to problems of potential theory and acoustic and electromagnetic scattering. It is desirable then, to consider using overlapping patches for dynamic surface problems, such as vortex sheet motion or fluid-fluid boundaries. We will discuss the obstacles faced when evolving patches in time, as well as the resolution of these obstacles. The talk will cover details of method, and attempts to solve a physical problem using the new techniques.

David Fox

NJIT-Rutgers, Department of Biological Sciences, Newark, NJ 07102, foxy1987@gmail.com

David Fox¹, Hua-an Tseng¹, Horacio Rotstein², Farzan Nadim^{1,2}

¹ Department of Biological Sciences, NJIT-Rutgers University, Newark, NJ 07102, USA

² Department of Mathematical Sciences, NJIT, Newark, NJ 07102, USA

Membrane Resonance of Bursting Neuron Captured with an I_{Ca}/I_h Model using Multi-objective Evolutionary Algorithms

Membrane potential resonance, a peak in the membrane impedance amplitude ($|Z|$) in response to oscillatory input current at a preferred frequency, is a common property of many neurons. It arises from interactions between passive membrane properties and voltage-gated ionic currents and has been implicated in the production of subthreshold and network oscillations. The PD neurons, one of the two cell types in the pyloric pacemaker group of the crab pyloric CPG, shows membrane resonance with a preferred frequency ($f_{max} \sim 1$ Hz) which is correlated with the network cycle frequency. The presence of membrane resonance in the PD neurons is sensitive to blockers of calcium currents I_{Ca} and the hyperpolarization-activated inward current I_h .

We used a single-compartment biophysical model comprising I_{leak} , a low-threshold inactivating I_{Ca} and I_h to capture the membrane impedance profile (Z vs. f_{input}) and the resonance in PD neurons. The impedance profile of the biological PD neuron and the model neuron were measured using a logarithmic sweeping-frequency (0.1 to 4 Hz) sinusoidal input ($A \sin(2\pi f(t))$) over 100 sec. The model parameters were constrained using biological data. We used the multi-objective evolutionary algorithm, non-dominated-sorting genetic algorithm (NSGA-II) to optimize five measurements defining the impedance profile: f_{max} , Z_{max} , Q (resonance power), $f_{1/2}$ (half-width) and Z_{fmax} which were characterized into objective functions to be minimized in the optimization process. The optimization process was constrained so that the solutions fit all five objectives to within the variability observed in the biological data to obtain a final optimal group of models, all of which would be considered a good fit to the experimental PD impedance profile. The dependence of the objectives on the parameters was explored by subjecting all 15 parameters for all models in the optimal group to a local sensitivity analysis. The distribution of the parameters, both in the optimal group and in the final generation, shows a tight constraint on the leak conductance as well as the half-activation ($V_{1/2_{Ca_{act}}}$) and half-inactivation ($V_{1/2_{Ca_{inact}}}$) of I_{Ca} , the half-activation ($V_{1/2_{h_{act}}}$) of I_h and the inactivation time constant of I_{Ca} but moderate constraints on g_{Ca} and g_h and little constraint on the activation/inactivation time constants and parameters associated with I_h . Most of the models are able to reproduce PD membrane resonance with just I_{Ca} alone. The parameter sensitivities show that, across all 48 models, positive changes in $V_{1/2_{Ca_{act}}}$ can increase Q and decrease $f_{1/2}$ (more peaky resonance profile)

whilst fixing f_{max} . The slope of the inactivation function of I_{ca} decreases the half-bandwidth and decreases power, and increasing the inactivation time constant decreases f_{max} . There is also an antagonistic relationship between $V_{1/2_Ca_act}$ and $V_{1/2_Ca_inact}$: the former decreases whereas the latter increases f_{max} . A pairwise-correlation analysis of all parameters showed that the mid-points for the steady-state activation and inactivation functions of I_{ca} were positively correlated, indicating that the calcium window current plays an important role in shaping resonance. We also show that some of these models can reproduce the shift in f_{max} when the voltage bounds of oscillation are changed.

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Gregory Funchess

University of Houston, Mathematics Department, Houston, TX 77096, gfunchess@gmail.com

Numerical Study of Anomalous Localized Resonance

We consider a slab of negative index material next to a charge distribution and observe the dissipated power. As the dissipation in the negative permittivity slab tends to zero the dissipated power has been shown to blow up to infinity. We observe that the rate the dissipated power blows up is highly sensitive to the surrounding permittivity.

