

# CONTRIBUTED PAPERS

Silas Alben

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## ***The Fin Ray as a Motion Transducer***

Our work considers the mechanics of swimming fish. In collaboration with the Lauder lab at Harvard, we are studying the structure of fish fin rays. Approximately half of all fish species utilize the same basic structure to transduce fin ray shape and motion from a given input force. We present a simple coupled elastica model which uses only geometry and a single elastic constant to obtain the scalings of forces and displacements. We will also present fin ray structures which are optimal for force output.

Christina Ambrosio

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## ***The Control of Frequency of an Excitable Network Simultaneously Subjected to Multiple Oscillatory Inputs***

Biological networks responsible for the generation of rhythmic motor output often involve a pair or pairs of reciprocally inhibitory neurons that burst in alternation. The triggering of such bursts often requires multiple rhythmic inputs, thus, making the network a conditional oscillator. Here, we study a set of reciprocally inhibitory neurons lying in the stomatogastric ganglion (STG) of the stomatogastric nervous system of the crab *Cancer borealis*. This pair of neurons is responsible for generating the gastric mill rhythm which is involved in the digestive process of the animal. The aim of this work is to mathematically explain the role of two oscillatory inputs, a fast pyloric input and a slow modulatory input, that act in coordination to set the frequency of the gastric mill rhythm. In particular, we mathematically explain experimental results in which it is shown that the pyloric input increases the gastric mill frequency when the modulatory input is tonic but does not increase the frequency when the modulatory input is rhythmic. Reduction techniques are used to reduce the modeling set of equations to a study on lower dimensional slow manifolds and the fast transitions between them. This enables us to geometrically show through phase plane analysis, the exact role that each of the inputs plays in determining the frequency of the gastric mill rhythm and it reveals the importance of the timing between such inputs. We conclude that for a small delay between the timing of the pyloric and modulatory inputs, the gastric mill rhythm frequency is only determined by the dynamics of the modulatory input as is seen experimentally in the biological network. For a larger delay, however, the inputs work together to speed the frequency. Joint work with Amitabha Bose (NJIT) and Farzan Nadim (NJIT and Rutgers University).

Roman Andrushkiw

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## ***On the Spectral Theory of Operator Valued Functions***

We study a class of operator-valued functions that are nonlinearly dependent on the spectral parameter and involve operators that may be unbounded and non-symmetric. Spectral properties of this class of functions are investigated in a Hilbert space setting, and sufficient conditions for the existence of the eigenvalues are derived. An iterative method for approximating the eigenvalues is developed, based on a variational characterization of the spectral problem, and some examples are given to illustrate the theory.

Eliana Antoniou

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## ***A Theoretical Simulation of Hematopoietic Stem Cells During Oxygen Fluctuations: Prediction Of Bone Marrow Responses During Hemorrhagic Shock***

Assembly of the human genome shows that the biological system of human cannot be explained by ~30,000-40,000 genes. This study is based on the premise that studies on bone marrow (BM) stem cells (lymphohematopoietic stem cell, LHSC) by proteomics, computational biology and genomics could be aided by mathematical models. We use a mathematical model of acute blood loss, which is associated with a sharp decrease in pO<sub>2</sub>, to predict the responses of LHSC in an area distant from the main sinus. The equations were modified to present the responses of two population of LHSC (Proliferating, P; Non-proliferating, N). Hematopoietic responses by the most primitive LHSC were simulated for otherwise healthy individuals who have been subjected to various degrees of blood loss, as represented by 3%, 5% and 20% O<sub>2</sub>. The model is robust and could predict for hematopoietic activity in the area close to the endosteum during low pO<sub>2</sub> when there is acute blood loss. Steady state hematopoiesis at physiological oxygen level (80% O<sub>2</sub>) could not be simulated with the equations. Functional assays tested the model with a modified long

term culture initiating cell assay. In the presence of 1%, 3-5% and 20% O<sub>2</sub>, highly purified LHSC showed significant increases in cell proliferation when compared to 80% O<sub>2</sub>. Thus, the functional studies show that the theoretical model is robust and could be used to gain insights into the biology of LHSC during different degrees of blood loss. The utility of such a model in surgical trauma is discussed.

Felix J. Apfaltrer

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***Population Density Methods in Two Spatial Dimensions and Application to Neural Networks with Realistic Synaptic Kinetics***

We explore the extension to two "spatial" dimensions of a computationally efficient method of simulating networks of neurons. The method is applied to integrate-and-fire neurons with realistic synaptic kinetics. In this method neurons are grouped into populations of similar biophysical properties, and for each population a probability density function (PDF) is constructed. This PDF represents the distribution of neurons over state-space. The evolution equation of the probability density functions is a partial differential-integral equation. To begin with, we model neurons with only excitatory synaptic input.

In the case where the unitary postsynaptic events are fast enough to be considered instantaneous (Nykamp and Tranchina, 2000), the PDF is one-dimensional, as the state of a neuron is completely determined by its transmembrane voltage. When synaptic kinetics are not assumed to be fast on the time-scale of the resting membrane time constant, and when the unitary postsynaptic conductance event has a single exponential time course, the state-space and the PDF are 2-dimensional; the state of the neuron is determined by its random membrane voltage and random excitatory postsynaptic conductance.

The population firing rate is given by the integral of the flux of probability per unit conductance across the threshold voltage over all possible excitatory postsynaptic conductance values.

We formulate a pair of coupled partial differential-integral equations, one for the neurons in their non-refractory state and the second one for the neurons in the refractory pool. The higher dimensionality causes an increase in computation time, which we tackle numerically by using an operator-splitting method to solve our partial-differential integral equations. We compare our two-dimensional results to Monte-Carlo simulations for simple neural networks and check for their speed and accuracy in such instances. We then extend the population density method by adding inhibitory synaptic input. We consider a method for reduction from three to two dimensions and we apply it to small sample neural networks, as well as to a model orientation selectivity network for 1 hypercolumn of the visual cortex.

Limitations of the method are discussed and possible improvements and directions for future study are suggested.

Paul Atzberger

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***A Stochastic Immersed Boundary Method for Biological Fluid Dynamics at Small-Length Scales***

In modeling many biological systems it is important to take into account the interaction of a fluid with deformable structures. At the length scale of individual cells and organelles thermal fluctuations of the aqueous environment become significant. To model and simulate the mechanics of such systems consistently taking into account these features presents a variety of theoretical and numerical challenges. For macroscopic systems the immersed boundary method has found wide use as an efficient numerical method for simulation of deformable structures in a fluid. In this work we show how the framework can be extended to small length scales to include thermal fluctuations. We then develop an efficient stochastic numerical method. Applications of the method, including simulation of diffusing particles, polymer knots, and self-avoiding membranes, are also presented.

Karim Azer

Merck & Co., Inc., Applied Computer Science & Mathematics, RY84-202, 126 E. Lincoln Avenue, Rahway, NJ 07065 and Courant Institute of Mathematical Sciences

***A One Dimensional Model with Friction of Blood Flow in Arteries: Analysis, Numerical Solution, Simulation and Validation***

In this poster, we present a one-dimensional model for computing blood flow in arteries, without assuming an a priori shape for the velocity profile across an artery. Combining the equations for conservation of mass and momentum with the Womersley model in an iterative way gives us a second order method. We are able to use this method to get the velocity profile at any particular location along an artery, which is very valuable in many applications. Moreover, we are able to get a more accurate representation of the flow and pressure waves in the arterial system since the friction term is based on the more realistic velocity profile that we compute. We also present flow simulations using both structured trees and pure resistance models for the small arteries, and the resulting flow and pressure waves under various friction models.

Joint work with Charles Peskin (Courant Institute of Mathematical Sciences).

Dipankar Bandyopadhyay

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***A Novel Approach to Testing Equality of Survival Distributions when the Group Memberships are Censored***

This paper introduces a novel nonparametric approach for testing the equality of two or more survival distributions when the group membership information is not available for the right censored individuals. Although such data structures arise in practice very often, this problem has received less than satisfactory treatment in the nonparametric testing literature. Currently there is no nonparametric test for this hypothesis in its full generality in the presence of right censored data. We propose a novel approach leading to a division of the samples that enables one to use any class of tests for comparing survival curves based on independent samples. We study a class of weighted log-rank tests obtained this way through extensive simulation. An asymptotic linear representation of our test statistic is obtained and two resampling alternatives were proposed which might be easier to use in practice. The testing methodology is illustrated using two real data sets. This is joint work with Prof. Somnath Datta, Dept of Statistics, University of Georgia.

Keywords: log-rank tests; competing risk model; independence; equality of survival curves.

Anisha Banerjee

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***Modeling Steady-State and Time-Dependent Oxygen Delivery in Working Muscle***

Advisor: Dr. Daniel Goldman

Oxygen delivery and distribution in muscle is studied using Krogh-type oxygen transport models. A series of modifications to the classic steady-state Krogh tissue cylinder model is used to study oxygen transport from individual capillaries in exercising skeletal muscle. Physiologically important features studied include intravascular resistance, myoglobin facilitation of oxygen diffusion, mitochondrial clustering near capillaries and Michaelis-Menten oxygen consumption kinetics. When consumption does not depend on oxygen concentration, intravascular resistance to oxygen diffusion is shown to significantly lower the partial pressure of oxygen in the tissue, suggesting a decrease in consumption rate. Mitochondrial clustering is shown to decrease the partial pressure of oxygen in most of the tissues, giving shallow tissue oxygen gradients as has been observed experimentally. Myoglobin facilitation is found to play only a minor role in steady state oxygen transport. By including oxygen-dependent consumption, the model makes it possible to study hypoxia as seen in working muscle. This also permits more accurate calculation of tissue oxygen distributions and the total oxygen consumption rate (oxygen extraction). The steady-state model is generalized to allow study of time dependent oxygen transport. In particular, time-dependent tissue oxygen distributions and oxygen consumption are calculated for coordinated changes in muscle activity and blood flow.

Sibabrata Banerjee

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***A Comparison Study of Models for the Human Sex Ratio***

The human sex ratio is always very close to unity. If it moves too far away from unity, we face the risk of extinction and thus it is a matter of great interest in population statistics. Overdispersion models are often used to fit the human sex ratio. Branching processes are also very powerful tools for the modeling human sex ratio. This study would involve fitting several models using classical and modern techniques and a comparison would be made between these methods.

Keywords: overdispersion, non-linear regression, quasi-likelihood (multiplicative) generalization of binomial model, double exponential family.

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***Numerical Simulations of Kelvin-Helmholtz Instability in Slightly Stratified Fluid in the Channel***

A system of density-stratified incompressible inviscid fluids in an infinite horizontal channel is considered. The approach is based on a boundary integral formulation in which the fluid interface is modeled as a free vortex sheet and the channel walls as bound vortex sheets. The density variations are assumed to be small (Boussinesq regime) and the motion of the interface between fluids is studied numerically using the vortex blob method. The goal is to simulate the flow in the inclined channel and compare the numerical results with the experimental results obtained by Thorpe [J. Fluid Mech. 46 (1971) 299-319]. Joint work with Robert Krasny.