Xinjun Guo

Brown University, School of Engineering, 184 Hope Street Box D, Providence, RI 02912, xinjun_guo@brown.edu

Xinjun Guo and Shreyas Mandre

Vortex Shedding in Flow Past an Airfoil using Boundary Layer Approximation

We investigate the flow passing by an airfoil at high Reynolds numbers for maximum energy extraction. The goal is to study the influence of unsteady dynamical effects like leading edge vortex, unsteady boundary layer separation, vortex recapture, etc. A conceptually simple and physically accurate method is proposed to account for the vortex shedding from structures at high Reynolds numbers. In the outer region far from the structure, the vortex methods are applied, which significantly reduces the computational cost compared to CFD in the whole domain. In order to describe accurately the location and strength of vortex shedding, we solve the simplified Navier-Stokes equations in the form of boundary layer approximation in the thin inner region close to the structure, rather than impose the Kutta condition.

Hamed Haddadi

Levich Institute, City College of New York, 140th Street and Convent Avenue, New York, NY 10031, haddadi.h81@gmail.com

Hamed Haddadi and Jeffrey Morris

Microstructure and Rheology of Neutrally Buoyant Spherical Suspensions at Finite Inertia

The role of particle scale inertia on microstructure and Rheology of mono-disperse suspensions of non-Brownian neutrally buoyant spherical particles has been studied. Inertia at particle scale is characterized by the Reynolds number defined as γ^+ , in which γ^+ is the shear rate, a is the particle

radius, and ν is the kinematic viscosity. The other dimensionless number is volume fraction which is denoted as ϕ . Trajectories and velocities of particles are extracted via numerical simulations using lattice-Boltzmann (LB). To study the microstructure the effect of fluctuating motions of particles due to interaction with other particles is screened and the advection flux of the pair probability, g , is calculated and compared with the result of simulations. In the next step, fluctuating motions are incorporated and the total flux of g is cast into an advection-diffusion equation which is solved numerically. The relationship between microstructure and stress system of suspensions has been examined by sampling the pair space and mapping the corresponding Stresslet at various pair separations on the shear plane. In addition, the contribution of acceleration stress and the Reynolds stress due to velocity fluctuations has also been detailed.

Muhammad Hameed

University of South Carolina, Div. of Mathematics & Computer Science, Spartanburg, SC 29303, mhameed@uscupstate.edu

Peristaltic Transport and Heat Transfer of a MHD Fluid of Variable Viscosity

The influence of temperature-dependent viscosity and magnetic field on the peristaltic flow of an incompressible, viscous Newtonian fluid is investigated. The governing equations are derived under the assumptions of long wavelength approximation. A regular perturbation expansion method is used to obtain the analytical solutions for the velocity and temperature fields. The expressions for the pressure rise, friction force and the relation between the flow rate and pressure gradient are obtained. In addition to analytical solutions, numerical results are also computed and compared with the analytical results with good agreement. The results are plotted for different values of variable viscosity parameter β , Hartmann number M , and amplitude ratio ϕ .

David Horntrop

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, horntrop@njit.edu

Todd Caskey, Albi Kavo, Mandeep Singh, David J. Horntrop

Variance Reduction Techniques for Stochastic Differential Equations

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

Stephen Keeley

New York University, Center for Neural Science, 4 Washington Place, 8th Floor, New York, NY 10003, StephenLKeeley@gmail.com

Modeling Fast and Slow Gamma Bands in the Rat Hippocampus

Gamma rhythms in rat hippocampus are thought to be important for a variety of cognitive tasks. When analysing LFP recording from CA1 in the hippocampus, two gamma regimes emerge in distinct parts of the theta cycle: slow (30-50 Hz) and fast (60-90 Hz). Here, we propose a model that suggests two types of interneurons and the differing time courses of their post-synaptic effects may be responsible for mediating oscillations in two distinct regimes. Using an integrate and fire model, we show how interplay between the excitatory population and two differing interneuronal

populations can cause the system to fall into one or two oscillatory regimes. Our model makes 3 explicit predictions about a network that works in such a way. One, it demonstrates that the slow inhibitory population must significantly limit its firing rate in the case of a fast gamma oscillations, but this need not be true for the fast inhibitory populations in the cases of slow gamma. Two, it shows that the increased input needed to switch a state from slow to fast gamma must act on both the inhibitory and excitatory population, and particularly in must lower the subthreshold voltage to increase the tendency for the fast inhibitory population to fire. 3, it illustrates a necessity for the fast and slow inhibitory populations to interact with each other, and particularly for the fast inhibitory population to have a selective ability to silence the slow inhibitory population. We corroborate this model with physiological network connectivity and interneuronal data from the experimental literature. We suggest that the fast gamma regime is mediated via basket or axoaxonic cells, and slow oscillatory regime mediated via bistratified cells.

Christopher Kim

University of Minnesota, School of Mathematics, Minneapolis, MN 55455, cmkim@math.umn.edu

Contracting Convex Torus in Hyperbolic Manifolds by its Harmonic Mean Curvature: Theoretical and Numerical Studies

We consider the harmonic mean curvature flow (HMCF) of convex torus around a closed geodesic in Hyperbolic 3-manifolds. Assuming the initial surface is axially symmetric, strictly convex and its $HMC < 1/2$, we show that the evolving surface becomes cylindrical as it converges to the closed geodesic by obtaining optimal asymptotic estimates of both principal curvatures: $\lambda_1 \approx e^{-t}$ and $\lambda_2 \approx e^t$, thus $\lambda_1 \lambda_2 \approx 1$. A numerical solution of general torus evolving under HMCF is studied using spectral methods. For axially symmetric surfaces, we verify that the numerical solution is in agreement with theoretical estimates and gives better curvature estimates. However, general torus found to be sensitive to the direction of initial perturbation and passes only low frequency components in θ direction.

Lenka Kovalcinova

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, lk58@njit.edu

Properties of Force Networks of Slowly Compressed Granular Matter

Force chains in granular material have been studied extensively by the scientific community over the years. Statistical approaches have been used to give some insights on the forces distribution inside the granular medium. They offer a quantitative perspective on the forces but no spatial information is being contained. We consider a set of circular particles confined in a square domain with rough walls composed of monodisperse particles and slowly squeeze the system. Using the numerical tools, we analyze our system around the jamming transition and for higher volume fractions. We look at the influence of various parameters on our system - such as system size, compression speed, polydispersity, etc. Statistical physics and recent results infer the universality and scaling laws of the mean cluster size, with several critical exponents. We try to find these parameters numerically using different approaches.

Michael Lam

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights,
Newark, NJ 07102, mal37@njit.edu

Thin Film Nematic Liquid Crystal Down an Incline Substrate: Two Dimensional Flow

In this presentation, the flow of nematic liquid crystals (NLC) down an inclined substrate is studied. Under the usual lubrication approximation, the Leslie Erickson equations for a NLC are reduced to a 4th order nonlinear partial differential equation of diffusion type. Furthermore, a precursor film and the relaxation of the preferred anchoring on the free surface are included into the model. Under these assumptions, standard linear stability theory is used to analyze the nematic effects on traveling wave solutions. Particularly, the regimes for stability, convective instability and absolute instability of such solutions are found. These results are then confirmed by the full numerical simulations of the non linear long wave model.

Weifan Liu

Worcester Polytechnic Institute, Mathematical Sciences Department, 100 Institute Road, Worcester,
MA 01609, weifanliu@wpi.edu

Modeling Calcium Dynamics and Muscle Mechanism

Currently, most models on muscle contraction do not account for the effect of calcium concentration on a microscopic level, which could significantly affect the cross-bridge attachment and thus the force. We investigate the role of calcium dynamics on muscle contraction by proposing a simplified two-compartment calcium movement model for skeletal muscle of frog. To capture the muscle contraction mechanism driven by calcium dynamics, we coupled the system of ODEs for the Distribution Moment Model to the calcium concentration and Hodgkin-Huxley equation. Additionally, we accounted for the effect of calcium inactivation mechanism, which enabled us to produce a more authentic cytosolic calcium concentration. We modified the velocity of muscle contraction to be a variant using a damped spring mass system, as opposed to the constant velocity used in previous models. With this coupled model, we are able to investigate the role of accounting for a time dependent calcium concentration on force generation of frog. Simulation results will be presented to show how the proposed model is an accurate and efficient model that captures the muscle contraction mechanism and calcium-force relationship observed in experiments.