Michael D. Bateman

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***Traveling Wave Solutions to a Coupled System of Spatially Discrete Nagumo Equations***

We consider a coupled system of discrete Nagumo equations and derive traveling wave solutions to this system using McKean's caricature of the cubic. A certain form of this system is used to model ephaptic coupling between pairs of nerve axons; we present the derivation of this particular system, but consider a slightly more general version. We study the difference  $g(c) = a_1 - a_2$  between the detuning parameters  $a_1$  that is required to make both waves move at the same speed  $c$ . Of particular interest is the effect of a coupling parameter  $\alpha$  and an "alignment" parameter  $A$  on the function  $g$ . The introduction of a time delay  $\beta$  is used to show that the effects of perturbation away from  $A = 0$  are minimal. Numerical investigation indicates that for fixed  $A$ , there exists a  $\beta$  value that results in  $g = 0$ ; and for large enough wave speeds, multiple such  $\beta$  values exist. Also, numerical results indicate that the perturbation of  $\alpha$  away from zero will yield additional solutions with positive wave speed when  $A = 1/2$ . We rely on both numerical and analytical results to demonstrate our claims. Joint work with Erik S. Van Vleck (University of Kansas).

John K. Bechtold

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#### ***Nonlinear Oscillations in Diffusion Flames***

Recent experiments of diffusion flames have identified fascinating nonlinear behavior, especially near the extinction limit. In this work, we carry out a systematic analysis of pulsating instabilities in diffusion flames. We consider the simple geometric configuration of a planar diffusion flame situated in a channel at the interface between a fuel being supplied from below, and oxidant diffusing in from a stream above. Lewis numbers are assumed greater than unity in order to focus on pulsating instabilities. We employ the asymptotic theory of Cheatham and Matalon, and carry out a bifurcation analysis to derive a nonlinear evolution for the amplitude of the perturbation. Our analysis predicts three possible flame responses. The planar flame may be stable, such that perturbations decay to zero. Second, the amplitude of a perturbation can eventually become unbounded in finite time, indicating flame quenching. And finally, our amplitude equation possesses time-periodic (limit cycle) solutions, although we find that this regime cannot be realized for parameter values typical of combustion systems. The various possible burning regimes are mapped out in parameter space, and our results are consistent with available experimental and numerical data. Joint work with H. Y. Wang and C. K. Law (Princeton University).

Manish C. Bhattacharjee

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#### ***Strong Versions of the DFR Property and Applications***

We explore two nonparametric classes of life distributions nested within the class of decreasing failure rate (DFR) distributions, motivated by the observation that the standard parametric families of such distributions possess properties which are stronger than the decreasing failure rate property. Our results characterize such distributions via several representation theorems. Associated consequences such as closure properties and reliability bounds are considered, along with examples of how such strongly DFR distributions arise naturally in many applied contexts.

Denis Blackmore

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#### ***Periodic and Quasiperiodic Motion of Point Vortices***

We study the dynamics of any finite number of point vortices moving in an ideal fluid in both the plane and half-plane. If there are  $n$  point vortices, the governing dynamical equations are Hamiltonian and have  $n$ -degrees of freedom. These equations are completely integrable for  $n$  small, but not integrable for larger numbers of point vortices. Among the results obtained is the following: If the vortices all have strengths of the same sign, there is a set of initial configurations of positive measure for which the Hamiltonian equations of motion have invariant KAM tori containing quasiperiodic orbits, as well as periodic solutions of arbitrarily large periods. This result is proved using a modified version of the KAM theorem, and a new version of the Poincaré-Birkhoff fixed point theorem that we developed to study small perturbation of completely integrable Hamiltonian systems. Joint work with Jyoti Champanerkar (William Paterson University).

Mark G. Blyth

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#### ***Stability of Two-Layer Channel Flow in the Presence of Surfactants***

The effect of an insoluble surfactant on the stability of two-layer viscous flow in an inclined channel confined by two parallel walls is considered both under conditions of Stokes flow and at arbitrary Reynolds numbers. At zero Reynolds number, a long-wave model is developed leading to a nonlinear evolution equation for the interfacial position. Numerical boundary-integral simulations for waves of arbitrary length agree with linear stability predictions at small amplitude, and predict that waves may grow and saturate into steep profiles or begin to overturn and break. The results are then extended to include inertia. A generalized form of the Orr-Sommerfeld equation is derived describing the growth of small disturbances at arbitrary Reynolds number and solved numerically. For general Reynolds numbers and arbitrary wavenumbers, the surfactant is found to either provoke instability or significantly lower the rate of decay of infinitesimal

perturbations, while inertial effects widen the range of unstable wavenumbers. The nonlinear evolution is computed numerically using a finite-difference method. The results are consistent with the linear theory and show that the interfacial waves steepen and eventually overturn under the influence of the shear flow.

**Michael R. Booty**

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***Scattering from a Thin Inhomogeneous Cylinder in a Waveguide***

A thin cylindrical target is placed with almost arbitrary orientation in a rectangular TE<sub>10</sub> waveguide and is subjected to an imposed electromagnetic field. The scattered far-field is expressed in terms of the scattered field inside the target and the far-field expansion of the dyadic Green's function for the waveguide. To capture features of interest in microwave heating applications, we allow the target material's electrical properties to be arbitrary functions of position along the target's axis. Reflection and transmission coefficients are derived together with an expression for the rate of deposition of electromagnetic energy within the target. Joint work with Gregory A. Kriegsmann (NJIT).

**Amitabha Bose**

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***Localized Activity Patterns in Excitatory Neuronal Networks***

The existence of localized activity patterns, or bumps, has been investigated in a variety of spatially distributed neuronal network models that contain both excitatory and inhibitory coupling between cells. Here we show that a neuronal network with purely excitatory synaptic coupling can exhibit localized activity. Bump formation ensues from an initial transient synchrony of a localized group of cells, followed by the emergence of desynchronized activity within the group. Transient synchrony is shown to promote recruitment of cells into the bump, while desynchrony is shown to be good for curtailing recruitment and sustaining oscillations of those cells already within the bump. These arguments are based on the geometric structure of the phase space in which solutions of the model equations evolve. We explain why bump formation and bump size are very sensitive to initial conditions and changes in parameters in this type of purely excitatory network, and we examine how short-term synaptic depression influences the characteristics of bump formation. Joint work with Jonathan Rubin.

**Bruce Bukiet**

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***Mathematical Modeling of Postural Stability***

Understanding postural stability (human balance) is important because millions of Americans experience dizziness and balance problems in their lifetimes. The quality of many people's lives could be improved through development of high quality diagnostic methods that could reliably determine who is in danger of falling. With this in mind, we have developed mathematical models of postural stability, including 2 and 4 link models. We have also created an index that can be used as a diagnostic tool to quantify postural stability. We discuss our model, the properties of our Postural Stability Index and applications of our work in the diagnosis and evaluation of treatment options. Joint work with Hans Chaudhry, Zhiming Ji, Thomas Findley, Karen Quigley, and Miriam Maney.

**Jean Cadet**

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***Robustness in Drosophila Melanogaster***

Driever and Nusslein-Volhard showed that the bicoid gene protein determines position in the Drosophila embryo in a concentration-dependent manner. We combine our knowledge of this result with the gene circuit model which is based on 4 steps: formulate a theoretical model, acquire data, optimize using simulated annealing and learn new biology. Finally, we propose a manner to characterize statistically biological robustness despite changes in the bicoid dosage.

**Jerry J. Chen**

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***Bifurcation and Chaos in Discrete Lotka-Volterra Equations***

A discrete Lotka-Volterra (L-V) population model for a pair of competing species is analyzed. It is known that the one-dimensional logistic map exhibits a variety of dynamical features such as period-doubling bifurcation and chaotic cobweb. It is shown that the L-V map demonstrates its own brands of period-doubling bifurcation and a two-dimensional twisted horseshoe. With initial values outside the Cantor-like set, the weaker species ultimately becomes extinct, which agrees with the continuous version of the Lotka-Volterra equations. A controlling scheme that diminishes the intrinsic growth rate of the dominant species is provided to prevent the probable extinction of the weaker species. Some numerical results are given to portray its effectiveness.

Yiming Cheng

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***Analysis of Equivalent Distorted Ratchet Potentials***

Separation technology is important in biotechnology for certain processes such as separation of microscopic particles undergoing Brownian motion. These particles can be separated by subjecting them periodically to an asymmetrical spatially periodic electric field, sometimes referred to as a Brownian ratchet. It has been found numerically that two different potentials under special equivalent distortions (Chen et al., 1999; Yan et al., 2001) can produce equal fluxes of particles. Although a simple physical explanation for this can be given, there is no analytical proof of this equivalency. Here, we pose the mathematical problem and discuss the difficulty in carrying out the analytical proof.

Shawn Chester

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***Discrete Element Simulations of Floor Pressure in a Granular Material in a Cylindrical Vessel***

Advisor: Anthony Rosato

At the end of the 19th century, H. A. Janssen discovered that the bottom floor pressure in a cylindrical container of granular material asymptotes exponentially to a value less than the weight of the material, i.e., the pressure becomes independent of the fill height of the column. Applications are prevalent in the handling, processing and transport of industrial bulk materials. Janssen's theoretical prediction is based on a constitutive assumption that the vertical (axial) stress in the material is proportional to the horizontal (radial) stress. We model this problem using particle level (discrete element) simulations in a cylindrical vessel in which the floor is slowly moved down. The objective of our investigation is to reproduce the theoretical prediction, and to make quantitative comparisons with experiments in the literature. A key parameter in the analysis is the selection of an appropriate friction coefficient between the particles and the cylinder walls, a topic which has seen much discussion in the literature. Results obtained thus far have shown a floor pressure that is smaller than the static value (due to the material weight), in qualitative agreement with the theory. However, the rate at which the graph of pressure versus fill height asymptotes to its constant value does not agree with the theory. We are now exploring a wide range of friction coefficients to understand how this parameter affects our simulated results. Work is also underway to test the major assumption in the model concerning the proportionality between the vertical and horizontal stresses.

Wooyoung Choi

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***Nonlinear Surface Waves in a Linear Shear Current***

Nonlinear surface gravity waves interacting with a linear shear current are studied for both infinitely deep and shallow water. For deep water, a closed system of the exact evolution equations is obtained using the conformal mapping technique and is solved numerically via a pseudo-spectral method to study the evolution of slowly modulated periodic surface waves. For shallow water, we consider an asymptotic model for long waves and discuss its solitary wave solutions including a solution with infinite slope.

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***Propagation of Large Amplitude Internal Waves Over Variable Bottom Topography***

The evolution of large amplitude internal waves is investigated using a strongly nonlinear long wave model for a system of two layers of different densities. A local stability analysis is presented to show that the solitary wave solution of this 'inviscid' model suffers from a Kelvin-Helmholtz type instability due to a velocity discontinuity across the interface between two layers. A numerical filter is used to eliminate the short-wave instability (that is absent in real observations) and its effects on long-term numerical simulations are discussed. Joint work with Taechang Jo (New Mexico Institute of Mining and Technology).