Kyle Mahady

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights,
Newark, NJ 07102, ktm4@njit.edu

Combined Mesoscopic-Macropscopic Computations of Thin Films and Contact Lines

When fluid is placed on a solid surface, the angle at which its surface meets the substrate will, at equilibrium, be equal to a specified contact angle. This angle arises due to van der Waals forces between particles of the liquid, solid, and ambient vapor, acting on the nanoscale. The Volume of Fluid (VoF) method is a popular method used to solve the two phase Navier Stokes equations, which conventionally treats contact angles geometrically by rigidly imposing an angle for the fluid surface on the substrate. Our work explores a physical approach which incorporates van der Waals forces into the VoF method, and allows it to treat physics which are ignored by the geometric implementation. In particular, we show that using this method we can capture film rupture, as well as dynamic and static features of the contact angle. This work has applications in nanofabrication, where bottom up nanoscale assembly is increasingly modeled by continuum fluid models.

Shreyas Mandre

Brown University, School of Engineering, 184 Hope Street Box D, Providence, RI 02912,

Shreyas_Mandre@brown.edu

Dissolution Driven Convection for Carbon Dioxide Sequestration: The Stability Problem

The dissolution-driven convection in porous media is potentially a rate limiting process for sequestering carbon dioxide in underground aquifers. Super critical carbon dioxide introduced in the aquifer is lighter than the water that fills the surrounding porous rock, and hence quickly rises to the top. However, the solution of carbon dioxide in water is heavier than water. Hence, as the layer of carbon dioxide dissolves in the water, convection may ensue. The threshold criteria for convection is obscured by the continually changing background density profile as the carbon dioxide diffuses through the pores. Commonly used techniques such as frozen coefficient analysis or non-modal theories using transient amplifications yield substantially different results for the threshold, which has been the cause of a debate in the scientific community.

We present a general theory for the linear stability of non-autonomous systems and present an example of its use for dissolution driven convection. The technique identifies the spectral radius of the propagator of the linear operator as the appropriate measure for the amplification of initial perturbations by the linearized dynamics. The technique unifies the classical modal stability theory using eigenvalues, the non-modal approaches using optimal growth of energy and the frozen coefficient analysis. We settle the debate, and demonstrate the existence of a threshold time for convection to commence. We also show that asymptotically the amplification rate grows as $\exp(C t^{1/2})$, for a dimensionless constant C and the most amplified wavenumber decays as $t^{-1/2}$.

John McClain

University of New Hampshire, Integrated Applied Mathematics Program, 33 Academic Way, Durham, NH 03824

A Wave Matching Method for Analysis of Low-Energy Electron Microscopy/Diffraction Spectra

The analysis of experimental data from low-energy electron microscopy/diffraction (LEEM/LEED) requires modeling the scattering of electrons off the system being probed. We present a computational method, using density-functional theory (DFT), to calculate LEEM reflection spectra of semiconductor thin-films, including graphene. We solve the Schrodinger equation for a three region domain with a Bloch wave matching approach, making use of self-consistent potentials obtained from supercell DFT calculations, which more accurately represent semiconductors than the muffin-tin potentials of traditional approaches. In the supercell approach, periodicity of the potential is assumed not only in the plane of the surface but also in the direction perpendicular to the surface; the supercell contains layers of a crystalline sample surrounded by a layer of vacuum on either side. We present successes and remaining challenges in using numerical solutions from this artificially periodic system to accurately reproduce experimental spectra. This includes comparisons to experiment for graphene systems, as well as investigations of simple model systems.

Michael Miller

Brown University, School of Engineering, 184 Hope Street Box D, Providence, RI 02912, michael.j.miller@brown.edu

Michael Miller, Khoi Nguyen, and Shreyas Mandre***Fluid Surface Deformation by Objects in the Cheerios Effect***

Small objects floating on a fluid/air interface deform the surface depending on material surface properties, density, and geometry. These objects attract each other through capillary interactions, a phenomenon dubbed the “Cheerios effect.” The attractive force and torque exerted on these objects by the interface can be estimated if the meniscus deformation is known. We present a series of

experiments focused on visualizing the motions of the floating objects and the deformation of the interface. The experiments involve thin laser-cut acrylic pieces attracting each other while floating in a water bath. A variety of methods are attempted to visualize and characterize the water surface deformation near the edge of the objects through techniques utilizing the optical distortion generated by a meniscus. This study of the deformation of the water surface around a floating object, a study of the attractive/repulsive forces, and of post-contact rotational dynamics are potentially instrumental in the study of self-assembly on a liquid interface.