Sohae Chung

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***Mathematical Erosion as a Measure for Osteoporosis: Quantifying Topological Change***

The evaluation of topological changes (hole formation, breakage) in the trabecular bone region provides insight into how trabecular bone protects itself against the effects of osteoporotic erosion and may provide essentials for fracture risk assessment at an early time point that are not reflected by density measurements (eg, bone mineral density). Based on 3D digital images obtained using micro-CT, a mathematical erosion model has been developed that enables the analysis of the relationship between virtual bone loss generated by mathematical erosion and the bone's structural alteration during progressive bone loss. The results demonstrate that erosion induced stresses are relieved through the preferential production of holes over breaks in the trabeculae. Trabecular bone appears constructed so that such preferential relief is

able to continue down to extremely eroded forms of the structure. Further, the topological analysis indicates that trabecular structure is better protected against isotropic rather than unidirectional erosive action. Joint work with W. Brent Lindquist and Yi-Xian Qin (Stony Brook University), and John Pinezich (Advanced Acoustic Concepts, Inc., Hauppauge, NY 11788).

Robert Clewley

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***Dynamical Models of Finger Biomechanics and Neuromuscular Control***

We analyze the periodic motor patterns of index finger control of a trackball, during a psychophysics task in which the subject has to match a constant angular velocity. We explore minimal hybrid (DAE) kinematic models of the system, and use parameter estimation to investigate what control strategies provide maximally-robust achievement of the target velocity. This work is also intended to develop the computational tools necessary to study a related question, in insect locomotion: What are the relative roles of 'pre-flex' and CNS feedback control strategies in cockroach locomotion? The cockroaches are mounted on a Kugel (a freely rotating styrofoam ball) at Robert Full's Berkeley laboratory, and so this resembles the finger manipulation problem under certain assumptions. Joint work with John Guckenheimer, Francisco Valero-Cuevas, Dan Brown, and Erik Sherwood.

Dean T. Crommelin

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***Extracting Low Order Stochastic Models from Data***

We present a numerical technique to derive optimal stochastic models (Markov chain or SDEs) for the description of the evolution of a few interesting collective variables in large-sized dynamical systems. The technique is based on constructing the stochastic model whose eigenfunctions and eigenvalues are the closest (in some appropriate norm) to the one gathered from the observations. The technique is validated on an example arising from climate dynamics, namely by extracting a stochastic model for the evolution of the first few principal orthogonal modes observed in a general circulation model. Joint work with E. Vanden-Eijnden.

R.E. Lee Deville

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***Self-Induced Stochastic Resonance for Excitable Systems***

Excitable systems arise in a wide variety of areas, including climate dynamics and lasers, and are especially common in biology. One can think of them schematically as dynamical systems possessing a rest state, an excited state, and a recovery state. Recently, there has been much interest in coherent response of these systems to small amplitude stochastic forcing. In particular, the well-known mechanism of coherence resonance has been successful in explaining some of these phenomena. Here we discuss an alternate mechanism to coherence resonance which takes place in different parameter regimes and gives rise to qualitatively different behavior. Moreover, in a suitable limit, we recover deterministic behavior which is far from the unforced dynamics. We will treat the cases of stochastically forcing excitable ODE and excitable media, i.e., the spatially extended PDE. This is joint work with E. Vanden-Eijnden (Courant Institute) and C. Muratov (NJIT).

Sunil K. Dhar

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***On the Characterization of a Bivariate Geometric Distribution***

In this paper it is shown that a bivariate random variable has constant failure rate and mixture geometric marginals if and only if it has the loss of memory property and the discrete Freund distribution. This characterization is achieved by extending a key lemma in this area. The mixture geometric can be collapsed to geometric marginals, thus validating the characterization as a generalization of the past work. Joint work with Srinivasan Balaji (George Washington University).

Sunil K. Dhar

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***Improved Methods for Establishing Noninferiority in Clinical Trials***

We consider a randomized, active-control clinical trial setting in which the objective is to test for noninferiority of the experimental treatment compared to control. An approach for defining a noninferiority margin is based on the concept of preserving a certain fraction of the active control effect. Noninferiority is established if the ratio of the lower limit of the two-sided 95% confidence interval for the treatment difference to the estimated mean of the active control is greater than a prespecified fraction. The nominal significance level, depending on values of location and scale parameters, may not be maintained by this confidence-interval approach to testing noninferiority. We examine bootstrap methods to derive a more accurate lower limit of the confidence interval for known functions of the treatment means. This, in turn, improves the power

of the test which will be demonstrated through simulation. Other methods of establishing noninferiority or equivalence will also be explored. Joint work with Michael Chen and Farid Kianifard (Biometrics, U.S. Clinical Development and Medical Affairs, Novartis Pharmaceuticals, East Hanover, NJ 07936).

**Ramana Dodla**

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***Dynamics of Weakly Coupled Kuramoto Oscillators***

Phase coupled Kuramoto oscillators have become classic examples of phaselocking among non-identical oscillators. While there are many studies on the limiting case of the number of oscillators becoming infinity, the dynamics of finitely large number of oscillators is still a largely unexplored and fascinating area of research. In this poster we present some preliminary results on the finitely large number of globally coupled phase oscillators when the coupling strength is weak. Under special frequency distributions, the oscillators could show signatures of a completely integrable system. For example, a perturbation decays in time, but can be recovered with a periodicity that is characteristic of the number of coupled oscillators.

**Brent Doiron**

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***Coding with Inter-Spike Intervals and Dendrites***

Many neurons use precise spike timing to reliably encode dynamic stimuli. We present experimental and computational results from sensory pyramidal neurons showing that the time interval between two precise spikes can also encode relevant sensory information. Electrosensory pyramidal neurons produce high frequency two spike bursts in response to upstrokes of dynamic stimuli. Using pattern classifier techniques we show that the inter-spike interval duration of a burst can accurately encode the scale of stimuli upstrokes. Electrosensory neurons have well characterized nonlinear dendritic processes that support backpropagation of action potentials along the dendritic arbor. We introduce a simple modified integrate-and-fire neuron that accounts for how nonlinear dendritic effects shape spike train statistics in response to dynamic stimuli. Using this model we study how active dendrites are critical for this inter-spike interval coding scheme. Specifically, the amplitude of the dendritic spike sets the range over stimuli space that the inter-spike intervals can accurately span. Interestingly, the amplitude of the dendritic spike that maximizes the information in the model's interval code is the value that best matches experimental observations of dendritic spikes in real electrosensory neurons.

**Graham Donovan**

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***Non-Gaussian Optical Field Statistics in a Long-Haul Soliton-Based DPSK Transmission System***

We demonstrate with importance-sampled Monte-Carlo simulations that the tails of the optical field's probability distribution at the end of a long-haul soliton-based differential phase-shift keyed (DPSK) transmission system are strongly non-Gaussian.

**Jonathan D. Drover**

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***Nonlinear Coupling Near a Degenerate Hopf Bifurcation***

A nonlinearly coupled network of oscillators near a Hopf bifurcation is analyzed. The equations are derived from the normal form of a subcritical Hopf bifurcation where the unstable branch of periodics 'turns around', creating a parameter dependent region of bistability. Solutions such as waves and localized regions of excitation, which may be analogous to patterns of activity used to model working memory, are found to exist numerically. A mechanism where waves do not exist because of large phase gradients is explored.

**Srabasti Dutta**

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***LES Simulations of Turbulent Combustion in a Type Ia Supernovae***

We propose a 2D axisymmetric model of a type Ia supernova explosion, based on a front tracking sharp flame model. The calculation is free from adjustable turbulent transport parameters, and in this sense it is in the spirit of Large Eddy Simulation (LES) turbulence simulations. Since the mixing is dominated by the largest eddies, we resolve these and not the smaller ones. We believe this method results in a tolerable error, which, in any case understates the success of the explosion. We report successful explosions. Both the 2D and the LES nature of the model greatly simplify parameter identification. The 2D model allows multiple simulations and an exploration of unknown parameters, while the LES model removes parameters from the simulation. Joint work with James Glimm and Yongmin Zhang (SUNY at Stony Brook).



Alan Elcrat

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***Free Surface Waves in Equilibrium with a Vortex***

Finite amplitude solitary waves of uniform depth which interact with a stationary point vortex are considered. Waves both with and without a submerged triangular obstacle are computed. The method of solution is collocation of Bernoulli's equation at a finite number of points on the free surface coupled with equations for the equilibrium of the point vortex. The stream function and vortex location are found by computing a conformal map from the flow domain to an infinite strip using Driscoll's SCTOOLBOX. The solutions are parameterized with respect to Froude number, vortex circulation, and, when an obstacle is present, obstacle height. When no obstacle is present there are two families of solutions. In one the amplitude increases with increasing circulation, while in the other it decreases. Beyond a certain critical Froude number the maximum amplitude wave has a sharp crest with an angle of 120 degrees. Similar behavior is observed for flow past an obstacle except that below a certain Froude number there is no solution at all.

Christopher E. Elmer

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***Functional Differential Equations of Mixed Type***

We illustrate techniques for deriving and for computing solutions to functional differential equations of mixed type. Also included are examples of applicable models.

Samiran Ghosh

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***Statistical Approach to Metabonomic Analysis of Rat Urine Following Surgical Trauma***

Motivation: Acute trauma is often associated with the progressive deterioration of multiple organ systems in humans and is the leading cause of death in trauma care units. Previous studies have suggested that multiple organ failure is likely related to uncontrolled systemic inflammation; however, causal mechanisms remain unknown. Current methods of assessing trauma patient status and predicting outcome are based on a variety of anatomical and/or physiological scoring models. While useful, these are labor intensive and do not allow for real-time analysis of patient status. In this study, we develop a metabonomic based approach using a rodent model of acute trauma in order to determine whether statistically significant differences exist between the quantitative and qualitative profile of urinary metabolites of control rats and rats that have experienced surgical trauma. This approach incorporates statistical, analytical and computational tools in order to identify metabolites that are unique to trauma and may be used to predict trauma outcome.

Results: We used electrospray ionization/time-of-flight (ES/TOF) mass spectrometry to analyze the urine metabonomes of eleven male rats 48 hours following surgical implantation of a biotelemetry transmitter and vessel cannulation as a model of surgical trauma. Statistical analysis showed significant differences between trauma and control urinary metabonomes. These included metabolites that were detected ES/TOF both positive and negative ionization modes. Principle component analysis was used to categorize metabonomes into either control or trauma with greater than 80% accuracy. We also show, using Bayesian methods that we could classify subjects as being traumatic or control with a given credible interval. These results suggest that metabonomics may prove useful for quantifying and identifying biomarkers of trauma status as well as trauma outcome in humans. Joint work with Dennis Hill, David F. Grant, and Dipak K. Dey (University of Connecticut).