Naga Munsunuri

New Jersey Institute of Technology, Department of Mechanical & Industrial Engineering, University Heights, Newark, NJ 07102, nam9@njit.edu

Naga Musunuri, Daniel Codjoe, Bhavin Dalal, Ian Fischer, and Pushpendra Singh

Transient Flow Induced by the Adsorption of Particles

When small particles, e.g., glass, our, pollen, etc., come in contact with a fluid-liquid interface they disperse so quickly to form a monolayer on the interface that it appears explosive, especially on the surface of mobile liquids like water. This is a consequence of the fact that the adsorption of a particle in an interface causes a lateral flow which on the interface away from the particle. In this study we use the particle image velocimetry (PIV) technique to measure the transient three-dimensional flow that arises due to the adsorption of spherical particles. The PIV measurements show that the flow develops a fraction of a second after the adsorption of the particle and persists for several seconds. The fluid below the particle rises upwards and on the surface moves away from the particle. These latter PIV results are consistent with the surface velocity measurements performed in earlier studies. The strength of the induced flow, and the time duration for which the flow persists, both decrease with decreasing particle size. For a spherical particle the flow is axisymmetric about the vertical line passing through the center of the particle.

Evgeni V. Nikolaev and Eduardo D. Sontag

Rutgers University, Department of Mathematics, Hill Center - Busch Campus, 110 Frelinghuysen Road, Piscataway, NJ 08854

To whom correspondence should be addressed: Professor Sontag, Tels.: (732) 445-2390, 3072;

Fax: (732) 445-5530; E-mails: sontag@math.rutgers.edu, eduardo.sontag@gmail.com.

Global Organization of Conserved-moiety Pools in Genome-scale Metabolic Reconstructions and Signaling Networks

The advent of bioinformatic and computational biology tools has greatly improved our ability to analyze genome-scale datasets obtained from high-throughput experimental measurements to infer the structure of complex networks. Despite the improvements, the existing deterministic and stochastic tools are not enough to get a deeper insight into the global molecular organization principles of conserved-moiety pools inherent in genome-scale metabolic reconstructions and signaling networks. As a result, the role that such pools can play in pure stoichiometric (e.g., non-allosteric) regulation of metabolic pathways and covalent modifications of signaling networks still remains essentially unknown. In this work, we present a novel theoretical and practical approach to elucidate the sparsest irreducible conserved-moiety pools with nonnegative coefficients from genome-scale reaction networks. To begin addressing the global organization and function of such pools, we discuss 26 stoichiometric models of metabolism and signaling pathways that represent species from all three domains of life (i) Archean, (ii) Bacteria, and (iii) Eukarya.

The complexity of the pathways ranges from the metabolism of *Mycoplasma pneumoniae*, a threatening pathogen with the smallest genome, TLR and EGFR signaling networks, up to a

comprehensive metabolic reconstruction of human metabolism (Recon-2). Implications of the analysis in biotechnology and human diseases are also discussed.

Motolani Olarinre

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, mto3@njit.edu

Motolani Olarinre, Horacio Rotstein, and Jorge Golowasch

A Modeling Study of Conductance Co-regulation in Neuronal Models

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

Archana Proddutur

UMDNJ, Department of Neurology and Neurosciences, 185 S. Orange Avenue, Newark, NJ 07103, ap269@njit.edu

Archana Proddutur¹, Jiandong Yu¹, Fatima S. Elgammal¹ and Vijayalakshmi Santhakumar^{1,2}

¹Department of Neurology and Neurosciences, ²Department of Pharmacology and Physiology, NJ Medical School, University of Medicine and Dentistry of NJ, Newark, NJ 07103

Seizure-induced Plasticity of Fast-spiking Basket Cell GABA Currents Modulate Frequency and Coherence of Gamma Oscillation in Network Simulations

Gamma frequency oscillations are crucial for memory formation and retrieval. Networks of fast-spiking basket cells (FS-BCs) interconnected by fast, high amplitude GABA synapses and gap junctions are known to underlie development of gamma oscillations. Recent studies have identified that, FS-BCs in the hippocampal dentate gyrus have GABAergic currents mediated by extrasynaptic receptors. Moreover, following experimental seizures, FS-BC extrasynaptic (tonic) GABA currents are enhanced and GABA reversal potential (EGABA) shifted to depolarizing potentials compared to controls. Here, we use homogeneous networks of biophysically realistic model FS-BCs to examine how the presence of extrasynaptic GABA conductance (gGABA-extra) and seizure-induced changes in gGABA-extra and EGABA influence network activity. Networks of FS-BCs interconnected by fast GABAergic synapses developed synchronous firing in the gamma frequency range. Systematic investigation of the effect of FS-BC interconnectivity on network synchrony revealed that the biologically realistic range of 30 to 40 connections between FS-BCs resulted in greater coherence at gamma frequency, when networks were activated by Poisson-distributed synaptic inputs rather than by heterogeneous current injections. Consistent with earlier studies, inclusion of gap junctions and distance-dependent conduction delay at synapses resulted in a modest enhancement of network coherence. In networks activated by heterogeneous current injections, increasing gGABA-extra modulated the frequency and coherence of network firing when EGABA was shunting (-74 mV), but