Daniel Goldman

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Calculations of Tissue Oxygen Delivery and Utilization During the Time Course of Microvascular Injury in a 6-Hour Acute Sepsis Model***

Sepsis produces severe disturbances to the microcirculation, including loss of functional capillary density (fCD) and increased blood flow heterogeneity. We have previously presented a mathematical model of microvascular oxygen delivery in rat skeletal muscle during sepsis (Goldman et al., AJP Heart, 2004), based on measurements of fCD, hemodynamics and blood oxygen saturation in a 24-hour cecal ligation and perforation (CLP) model. Here we utilize recent measurements of these same transport parameters, as well as capillary geometry, in a single microvascular network at two, three and four hours after surgery in an acute 6-hour CLP model. This data was obtained to study changes in microvascular blood flow during the time course of sepsis, but also allows us to study progressive changes in oxygen delivery and utilization. We will present results showing how changes in functional microvascular geometry and blood flow result in changes

in oxygen transport, as the effects of sepsis on the microcirculation become more severe over time. Joint work with Graham Fraser and Christopher Ellis (University of Western Ontario, London, Ontario, Canada).

## Jorge Golowasch

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

### ***Gap-Junction Conductance Determines an Optimal Coupling Diameter in Passive Fibers***

Neurons communicate via chemical synapses but also via direct electrical connections called gap junctions. These are molecular channels that directly link cells for electrical and biochemical signal transfer. Gap junctions, although discovered almost 50 years ago, are only now being studied in more detail at the molecular level. At the computational level gap junctions are thought to have a synchronizing role of the electric behavior of coupled cells. However, even some very basic questions have not been addressed. We are interested in understanding the behaviors that may arise from the combination of current flow along cables and their coupling gap junctions. Current flow through gap junctions depends on their conductance as well as the electrical properties of the coupled cells. We show that an optimal current transfer between two gap-junctionally coupled cables occurs as a function of cable diameter as well as a function of the gap junctional conductance. This non-monotonic behavior does not depend on any active properties. The optimal current transfer is a local phenomenon that depends on the diameters of only the coupled processes. We predict that in biological networks coupled processes may have optimal diameters that maximize current transfer between neurons. Supported by NIH grants MH-60605 (F.N.) and MH-64711 (J.G.). Joint work with Farzan Nadim (NJIT).

## Roy Goodman

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

### ***Heads Up! A Capstone Applied Math Course in the Mechanics of Coin Flipping***

In a recent preprint, Diaconis, Holmes, and Montgomery have shown that under general conditions, a coin tossed in the air that starts heads up spends more than half of its time in the air heads up, and thus is inherently biased to land that way. This effect does not diminish as the coin is thrown higher or with more vigorous rotation. This result formed the basis of my capstone course for graduating seniors in applied mathematics at NJIT. This bias arises because the coin precesses as it tumbles, and is a straightforward, though novel, application of results due to Euler in about 1750! We reproduce experiments in which flipping coins are filmed using a high speed video camera. We use Matlab's image processing toolbox to analyze the motion and quantify the bias. We also analyze at "Feynman's plate" and the motion of gyroscope under the influence of gravity using the same techniques. The experiments are incredibly simple, yet analyzing them in the framework of Euler's equation requires a great deal of knowledge and computational work. Joint work with the students of Math 451H-04.

## Arnaud Goulet

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### ***Control of Mixing***

In this work, we address the control of Lagrangian chaos or chaotic advection in a two-dimensional incompressible fluid flow. Due to the fact that the motion of passive tracers (particles) can be described by a Hamiltonian function, we apply a control technique recently developed for Hamiltonian systems. The control is performed by introducing a suitable small term in the original Hamiltonian which is derived explicitly. The control term is in the form of a secondary flow which slightly deforms the streamlines of the original flow and reduces the chaoticity of the particle trajectories.

The technique is implemented on two different fluid flow systems consisting of Rossby waves and Rayleigh-Bénard convection which can both exhibit chaotic advection for certain parameter values. For each system, we derive the control term and demonstrate its effect on chaotic advection through numerical simulations of the time dependent material lines as well as Poincaré sections. Joint work with Nadine Aubry (NJIT).

## Muhammad Hameed

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

### ***Influence of Surfactant on Necking and Pinch-Off in Two Fluid Jets***

The effect of surfactant on the breakup of a periodic fluid jet immersed in another viscous fluid at low Reynolds number is studied both numerically and experimentally. Evolution equations for the jet interface and surfactant concentration are derived using long wavelength approximations. These one dimensional partial differential equations are solved numerically for given initial interface and surfactant concentration. It is found that the presence of surfactant at the interface retards pinch-off and results in the formation of a thin and long filament. To check the predictions of our model, we performed experiments both for clean interface and as well as in presence of surfactants. The experimental results support the prediction of theoretical model that the presence of surfactant slows down the pinch-off process.

Alex Haro

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***Invariant Manifolds in Quasiperiodic Systems: Theory, Computation and Applications***

The parameterization method is useful to prove the existence of invariant manifolds in quasi-periodic systems, and it also provides effective algorithms to compute these manifolds. We apply the method to two paradigmatic examples: the quasiperiodic Hénon map and the quasiperiodic standard map. Joint work with Rafael de la Llave.

Cristel Hohenegger

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***Statistical Reconstruction of Velocity Profiles for Nano-PIV***

Velocities and Brownian effects at nano-scales near microchannel walls have been measured by evanescent-wave illumination techniques [R. Sadr et al., J. Fluid Mech. 506, 357-367 (2004)]. Assuming mobility of spherical particles is dominated by hydrodynamic interaction between the particle and wall, and that fluid velocity is directed in one in-plane direction, the out-of-plane dependence of mobility and velocity are clearly coupled. We investigate such systems computationally, using a Milstein algorithm that is both weak- and strong-order 1. We demonstrate that a maximum likelihood algorithm can reconstruct the out-of-plane velocity profile given known mobility dependence and ideal particle identification. We further test this reconstruction for measurements obtained by cross-correlation techniques applied to windowed simulation data. Application to physical data is proposed via analytical results about the influence of Brownian motion in this setting on the correlation peak, combined with simulation results to help identify nearly-optimal parameters. Joint work with P.J. Mucha (School of Mathematics, Georgia Institute of Technology).

David Horntrop

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Mesoscopic Simulation of Domain Coarsening in Surface Processes***

Self-organization of components of two phase mixtures through a diffusive mechanism is known as Ostwald ripening and is an example of a multiscale phenomenon which is well-suited to study using mesoscopic models. Mesoscopic models are stochastic partial differential equations which are directly derived from the underlying microscale behavior. In order to computationally study these models, new spectral schemes for stochastic partial differential equations are introduced and validated using exactly solvable benchmark problems. These schemes are then applied to the mesoscopic model and simulation results are compared with various theoretical results such as the Lifshitz-Slyozov growth law.

Maureen Howley

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***A Comparison of One-Dimensional Traveling Waves in Inverse and Normal Fluidized Beds***

The state of uniform fluidization is usually unstable to small disturbances, and this can lead to the formation of vertically traveling voidage waves. In inverse fluidization, when particle density is less than fluid density ( $\rho_p < \rho_f$ ), particles fluidize in the direction of gravity when the drag force exerted by the fluid overcomes buoyancy. Inverse fluidization thus provides a unique parameter space, which augments the study of instability behavior in normal fluidization when  $\rho_f < \rho_p$ . Using continuum equations of continuity and motion, we compared the linear stability of normal and inverse bed modes to examine the effect of the Froude number  $Fr$  and fluid to solid density ratio ( $\delta = \rho_f / \rho_p$ ). Making use of numerical bifurcation analysis and continuation, periodic solutions in the form of one-dimensional traveling waves (1D-TWs) were computed. Based on wave growth rates and bifurcation structure, we identified the  $Fr$  as an important parameter for predicting instability strength. However,  $\delta$  affects instability onset, or the point at which the base state is rendered unstable. In the case studies we examined, traveling waves were shown to propagate in the direction of fluidization, and asymmetrical, high amplitude 1D-TW profiles suggest fully developed bubble-like structures are oriented in the direction of fluidization.

Aridaman K. Jain

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***Small-Sample Non-Parametric Tests for the Effectiveness of Liposuction Surgery for Breast Hypertrophy***

Previous studies on the effectiveness of treatments for breast hypertrophy have been based on the use of normal approximations for the averages of the responses from a large number of patients treated at several plastic surgeon practices. In those studies, patients were asked to fill out questionnaires containing many questions on measures of health/pain, on a 3-point or a 5-point scale, both before and after the surgery. We describe the results from a prospective research study of breast-reduction, which is unique in two aspects: (i) it is the first such study focused exclusively on African-American women, (ii) it investigates the liposuction breast reduction technique. Due to the newness of this surgical procedure, data are available only for a limited

number of patients. Since the use of the normal approximation for a small sample number of patients may be questionable, we decided to use non-parametric tests that do not make any assumptions about the shape of the probability distribution for the self-reported responses on 3-point or 5-point scales. After the surgery, the pain was reduced and the general health was improved, when compared with those reported before the surgery ( $p \leq 0.05$ ). Joint work with Martin J. Moskovitz, Sherwood A. Baxt, and Robert E. Hausman.

Shidong Jiang

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***The Hyperpolarizabilities for One-Dimensional Infinite Single-Electron Periodic Systems***

The analytical solutions for the general-four-wave-mixing hyperpolarizabilities on infinite chains under both Su-Shrieffer-Heeger and Takayama-Lin-Liu-Maki models of trans-polyacetylene are obtained through the scheme of dipole-dipole correlation. Analytical forms of DC Kerr effect, DC-induced second harmonic generation, optical Kerr effect and DC-electric-field-induced optical rectification are derived. By including or excluding the gradient terms in the calculations, comparisons show that the intraband contributions dominate the hyperpolarizabilities. The intraband transition leads to the break of the overall permutation symmetry in hyperpolarizabilities even for the low frequency and non-resonant region. Since the Kleinman symmetry is directly based on the overall permutation symmetry, our calculations provide a clear understanding about the break of the Kleinman symmetry that are widely observed in many experiments.

Ning Ju

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***Vorticity Geometry and Regularity of 3D Incompressible Flow***

New geometric constraints on vorticity are obtained which suppress possible development of finite-time singularity from the nonlinear vortex stretching mechanism. The continuity conditions of Constantin-Fefferman and Beirao da Veiga-Berselli for the direction of vorticity which yield the regularity of the solution to the 3D Navier-Stokes equations are further relaxed. The important role of the "critical plane" is recognized. This leads to two broad classes of geometric configurations which allow non-continuity of vorticity direction. This also leads to improvement of the results of Beirao da Veiga and Grujic and Ruzmaikina for 3D Navier-Stokes equations and a result of Constantin for 3D Euler equations.

Yeona Kang

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***A Constrained Kinetic Approach to Fast Algorithms for the Protein Folding Dynamic***

The Einstein Relation defines the ratio of diffusion constant to a field driven drift constant. A new Einstein Relation for charges constrained to move as an integral part of a shape changing protein structure was derived and applied to protein folding. The partitioning of free energy into structural and electrostatic (and/or any other easily mapped energy form) provides a constrained trajectory for environmentally induced protein shape change. Lagrange methods ensure that the simultaneous minimization of two or more energy forms is describable in terms of the free energies gradients or forces. Using an analysis based on gradients and measurable physical parameters such as: total free energy change, molecular mobility (and diffusion), and the steady-state key mechanisms of protein shape change were elucidated. Protein folding involves pivoting of large groups of atoms specific bonds. The functional atomic group of folding can be viewed as a wishbone comprised of a pivot bond and of two (or more) charged regions held distant from the pivot bond by inert lever arm regions. A computation using a Markov sequence of wishbone-based rotations was carried out. These considerations lead naturally to a description in which the cooperative motions of large numbers of protein atoms move simultaneously.

The goal of this work is to build upon known processes to provide and demonstrate a thermodynamic framework that simulates protein folding and elucidates the key mechanisms and structures related to protein folding. Furthermore another goal for the model is to wherever possible link input parameters to laboratory parameters using the mathematical description. In some cases this required the development of new relationships. For example, the well known Einstein relation links the diffusion constant to the drift mobility of a given species, thereby making it possible to link the potential energy gradient to the concentration gradient. Einstein relations are specifically developed for charged species constrained to move as part of a molecular chain that could itself store energy independently of the electric potential. Joint work with E. L. Jaen, J. H. Coleman, and C. M. Fortmann (SUNY at Stony Brook).

Said Kas-Danouche

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***A Mathematical Model for Core-Annular Flows with Surfactants and No Basic Flow***

For oil companies, transport techniques are very important. One technique is transporting crude through water lubricated pipelinings. This is an example of core-annular flows. In our case, the annular fluid (water) lubricates the movement of the core fluid (crude). Instabilities occur at the interface of both fluids

giving rise to not wanted final products as, for example, emulsification. On the other hand, it is known that most of surfactants affect the interfacial dynamics since they reduce the interfacial tension and introduce the Marangoni force. We derive a mathematical model for core-annular flows without basic flow and with surfactants using asymptotic methods. We assume that the annulus is thin compared with the core radius. We obtain a coupled system of two nonlinear partial differential equations. One describes the evolution of the interface and the other the evolution of the concentration of surfactants at the interface. Joint work with Michael Siegel and Demetrios Papageorgiou (NJIT).

**Aslan R. Kasimov**

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***Asymptotic Theory of Self-Sustained Detonations***

A self-sustained detonation wave is a shock wave propagating in a reactive medium so that its motion is sustained only by the chemical energy released behind the shock. An important property that distinguishes self-sustained detonations from supported (also called overdriven) detonations is that in the former a sonic locus exists at the end of the reaction zone. We propose general sonic conditions for detonation waves with smoothly evolving reaction zone as compatibility conditions in the limiting forward characteristic surface, which defines a general sonic locus. Such a surface is an information boundary that isolates the lead shock from the influence of the downstream flow of burnt products. The sonic conditions are derived from the general system of reactive Euler equations. A numerical illustration of their properties in the simplest case of a pulsating one-dimensional detonation is given. The sonic conditions are essential ingredients of an asymptotic theory of a slowly evolving weakly curved detonation. We derive a reduced evolution equation for such detonations that relates the detonation-shock curvature, speed, and acceleration. Some properties of the evolution equation will be illustrated with an analysis of strong-blast initiation of a gaseous detonation.

**Navodit Kaushik**

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***Solving Second Order ODEs with the Local Discontinuous Galerkin Method: Effect of Stencil Selection on Accuracy***

The Runge Kutta Discontinuous Galerkin (RKDG) method has been well established for compressible Euler equations by Cockburn, Shu and coworkers. Following the initial idea of Bassi and Rebay of writing the compressible Navier-Stokes equations as a system of first order equations, the Local Discontinuous Galerkin (LDG) method was also developed by Cockburn and Shu among others. Recent interests are in extending the Discontinuous Galerkin approach to elliptic equations and to the incompressible Navier Stokes equations.

We focus on the application of the LDG method to the following one-dimensional equation:

$\frac{d^2u}{dx^2} = f(x)$ . According to literature, one of the salient features of LDG method is that one can obtain high

orders of accuracy using a highly compact stencil. We show that the choice of stencil has a major effect on the accuracy of the method for the above model problem. In particular, it is shown that for a three point stencil, using Legendre polynomial bases, the resulting scheme is at best second order accurate, for the numerical fluxes considered in this work irrespective of the cell size and order of polynomials. The extension of the current work to two-dimensional cases is currently under study. Joint work with Beddhu Murali.

**Adnan A. Khan**

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***Turbulent Transport in the Presence of Periodic Fluctuations and Strong Mean Flow***

The transport of passive scalars has been well studied using the advection-diffusion equation in the case of periodic fluctuations with a weak mean flow or a mean flow of equal strength through homogenization techniques. However, as the mean flow becomes stronger, homogenization seems to break down. We study the transport of passive scalars using Monte Carlo simulations for the stochastic differential equations describing the tracer trajectories, and study the transport properties as the mean flow is made stronger. We benchmark our numerical experiments by starting in a regime where homogenization works and agrees with our Monte Carlo results, and then we increase the mean flow strength and seek to describe how the breakdown in homogenization is manifested in the statistics of the tracer trajectories. Joint work with Peter R. Kramer (Rensselaer Polytechnic Institute).

**Hafiz M. R. Khan**

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Predictive Distributions for Responses from the Weibull Life Testing Model***

The Weibull distribution has been widely used for modelling life data, and most studies on this distribution concentrate on inference about the parameters or on the reliability and hazard functions. This

presentation is concerned with predictive inference for future responses from a Weibull distribution in a Bayesian framework. It considers both the two-parameter and the three-parameter Weibull distributions. A numerical example is provided, and predictive bounds are determined for various values of the hyperparameters of the prior distribution.

Christopher E. Khedouri

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***Everyday Challenges of a Statistical Reviewer at the Food and Drug Administration (FDA)***

This presentation provides a brief overview of the drug review process in the Center for Drug Evaluation and Research (CDER) at the Food and Drug Administration (FDA). The primary objective is to describe the everyday challenges that a statistical reviewer may face throughout the review process. Examples of actual statistical and/or design issues relevant to the Division of Anti-Infective Drug Products (DAIDP) at CDER will be discussed. (The views expressed are those of the author and not necessarily those of the FDA.)

Nickolas Kintos

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***Modeling Actions of a Neuromodulator on a Rhythmic Neuronal Network***

The stomatogastric ganglion (STG) of the crab, *Cancer borealis*, houses the rhythmic networks that control chewing (gastric mill) and filtering (pyloric) of food. These STG networks are modulated by several substances which are released by projection neurons. One such neuron is the modulatory commissural neuron 1 (MCN1), whose activity elicits a gastric mill rhythm. Previous modeling and experimental work studied the frequency regulation of the MCN1-elicited rhythm by the pyloric rhythm. Recent experimental work, however, showed that bath application of the neuropeptide, pevpyrokinin elicits a gastric mill rhythm that is very similar to the MCN1-elicited rhythm. Using a 3D model of the MCN1-elicited rhythm, we reduce to 2D by exploiting the difference in time scales. Then, we investigate possible mechanisms by which the neuropeptide can elicit a gastric mill rhythm that mimics the MCN1-elicited rhythm. We also use a biophysically-detailed model to compare the MCN1-elicited and peptide-elicited rhythms.

Lou Kondic

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Thin Liquid Films with Contact Lines: Instabilities, Coalescence and Rupture***

This contribution will concentrate on computational and experimental results involving dynamics of thin film flows on homogeneous and heterogeneous surfaces. In particular, I will present the dynamics of the fluid fronts, i.e., contact line. The presence of contact lines introduces microscales in a macroscale flow and therefore requires bridging the scales and careful modeling and numerical simulations. After presenting basic features of the flow, we will consider several flow configurations. One of these is an unstable configuration involving gravity driven flow on homogeneous and heterogeneous inclined solid surfaces, leading to pattern formation in the form of fingers and rivulets. In particular, the flow on heterogeneous surfaces is interesting since the effect of heterogeneity often competes with the basic instability mechanism, leading to an elaborate interplay of various sources of instability. The computational results are then related to the pattern formation process observed in the experiments performed at NJIT. Other topics of discussion include modeling of the problems involving topological changes, such as drop coalescence and formation of dry spots.

Gregory A. Kriegsmann

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***Propagation in Periodic Dielectric Media***

We have employed a homogenization procedure to describe the propagation of electromagnetic waves in a dielectric structure which is periodic in the X-Y plane and translationally invariant in the direction of propagation, Z. The fundamental cell is composed of an arbitrarily shaped pore filled with a dielectric and the host by another. The pore shape is allowed to depend upon Z.

Our analysis yields the structure of the electromagnetic fields at the micro level and gives an effective medium equation at the macro level. The latter contains a simple arithmetic average of the dielectric constants and a correction term which involves a line integral around the pore. The integrand of this integral depends upon the polarization of the wave and the solution to a canonical potential problem which has an equivalent variational formulation. We have used this to obtain a simple macroscopic description of the dielectric structure.

Stephen Kunec

Boston University, Center for Biodynamics and Department of Mathematics and Statistics, Boston, MA 02215

***Encoding and Retrieval in the CA3 Region of the Hippocampus: A Model of Theta Phase Separation***

Past research (Hasselmo et al. 2002) suggests that some fundamental tasks are better accomplished if memories are encoded and recovered during different parts of the theta cycle. A model of the CA3 subfield of the hippocampus is presented, using biophysical representations of the major cell types including pyramidal cells and two types of interneurons. Inputs to the network come from the septum and the entorhinal cortex (directly and via the dentate gyrus). A mechanism for parsing the theta rhythm into two epochs is proposed and simulated: in the first half, the strong, proximal input from the dentate to a subset of CA3 pyramidal cells and coincident, direct input from the entorhinal cortex to other pyramidal cells creates an environment for strengthening synapses between cells, thus encoding information. During the second half of theta, cueing signals from the entorhinal cortex, via the dentate, activate previously strengthened synapses, retrieving memories. Slow inhibitory neurons (O-LM cells) play a role in the disambiguation during retrieval. We compare and contrast our computational results with existing experimental data and other contemporary models. Joint work with M. Hasselmo and N. Kopell (Boston University).

**Soumi Lahiri**

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***Linear and Log-Linear Models Based on Generalized Inverse Sampling Scheme***

The linear and log-linear models based on generalized inverse sampling scheme, have a broad application to the research of biological and environmental sciences. Model parameters are estimated using maximum likelihood and modified minimum chi-square estimation methods. The model efficiency is verified based on Wald test. Some applications of these models will be demonstrated. Joint work with Sunil K. Dhar (NJIT).