failed to alter network firing when EGABA was depolarizing (-54 mV). When FS-BCs were activated by dendritic synaptic inputs, enhancing gGABA-extra reduced the frequency and coherence of FS-BC firing when EGABA was shunting and increased firing frequency when EGABA was depolarizing. Shifting EGABA to depolarizing potentials consistently enhanced firing by over 30 Hz shifting network firing to the high gamma frequency range (>80 Hz). Our demonstration that network oscillations are modulated by extrasynaptic inhibition in FS-BCs suggests that neuroactive compounds that act on extrasynaptic GABA receptors may impact memory formation by modulating hippocampal gamma oscillations. The simulation results indicate that the depolarized FS-BC EGABA, observed after experimental seizures, together with enhanced spillover extrasynaptic GABA currents are likely to promote generation of high gamma frequency activity associated with epileptic networks.

Aminur Rahman

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, ar276@njit.edu

Aminur Rahman and Denis Blackmore

A Scheme for Modeling and Analyzing the Dynamics of Logical Circuits

An algorithm is developed to map Boolean algebraic functions of discrete circuits to elementary algebraic functions. In the paper by Blackmore, Rahman, and Shah, it is shown how a rather simple discrete planar algebraic dynamical model of the R-S flip-flop circuit can mimic the dynamical behavior observed for its physical realizations. However, the model was developed in an ad-hoc manner, rather than from first principles. A systematic - algorithmic - first principles based approach is developed in order for such dynamical models to more accurately reflect observed behavior and facilitate further investigation. Also, it is demonstrated how this fundamental algorithmic approach can, with similar ease, be used to obtain discrete dynamical models of other more complicated logical circuits.

Jaime Gomez Ramirez

Universidad Politecnica de Madrid, Autonomous Systems Laboratory, Jose Gutierrez Abascal, 2 Madrid 28006, Spain, jd.gomez@upm.es

Understanding the Inverse Problem in Biological Modeling: Lessons from Neuroscience

The inverse problem is to infer the value of parameters of interest for a given phenomenon, based on the direct measurement of observables. This form of inference is ill-posed in the sense that solutions to the problem may not exist, be multiple, and be unstable, that is, small errors in the measurements lead to large differences in the solution (Hadamard, 1923).

In (Brenner, 2010), Brenner has pointed out that deducing function models based on behavior is an inverse problem impossible to solve. According to this view, the standard approach followed by systems biologists which mainly relies upon system identification is flawed. The working hypothesis of this presentation is in frontal opposition with that rationale. Here it is argued that rather than abandon the inverse problem, it is precisely by adopting a "inverse thinking approach" in biological systems modeling, that effective progress can be made. In the presentation we attempt to clarify the conceptual and methodological obstacles that lie in the inverse problem in biological systems modeling. We review the recent progress made in the study of the Neural Coding Problem i.e., the uncertain relationship between cognition and neural activity, highlighting its major technical and conceptual challenges. It will be explained why the difficulties in characterising the neural patterns associated with external stimuli, which are commonly attributed to the high dimensionality and complexity in either neural and stimuli space or to technical limitations in the measurement of brain activity, reside in a more fundamental reason which is the ill-posed nature of the inverse problem. The classical approach to the inverse problem in biological modeling which is general and optimal is

critically revised here and a theoretical framework which describes probability distributions conditional on biophysical mechanisms is presented (Gomez-Ramirez, Sanz, 2013).