**Sanyogita Lakhera**

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***Computing Numerical Derivatives Using Bernstein Functions***

We examine the problem of estimating derivatives of grid functions based on non-compact, non-polynomial estimators built using stochastic interpolation and approximation methods, with particular attention to methods derived using Bernstein functions.

Bernstein functions arise naturally as an extension of the Bernstein polynomials in which the binomial probability density function (pdf) is replaced appropriately with a Gaussian pdf. These lead to row stochastic matrices which can be interpreted as convolution-deconvolution operators that can be used to construct Bernstein polynomial and Bernstein function interpolants.

These methods yield errors which are rapidly convergent (typically in the range of second to sixth order for smooth functions), however they appear to have advantages for non-smooth functions, providing robust interpolants even for very noisy data. Difficulties arise, though, in dealing with the boundaries of the domain as the errors typically decrease to first order near the boundary. Joint work with Joseph Kolibal (University of Southern Mississippi).

**Joe Latulippe**

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***Weakly Non-Autonomous Bursting Model for Visual Neurons***

Certain visual system neurons exhibit On and Off responses when given a light stimulus. By drawing analogies to Hodgkin-Huxley type models, we systematically develop a phenomenological model which replicates On and Off behaviors. This model is also shown to (numerically) replicate the simultaneous stimuli case measured by Kuffler (1953). An examination of the fast-slow dynamics of the model is divided into two cases: constant and non-constant post-synaptic currents. In the constant stimuli case, singular perturbation methods are used to show the dependence of the cell's response for various combinations of stimulus intensity and duration. When the (slowly varying) synaptic current is non-constant the model is weakly non-autonomous. However, we show that by embedding the non-autonomous problem into a higher dimensional autonomous system, much of the analysis for the constant case extends. Preliminary results of this will be shown.

**Eric Lauga**

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***Bacteria Swimming in Circles***

Near a solid boundary, *E. coli* does not swim in a straight line but performs a clockwise circular motion. We provide a hydrodynamic model for the motion of such bacteria near solid surfaces. We show that circular trajectories are natural consequences of force-free and torque-free swimming with account taken of hydrodynamic interactions with the boundary. Results of the model are compared to a new set of experimental data and reasonable agreement is obtained. Joint work with Willow DiLuzio, George M. Whitesides, and Howard A. Stone (Harvard University).

Kevin K. Lin

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***Entrainment and Chaos in the Pulse-Driven Hodgkin-Huxley Oscillator***

The Hodgkin-Huxley system of differential equations was derived to model action potential generation in the squid giant axon, and has long served as a paradigm for quantitative models of neurons. I present numerical evidence that a surprisingly rich range of qualitatively distinct responses may be elicited from the Hodgkin-Huxley model by the addition of a periodic impulse train. These response types include

- \* Stable entrainment to the input pulse train;
- \* Transient chaos followed by entrainment;
- \* Fully chaotic behavior characterized by a positive Lyapunov exponent, exponential decay of correlations, and the existence of a (unique) SRB measure.

These results are consistent with the predictions of Qiudong Wang and Lai-Sang Young, whose theory of kicked nonlinear oscillators motivated this work.

Xinfeng Liu

SUNY at Stony Brook, Applied Mathematics and Statistics, Stony Brook, NY 11794

***Computational Algorithms for Dynamic Interface Tracking in Three Dimensions***

A major challenge to this method is to handle changes in the interface topology. Two tracking methods, one named grid-free tracking and the other named grid-based tracking have been used to handle the three dimensional interface propagation and topological bifurcation. The former is a pure Lagrangian method in which the interface propagation and redistribution are independent of the underlying Eulerian grid. The detection and resolution of topological bifurcation is fully determined by the interface itself. This method is more accurate in the propagation of the interface position, but it is not robust in resolving the topological bifurcations. The latter is just the opposite. I developed locally grid based method, which uses Lagrangian propagation and redistribution, but applies Eulerian reconstruction for the bifurcation of Topology. This new method takes advantage of grid based method and grid free method, and reduces the use of Eulerian reconstruction to a minimum. It is particularly useful for the computation of an interface motion in which the interface forms sharp corners. It will also reduce the unphysical disappearance of the fragmented components of the material after bifurcation. The success of this improved algorithm is shown by simulations of turbulent mixing, such as the acceleration driven Rayleigh-Taylor instability, we found our simulations are now too fast, in disagreement with experiment, but when we include physical values of surface tension (we have implemented the revised calculation of curvature for a three dimensional surface into our code) and mass diffusion, we recover consistency with experimental values. Joint work with James Glimm and Xiaolin Li.

Xing Liu

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***Optimization in 2D Gel Image Alignment***

A new method for aligning families of two-dimensional polyacrylamide gel electrophoresis (2D-PAGE) images arising in proteomics studies is presented. Piecewise polynomial transformations via a multi-resolution approach is used to align the family of gels to an ideal gel. Both the ideal gel and the coefficients defining the transformations are obtained by solving a quadratic programming problem. Numerical results for a family of 123 gels are reported. Joint work with Florian Potra.

Dawn A. Lott

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***The Configuration of the Aneurysm Neck and Proximal Dome Profoundly Affects Shear Stress and Flow Velocities within an Aneurysm and its Parent Vessel***

Introduction: Flow characteristics of aneurysms depend upon the input flow and size of the parent vessel and aneurysm. Little is written describing the role of neck and dome configuration in establishing areas of shear stress as a potential for aneurysm growth. We developed a side-wall aneurysm model and compared different neck and dome configurations with regards to shear stress, velocity and pressure.

Methods: A finite-volume based package for modeling complex flow was utilized. A 5.3mm side-wall aneurysm with a 3.1mm neck was created and analyzed under pulsed-flow conditions. Shear stresses and velocities within the parent vessel, aneurysm, and interface were determined along several points of the cycle. Changes in neck and proximal dome geometry were made, and the analysis repeated. Comparisons in maximum velocities, pressures and shear stress were made.

Results: Changes in configuration of the neck, while maintaining its 3.1mm size altered the flow velocity, pressure and shear stress along the distal portion of the aneurysm, neck and parent vessel. Vorticeal flow patterns within the aneurysm dome changed, with flow velocities increasing at the interface between the aneurysm neck and parent vessel. The velocities at the distal neck (inflow zone) significantly increased when proximal dome configurations were modified as well.



Conclusion: The configuration of the neck and proximal dome, independent of the actual neck and aneurysm size, dramatically affects flow characteristics within the aneurysm and the aneurysm/parent vessel interface. Further benefits of the 2-D model as a possible predictor of aneurysm behavior will be explored. (Joint work with Hans Chaudhry and Michael Siegel (NJIT), and Charles J. Prestigiacomo (NJIT and UMDNJ).

Tianshi Lu

SUNY at Stony Brook, Department of Applied Math and Statistics, Stony Brook, NY 11794

***Direct Numerical Simulation of Bubbly Flows and Application to the Mitigation of Cavitation Erosion***

We have investigated the propagation of acoustic and shock waves in bubbly flows using direct numerical simulation. In this method, the liquid and the gas bubbles are represented by single-phase domains separated by free interfaces. FronTier, a front tracking hydro code was used for numerical simulations. It is capable of tracking simultaneously a large number of interfaces and resolving their topological changes in two- and three-dimensional spaces. We have compared results of our numerical simulations with theoretical predictions and experimental data on the propagation of linear sound waves and shock waves in bubbly fluids. The method has been applied to estimate the efficiency of gas bubble mitigation in reducing the cavitation erosion of the container of the Spallation Neutron Source liquid mercury target. Joint work with R. Samulyak (Brookhaven National Lab) and J. Glimm (SUNY at Stony Brook).

Jonathan H. C. Luke

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***An Effective Fluid Model for the Decay of Velocity Fluctuations in a Sedimenting Suspension***

Effective fluid models for sedimentation have often neglected fluctuations in the particle density. For well-stirred suspensions, however, these fluctuations produce enormous velocity fluctuations in large containers. We use an effective fluid model to study the transition from the large fluctuations typical of well-stirred suspensions to the small-fluctuations seen in "steady" sedimentation. We present the time-scales of the fluctuation decay and an assessment of the short-time asymptotics of the system energy and velocity fluctuations.

Valeriy V. Lukyanov

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***Analytical Modeling of Rayleigh-Bloch Surface Waves Along Metallic Rectangular Rods***

We develop an analytical method to analyze and to study Rayleigh-Bloch surface waves propagating along a two-dimensional diffraction grating which again consists of a periodic array of rods with rectangular cross sections. The method is based on mode matching. By taking into account all propagating and only a finite number of evanescent modes in a specific portion of the waveguide, we show that the surface waves correspond to the zeros of the determinant of a Hermitian matrix. We demonstrate numerically that the method gives an accurate result if we take into account only several evanescent waves. Joint work with Gregory A. Kriegsmann (NJIT).

Marc Q. Ma

NJ Institute of Technology, Computer Science Department and Center for Applied Mathematics and Statistics, University Heights, Newark, NJ 07102

***A Molecular Dynamics Study of the Effect of YC-1's Binding Modes on the Structure of Soluble Guanylyl Cyclase***

Soluble guanylyl cyclase (sGC) is an enzyme that can be allosterically activated by synthetic compounds such as YC-1 and its derivatives. sGC catalyzes the cyclization of the substrate guanosine 5'-triphosphate (GTP) to guanosine 3',5'-cyclic monophosphate (cGMP). cGMP is a second messenger molecule that regulates lots of biological processes including vasodilation. The mechanisms regulating the catalytic activity of sGC remain unclear. Recently, however, a mutagenesis study has been reported, in which a variety of point mutations were made in wild-type (WT) sGC that affect the catalytic activity and YC-1 allosteric activation of sGC. These new data still do not immediately point to a unifying molecular mechanism to explain sGC's regulatory processes. We present preliminary results in using all-atom, classical molecular dynamics (MD) simulations to study the pre-chemistry conformational changes induced by YC-1 with the ultimate goal of establishing a valid detailed molecular model of allosteric regulation in sGC. The details of our simulation protocol and some novel discoveries will be presented. Joint work with Kentaro Sugino and Yu Wang (NJIT), and Annie V. Beuve (UMDNJ).

Marc Q. Ma

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***GO-LinkGenes, A Multiple Component Data Mining Framework for Knowledge Discovery in Microarrays***

We present the design and evaluation of GO-LinkGenes, a data mining framework to facilitate exploration and knowledge discovery in DNA microarray experiments. GO-LinkGenes consists of two components, GO-Chart and LinkGenes. Each component can work independently of each other, or together in a unified fashion. GO-Chart is designed to visualize more conveniently the output from GOTM (GOTree Machine), while adjusting the p-values for multiple testing. GO-Chart allows users to analyze genes by Gene Ontology functional categories, occurrence, multiple parents-children relationships. LinkGenes is designed as a web-based tool for linking multiple genes to physical locations on human chromosomes and visualizing these genes. Feeding the output of genes identified using GO-Chart to LinkGenes, we are able to identify several human chromosomal regions that could be linked to either gene expression phenotypes or metabolic pathways. Genetic disease information associated with these genes is also obtainable through this tool. Joint work with Tongsheng Wang (NJIT and Public Health Research Institute, Newark, NJ 07103), Deepali Shah and Jason Wang (NJIT), Gerard Tromp (Wayne State University-School of Medicine), and Patricia Soteropoulos (Public Health Research Institute, Newark, NJ 07103).