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Horacio Rotstein

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, horacio@njit.edu

Eran Stark, Gyorgy Buzsaki, Horacio G. Rotstein

Mechanism of Generation of Theta Spiking Resonance in a Hippocampal Network

This work is based on recent experimental results using optogenetic tools to stimulate both pyramidal cells (PYR) and parvalbumin-immunoreactive interneurons (INT) in the hippocampus of freely-behaving rodents. In vitro, PYR-cells exhibit theta range subthreshold (membrane potential) resonance, a peak in the subthreshold voltage response to sinusoidal input currents at a preferred (resonant) frequency. Whether and how this preferred frequency response translates to spiking resonance in behaving animals is unknown. In vivo, individual directly stimulated PYR-cells exhibited narrow-band spiking centered on a wide range of frequencies rather than spiking predominantly at theta. In contrast, in vivo INT photostimulation indirectly induced theta band-limited spiking in pyramidal cells accompanied by post-inhibitory rebound spiking. We present a minimal biophysical (conductance-based) model of CA1 hippocampal network that qualitatively reproduces the experimental results. This model includes three cell types: PYR, INT and OLM (oriens-lacunosum moleculare) cells. We find that the presence of subthreshold resonance in isolated PYR-cells is not enough to generate robust theta-band spiking resonance in PYR cells embedded in this network model. Theta-band spiking resonance was especially robust when the model included a timing mechanism, implemented by either a network-mediated time inhibition provided by the OLM cell or synaptic depression of the INT synapses.

Ivana Seric

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, is28@njit.edu

Long-wave Approximation of a Ferrofluid Film under an External Magnetic Field

We consider a thin layer of viscous and non-conducting ferrofluid film subjected to an applied uniform magnetic field with a non-magnetizable passive gas atop. Governing equations are the static Maxwell equations coupled with the incompressible Navier–Stokes equations. We derive a thin film equation that governs the non-linear evolution of the interface and study the linear stability of the interface in the long-wave limit. The thin film equation is solved numerically and the results are compared with the linear stability analysis.

Ryohei Seto

Levich Institute, City College of New York, 160 Convent Avenue, New York, NY 10031, setoryohei@me.com

Ryohei Seto, Romain Mari, Jeffery Morris, and Morton Denn

Discontinuous Shear Thickening Simulation: Contact Dynamics in Viscous Fluids

We introduce a simulation model to capture abrupt shear thickening (ST) of non-Brownian concentrated suspensions. Historically, with simulation schemes born in the field of hydrodynamics, particle surfaces have been considered as a boundary condition of (Navier-)Stokes equations. Close particles are interacting through lubrication, which shows a diverging resistance at contact. These simulations have succeeded to capture mild ST of semi-dilute suspensions, but do not capture the discontinuous ST observed at high volume fractions. In this work, unlike previous works with lubrication force models, we allow particles to come into contact, assuming that there is some breakdown in the lubrication singularity. To simulate the contacting particles, we borrow a frictional contact model from granular physics. We are able to recover the discontinuous shear thickening, which appears as a dynamic jamming transition. We point out the essential role of friction and colloidal forces, and discuss the relation with the static jamming transition.

Umeshkanta S. Thounaojam¹, Sharon E. Norman³, Srisairam Achuthan¹, Jianxia Cui², Robert J. Butera,³ and Carmen C. Canavier¹

¹ Department of Cell Biology and Anatomy, LSU Health Sciences Center, New Orleans, LA 70112, USA

² BioCircuits Institute, University of California, San Diego, La Jolla, CA, 92093, USA

³ Laboratory for Neuroengineering, School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, GA, 30332, USA

Intrinsic Noise Drift Accounts for Variability in Hybrid Neural Circuits

Synchrony within and between brain regions has been implicated in many aspects of cognition, movement, and disease. In order to explore general principles of synchronization between synaptically coupled neurons, we constructed hybrid circuits of one model and one biological neuron using the dynamic clamp. The synchronization tendencies of each isolated neuron were characterized by measuring how much a single input from the other neuron transiently shortened or lengthened the cycle period of the oscillation. We used this information to construct a map to predict the cycle by cycle dynamics of the hybrid circuits. Most experiments exhibited transitions between phase locking and phase walkthrough. We hypothesize that these transitions result from bifurcations in which fixed points of the map emerged or disappeared. We tested the ability of three noise models to account for these transitions. A model in which the intrinsic period of the biological neuron evolved as a slow random process best explained the data. Our main result is that both the bifurcation structure and the form of the dynamical noise are critical for understanding episodes of phase-locked activity in neural systems.

Oleksiy Varfolomiyev

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, ov5@njit.edu

A Non-stiff Boundary Integral Method for Internal Waves

We study the internal waves as the evolution of the interface between two immiscible, inviscid, incompressible, irrotational fluids of different density in three dimensions. Motion of the interface and fluids is driven by the action of gravity, surface tension, and/or a prescribed far-field pressure gradient. The model includes derived equations for the evolution of the interface and surfaces density. Presence of the surface tension introduces high order derivatives into the evolution equations. This makes the considered problem stiff and the application of the standard explicit time-integration methods suffers strong time-step stability constraints.