**Victor Matveev**

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

#### ***A Bound-Calcium Mechanism of Synaptic Facilitation Revisited***

Synaptic facilitation (SF) is a form of a transient increase in synaptic strength elicited with just one or several stimulation pulses, and decaying with time constants from tens to hundreds of milliseconds. At some synapses, SF may be caused by the increase in the activity-induced  $\text{Ca}^{2+}$  influx; however, in many other synaptic types SF is believed to result from the presynaptic accumulation of residual  $\text{Ca}^{2+}$ , under conditions of constant  $\text{Ca}^{2+}$  current from one pulse to the next. In the latter case, it is not known whether it is free or bound residual  $\text{Ca}^{2+}$  that underlies SF. Experimental work has demonstrated that an increase in intrasynaptic  $\text{Ca}^{2+}$  buffering capacity leads to a rapid reduction in both the baseline synaptic response and in the magnitude of SF; this is often viewed as a proof that SF is caused by the accumulation of  $\text{Ca}^{2+}$  in free form. In the past we have explored two variations of such free residual  $\text{Ca}^{2+}$  hypothesis of SF: the so-called two-site model, and the buffer saturation mechanism. However, here we show that a model including the contribution of bound  $\text{Ca}^{2+}$  to SF is also consistent with the observed effect of exogenous  $\text{Ca}^{2+}$  buffers on synaptic response, and thus represents a viable alternative to the two-site free residual  $\text{Ca}^{2+}$  model. In particular, we show that such hybrid free/bound  $\text{Ca}^{2+}$  model is not in contradiction with the Kamiya-Zucker protocol (1994, Nature 371:603), whereby the synaptic strength of the crayfish neuromuscular junction is seen to decrease within few milliseconds of a UV-flash photolysis liberating a  $\text{Ca}^{2+}$  buffering compound. While evidence indicates that buffer saturation may underlie SF at calbindin-positive central synapses, we conclude that SF at other synaptic types may well involve a slow  $\text{Ca}^{2+}$  unbinding step from a putative  $\text{Ca}^{2+}$  release sensor. Joint work with Richard Bertram (Florida State University) and Arthur Sherman (NIH).

**Roberto Mauri**

University of Pisa, Department of Chemical Engineering, Pisa, Italy

#### ***Mixing of Viscous Liquid Mixtures***

We simulate the mixing process of a quiescent binary mixture that is instantaneously brought from the two- to the one-phase region of its phase diagram. Our theoretical approach follows the diffuse interface model, where convection and diffusion are coupled via a body force, expressing the tendency of the demixing system to minimize its free energy. In liquid systems, as this driving force induces a material flux which is much larger than that due to pure molecular diffusion, drops tend to coalesce and form larger domains which eventually must dissolve by diffusion. Therefore, in macroscopically quiescent mixtures, while convection speeds up phase separation, it effectively slows down mixing, which therefore is faster when the mixtures have large viscosities. In addition, the mixing rate is also influenced by the Margules parameter, which describes the relative weight of enthalpic versus entropic forces. In the late stage of the process, this influence can approximately be described assuming that mixing is purely diffusive and is therefore characterized by a self-similar solution of the governing equations, which leads to a  $1/t$  power-law decay for the degree of mixing, i.e. the mean square value of the composition field. Joint work with A.G. Lamorgese (Cornell University).

**Zoi-Heleni Michalopoulou**

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#### ***Using Time-Frequency Analysis and the Bayesian Paradigm to Extract Modal Arrivals in Underwater Acoustics***

Time-frequency analysis of signals that have propagated in an oceanic waveguide demonstrate modal dispersion in an informative manner. Identifying precise modal arrival times at specific frequencies can then be used for localization and geoacoustic inversion. Simple spectrograms, however, do not always allow accurate estimation of an arrival time - frequency pair for a given mode; especially in the presence of ambient noise, uncertainty characterizes such estimates. We here show how we can improve modal arrival estimates

using a Bayesian approach for time-frequency surface estimation as has been proposed for audio signals [Wolfe et al, Journal of the Royal Statistical Society, Series B, vol. 66, 2004].

Yuriy Mileyko

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#### **Algorithms for Swept Surface Intersections**

A new class of geometric objects called swept surfaces is studied and the problem of finding intersections of such objects is considered. Three algorithms for computing swept surface intersections are presented. The algorithms are based on ideas from existing intersection methods and utilize properties specific to swept surfaces to achieve the desired efficiency. Some of the employed properties of swept surfaces are also discussed.

Petronije Milojevic

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#### **Fredholm Theory for Hammerstein Equations**

Let  $X$  and  $Y$  be Banach spaces,  $K : Y \rightarrow X$  be a linear map and  $F : X \rightarrow Y$  be asymptotically positively homogeneous and odd, i.e.,  $F = F_1 + F_2$  with  $F_1$  positively homogeneous and odd outside some ball and  $\|F_2x\| \leq a \|x\| + b$  for large  $\|x\|$  and some constants  $a$  and  $b$ . Assuming that  $x + KF_1x = 0$  has only the trivial solution, we discuss various conditions on  $K$  and  $F$  that imply the solvability of the Hammerstein equation (\*)  $x + KF_x = f$  for each  $f$  in  $X$  (a generalized first Fredholm theorem). We require that  $I + KF$  be a (pseudo) approximation-proper map. In particular, we consider the cases when  $K$  is compact, or monotone and possibly nonselfadjoint, while  $F$  is of ball contractive or monotone type. The number of solutions of (\*) is discussed when  $I + KF$  is approximation-proper. Under suitable conditions, we also prove a complete extension of the Fredholm alternative to these classes of maps. Applications to Hammerstein integral equations and to BV problems for differential equations are also given.

Victor A. Miroshnikov

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#### **The General Solution for the Two-Dimensional Poiseuille Flow**

In two dimensions, general solutions of the unsteady Navier-Stokes equations are computed symbolically in the form of the Boussinesq-Rayleigh series and evaluated numerically. For finite Reynolds numbers, a nonlinear system of differential recurrent relations admits the following general solutions: the series solution for flows forced by the dynamic pressure and the series solution for freestreams. For generating functions, which are bounded together with their derivatives, the absolute convergence of the series solutions is shown by converting the differential recurrent relations into tensor recurrent relations and using the comparison and ratio tests. A triangular structure of three tensors of derivatives, which is employed in the tensor recurrent relations, is obtained by induction. It is shown that the general solutions away from boundaries are nonlinear superpositions of the Stokes flow, the Bernoulli flow, the Couette flow, and the Poiseuille flow. The general solution for the Poiseuille flow is specified by periodic generating functions, which model mixing of two-dimensional flows away from boundaries.

Milind Misra

NJ Institute of Technology, Department of Chemistry and Environmental Science, University Heights, Newark, NJ 07102

#### **Fuzzy Relational Clustering of Molecular Conformations Using Novel Features Based on DNA Base-Pair Step Parameters**

Six rigid-body parameters (Tilt, Roll, Twist, Shift, Slide, Rise) are commonly used to describe the relative orientation and positioning of any two base pairs in a nucleic acid structure. The present work generalizes the algorithms of the 3DNA software package (*Nucleic Acids Res.*, 31, 5108-21, 2001) to describe the relative orientation of any two planes in a molecule—for example, planes which contain important pharmacophore elements. Fuzzy relational clustering is used to classify molecular conformations using the six base-pair step parameters as features. This approach is applied to an analog of GBR 12909, a flexible inhibitor of the dopamine transporter potentially useful in the treatment of cocaine abuse. The results of this approach provide representative conformers to be used as templates for future 3D-QSAR (CoMFA) analysis. Joint work with Amit Banerjee, Deepa Pai, Rohan Woodley, Rajesh N. Davé, Liang-Yu Shih, Carol A. Venanzi (NJIT), and Xiang-Jun Lu, A. R. Srinivasan, and Wilma K. Olson (Rutgers University, Piscataway, NJ).

Robert M. Miura

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#### **Modeling Nonlinear Waves of Spreading Depression**

Slow chemical waves of spreading cortical depression (SD) have been observed during experiments in a variety of brain structures in different animals. Several mechanisms that are believed to be important in

modeling SD will be described, including ion diffusion, the spatial buffer mechanism, membrane ionic currents, osmotic effects, neurotransmitter substances, gap junctions, metabolic pumps, and synaptic connections. Ion diffusion and spatial buffering have been treated both theoretically and numerically, in simplified geometries, and several of the other mechanisms have been investigated numerically. In this talk, I will describe continuum models that consist of coupled nonlinear diffusion equations for the ion concentrations, and a discrete model that corresponds to treating the brain-cell microenvironment using a lattice Boltzmann method.

Brian E. Moore

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#### ***Modified Equations for Multi-Symplectic Integrators***

A useful way to understand symplectic integration of Hamiltonian ODEs is through the system of equations, known as the modified equations, which are solved by the numerical solution. Here, the ideas of symplectic integration are extended to Hamiltonian PDEs, such that the symplectic structure in both space and time is exactly preserved. This paves the way for the development of a local modified equation analysis solely as a useful diagnostic tool for the study of these methods. In particular, the modified equations are used to derive modified conservation laws of energy and momentum that are preserved to higher order along the numerical solution. Results on the behavior of the modified equations are also demonstrated through an application to traveling wave solutions.

Richard O. Moore

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#### ***Thermally Induced Dynamics and Pattern Formation in Optical Parametric Oscillators***

Optical parametric oscillators (OPOs) are an important source of laser-quality light in the far infrared. When operated at high average powers, absorption can lead to significant heating of the gain medium, changing the cavity properties and leading to thermal lensing and deformation of the transverse beam profile. To understand this process better, we consider the formation and evolution of patterns in reduced models of OPOs coupled to a diffusion equation for the temperature.

Pascal Moyal

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#### ***Stationarity of Some Queues with Impatient Customers***

Consider a queueing system with one server and infinite capacity, where the customers enter following an ergodic sequence  $(U_n, n \in \mathbb{N})$ , requesting ergodic services  $(\sigma_n, n \in \mathbb{N})$ . The customers are furthermore impatient: they must meet their requirement before a fixed due-date, and leave the system if they did not reach the server before. Their *patiences*  $(D_n, n \in \mathbb{N})$  are ergodic. We denote such a queue by  $G/G/1+G$ . Such a model has first been used to describe call centers with impatient customers, and applies furthermore in many time-sensitive computer networks or multimedia systems.