Our proposed numerical method employs a special interface parameterization that enables the use of implicit time-integration methods via a small-scale decomposition. This approach allows us to

capture the nonlinear growth of normal modes for the case of Rayleigh-Taylor instability with the heavier fluid on the top. In addition, in the given test problem with the prescribed initial disturbance to a flat interface under an action of the surface tension dominating the gravity, the surface relaxes to a flat interface. Linear stability analysis is performed and the numerical results are validated by comparison to the obtained analytic solution of the linearized problem for a short time. The developed model and numerical method can be efficiently applied to study the motion of internal waves for doubly periodic interfacial flows with surface tension.

Shaobo Wang

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, sw228@njit.edu

Shaobo Wang and Shidong Jiang

Fast Algorithms for Vector Spherical Harmonic Transforms

Vector spherical harmonic transforms have been useful for many problems in scientific computing. Some applications include scattering problem for Maxwell's equations by a sphere, weather prediction and climate modeling, and cosmic microwave background radiation data analysis. The classical algorithms for vector spherical harmonic transforms require $O(L^3)$ operations, where L is the highest degree of the spherical harmonics in the expansion. We have developed a fast algorithm for vector spherical harmonic transforms. The complexity of the fast algorithm is $O(L^2 \log L)$. The algorithm is an extension of Mark Tygert's fast algorithm for scalar spherical harmonic transforms using the butterfly algorithm. The performance of our algorithm is illustrated via several numerical examples.

Hao Wu

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights, Newark, NJ 07102, wh45@njit.edu

Hao Wu and Denis Blackmore

Investigation of an Integro-PDE Model for Granular Flow

The BSR model is an integro-partial differential equation developed by Blackmore, Samulyak, and Rosato to predict a wide variety of granular flow regimes. Using techniques similar to those employed for the Boltzmann-Enskog equation, we prove that under fairly general assumptions, the BSR model has a unique global solution that depends continuously on auxiliary conditions. Our proofs inspired the creation of a semi-discrete numerical scheme for obtaining approximate solutions of the BSR model, which was used to produce the results of simulations that will be presented. The analytical results obtained are compared with the simulations for the case of periodically tapping a vertical column of particles and good agreement is observed. We also investigate the existence and stability of travelling wave solutions.

Yang Zhang

New Jersey Institute of Technology, Department of Mathematical Sciences, University Heights,
Newark, NJ 07102, yz83@njit.edu

Predicting the History-Dependence of Conduction Delay in an Unmyelinated Axon Using a Computational Model

Yang Zhang¹, Dirk Bucher^{2,3}, Farzan Nadim^{4,1}

¹ Department of Mathematical Sciences, New Jersey Institute of Technology, Newark, NJ 07102

² The Whitney Laboratory for Marine Bioscience, University of Florida, St. Augustine, FL 32080

³ Department of Neuroscience, University of Florida, Gainesville, FL 32603

⁴ Federated Department of Biological Sciences, NJIT and Rutgers University, Newark, NJ 07102

Conduction delay in axons is defined as the time required for an action potential to propagate from one point to another. It is a function of the axon's passive membrane properties, voltage-gated ion channels and the Na^+/K^+ pump. It also can be substantially affected by neuromodulators. Conduction delay of action potential generated by motor axon in stomatogastric ganglion (STG) shows significant variability with ongoing bursting or Poisson stimulation. The mean value (D_{mean}) and coefficient variation of conduction delay (CV-D) increase with time, and the relationship between delay and instantaneous stimulus frequency (F_{inst}) is non-monotonic. In order to investigate the temporal fidelity of spike propagation of conduction delay, we built a biophysical model of an unmyelinated axon to examine the contribution of different ionic currents in shaping the slow and fast timescale effects of conduction delay. The biophysical model captures most of the changes at the slow and fast timescale effects of conduction delay with burst and Poisson stimulations at different mean rates, as seen experimentally. We developed an empirical formula as a linear function of trough and peak voltages of each spike, which can be used to predict conduction delay both for biophysical model and experimental results. These results indicate that conduction delay of action potentials depend on both short- and long-term history of activity, with potentially significant effects on temporal fidelity of spike propagation and temporal coding.