We investigate the stability of the queue: is 0 positive recurrent for the congestion process (*regenerativity*)? These questions have only been answered in the FIFO (*First in, First out*) context, where the arrival process is a renewal process, and the service durations as well as the patiences are i.i.d. ( $GI/GI/1+GI$  system): a sufficient condition for the system to be regenerative is given by  $P[\sigma < U] > 0$ . But in a general  $G/G/1/1+G$  system under any service discipline (as the EDF -*Earliest Deadline First-one*), the results are so far restricted, due to a higher stochastic instability. We prove the following more general statements:

1. any  $GI/GI/1/1+GI$  system satisfying  $P[D + \sigma < U] > 0$  is regenerative,
2. for any  $G/G/1/1+G$  system, there exists a monodimensional description of the system  $(Y_n, n \in \mathbb{N})$  tending to a stationary distribution  $Y$  as finite,
3. under further assumptions,  $Y$  is unique and the queue is regenerative.

Cyrill Muratov

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

#### ***Signal Propagation and Failure in Discrete Autocrine Relays***

This poster presentation is of my recent joint work with S. Shvartsman on modeling cell communication mechanisms in epithelial layers. The main mechanism at work here is ligand-induced ligand release coupled to the diffusion of ligands in the extracellular matrix. It is believed that under physiologically relevant range of parameters cell discreteness plays an important role in cell-to-cell communication. We formulated a fully discrete model of an autocrine relay, in which under physiologically reasonable assumptions it was possible to completely characterize propagation and failure. In particular, we obtained exact closed form discrete traveling wave solutions in this cell communication system.

Duane Nykamp

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***Reconstructing Subpopulation Connectivity Within Neuronal Networks***

To understand the function of neuronal networks within the brain, one would, at minimum, like to characterize the connectivity patterns that underlie these networks. Since one can simultaneously measure only a tiny fraction of neurons, the presence of vast numbers of unmeasured neurons can confound attempts to determine the subnetwork connecting the measured neurons.

A suitable mathematical framework can provide the structure to account for the presence of unmeasured neurons. Using a simple probabilistic model of a neuronal network, we demonstrate how to analyze connections among a subset of measured neurons embedded in the larger network. One obtains connectivity patterns in terms of certain neural subpopulations, which are groups of neurons with a similar response to a stimulus. This subpopulation connectivity can capture how network connections depend on the response properties of neurons.

Although the results are presented in terms of neuronal networks, the mathematical framework is applicable to other networks, such as gene regulatory networks.

Ozgur Ozen

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Experiments on Electrohydrodynamic Instability of Two-Layer Flow in a Square Channel***

The stability of two-fluid flow in a channel is of importance in the design of microfluidic systems. Due to the low Reynolds numbers in micro-channels, it is relatively difficult to attain mixing in these geometries. Recent studies using miscible fluids have shown that applying electric fields to these systems drastically enhances mixing over a short distance and in short times. However, in a class of applications, the fluids in contact are not miscible, and the interfacial tension stabilizes the interface; an effect absent in the physics of miscible fluids.

We have performed experiments where two immiscible fluids of different electrical properties flowing in a square channel are subjected to an electrical field normal to the liquid-liquid interface. Our experiments show that electric fields indeed affect the stability of the interface between two immiscible fluids and careful application of electrohydrodynamic instability can be used to cause a controlled deflection of the interface.

The experiments are also compared qualitatively to the theoretical study of the problem where the linear stability analysis of the two-fluid flow subject to a normal electric field is carried out using the Chebyshev Spectral Tau method. Joint work with N. Aubry, D. T. Papageorgiou, and P. Petropoulos (NJIT).

Demetrios T. Papageorgiou

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Nonlinear Dynamics of a Leaky Dielectric Fluid Sheet Under Horizontal Electric Fields***

In related work we have shown that a horizontal electric field applied to a fluid sheet comprised of a leaky dielectric can become unstable. This instability is not present for perfect dielectrics and arises due to the build-up of charge at the interface and the ensuing modification of the tangential stress balance there. In the linear regime we identify a canonical asymptotic limit that yields a rational long wave nonlinear model. This limit occurs as the electric field parameter,  $E_b$  say, tends to zero and a band of unstable waves is seen with a cut-off wavenumber  $E_b^{1/2}$  and growth rate  $E_b$ . This leads to nonlinear long waves of size  $E_b^{1/2}$  which is a measurable physical parameter (in general long wave theories assume the existence of an arbitrary long wavelength). A nonlinear system of evolution equations is derived asymptotically and it is found that the electric field in the surrounding medium enters in a local manner due to the smallness of  $E_b$ . The equations are studied for nonlinear traveling waves and the initial value problem is addressed to study possible rupture of the sheet. Joint work with Ozgur Ozen and Peter G. Petropoulos (NJIT).

John A. Pelesko

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***The MEC Lab, Hands-On Mathematics at the University of Delaware***

Just about everyone expects to find mathematics being used in the laboratory, but few of us expect to find mathematicians in the laboratory. Well, at the University of Delaware in the Department of Mathematical Sciences, finding mathematicians in the laboratory is quickly becoming a commonplace event. This was made possible with the establishment of the MEC Lab in the fall of 2002. This experimental laboratory, housed in the Department of Mathematical Sciences, takes its name from the words Modeling, Experiment, and Computation. These three words capture the hands-on philosophy of the lab; in the MEC Lab, math is meant to be experienced from every possible direction. This means carrying out real-world, often-dirty, hands-on experiments, constructing mathematical models, and analyzing them with the aid of

computers. In this poster, we showcase the many ways the MEC Lab has been incorporated into teaching and research in the Department of Mathematical Sciences at the University of Delaware. Joint work with Louis Rossi.

Mark Pernarowski

Montana State University, Mathematical Sciences, Bozeman, MT 59717

***Return Map Characterizations for a Model of Bursting with Two Slow Variables***

Many neurons and endocrine cells exhibit periodic bursting oscillations in their transmembrane electrical potential. The fast subsystems of the corresponding models exhibit bistability between stable equilibria and periodic orbits. Slow variables evolve in a manner which causes the solutions to switch between pseudo-stationary and oscillatory states resulting in a characteristic bursting pattern.

Most recent models involve two slow variables which tends to complicate their analyses. Using singular perturbation techniques we show that bursting solutions of such models correspond to fixed points of a one dimensional map constructed from the fast and slow subsystems. We further show that for some parameter values, bistability between bursting solutions and stable equilibria is possible. Joint work with Roger Griffiths (Mercyhurst College).

Peter G. Petropoulos

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Chemical Oscillations & Waves in the Undergraduate Applied Mathematics Laboratory: The Belousov-Zhabotinsky (BZ) Reaction***

By considering the modeling of the BZ reaction in a closed reactor (glass beaker) with continuous stirring (spatially homogeneous reaction modeled by a 3x3 system of nonlinear ordinary differential equations) the students make the connection between topics from nonlinear dynamics theory (stability of steady-states and birth/death of limit cycles through super/sub-critical bifurcations) and a real-world problem where chemical oscillations arise. Then, the students perform the actual experiment where potentiometric methods are employed to measure the two most important chemical concentrations as the reaction proceeds to equilibrium. Finally, the students identify the theoretical attributes of the BZ mathematical model in the measured time traces by constructing the phase plane from the measurements.

By considering the modeling of the BZ reaction in Petri dishes (spatially inhomogeneous reaction) the students study how systems of parabolic reaction-diffusion partial differential equations arise and how traveling waves are then possible in such systems. By performing the actual experiment and capturing sequences of images the students experimentally measure the speed of propagation of reaction fronts and compare to the theoretically obtained results for the speed of traveling waves.

A web diary of our progress can be found at <http://web.njit.edu/~peterp/Capstone.html>.

Valentin Polishchuk

SUNY at Stony Brook, Applied Mathematics and Statistics, Stony Brook, NY 11794-3600

***Touring Convex Polytopes – A Conic Programming Solution***

We study the problem of finding a shortest tour visiting a given sequence of convex bodies in  $R^d$ . To our knowledge, this is the first attempt to attack the problem in its full generality: we investigate high-dimensional case ( $d \geq 2$ ); we consider convex bodies bounded by (hyper)planes and/or (hyper)spheres; we allow a different cost of travel through each of the bodies; we do not restrict the start and the goal positions of the path to be single points, etc. Formulating the problem as a second order cone program (SOCP) makes it possible to incorporate distance constraints, which cannot be handled by a purely geometric algorithm.

Next, we focus on the planar case ( $d = 2$ ), with the convex bodies being just straight line segments – adjacent edges in a triangulation of a polygonal domain. In this setting we introduce a set of separation constraints on the path and observe that the new constraints can naturally be handled by the conic program. We also consider the case in which each face of the triangulation is assigned a weight, and the length of the path is measured according to the weighted region metric.

We implemented the SOCP program in MATLAB and obtained its solution with the SeDuMi package. We ran computational experiments, which suggest that the proposed solution is practical. Finally, we present NP-hardness results, showing that the assumptions we make in the statement of our problems are crucial for the problems to be tractable. Joint work with Joseph S. B. Mitchell (Stony Brook University).

Keywords: Computational Geometry, Weighted Region Metric, Conic Programming, Algorithms Complexity.

Joshua L. Proctor

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***Theory of Q-Switching in Actively Mode-Locked Lasers***

An analytic theory is proposed which characterizes Q-switching in an active mode-locked cavity as the nonlinear interaction of two unstable modes: one symmetric, another anti-symmetric. The phase difference between these modes generates a nonlinear beating interaction which gives rise to quasi-periodic behavior in the laser cavity. This quasi-periodic behavior is responsible for the Q-switching phenomena and is controlled by the interaction and overlap between neighboring pulses. Using a linear stability analysis, a

simple qualitative description of the Q-switching phenomena is given which is verified with numerical simulations of the governing active mode-locked equations. This model characterizes the Q-switching as a function of the physical parameters of the laser cavity and elucidates the mechanisms for controlling its behavior.

**Christopher Raymond**

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Effect of Reversible Chemistry on Immunocolloid Labeling***

We investigate the effect of reversible chemistry on the time course of a surface-volume biochemical reaction. We show how to modify asymptotic techniques developed for the irreversible case to produce approximate analytical solutions for arbitrarily strong reversibility and validate these approximate solutions by comparison to full numerical solutions.

**Gregory T. Reeves**

Princeton University, Chemical Engineering Department, Princeton, NJ

***Computational Analysis of EGFR Inhibition by Argos***

Argos, a secreted inhibitor of Drosophila epidermal growth factor receptor, and the only known secreted inhibitor of receptor tyrosine kinases, acts by sequestering the EGFR ligand Spitz. We use computational modeling to show that the biochemically-derived mechanism of Argos action is consistent with genetic data on EGFR/Spitz/Argos interactions in vivo. We find that efficient Spitz sequestration by Argos is key for explaining the existing data and for providing a robust feedback loop that modulates the Spitz gradient in patterning of the embryonic ventral ectoderm. Our analysis of the EGFR/Spitz/Argos module shows that Argos need not be long-ranged in order to account for genetic data in the ventral ectoderm. In our models, Argos action over both long and short length scales can effectively limit the range of secreted Spitz. Thus, the spatial range of Argos does not have to be tightly regulated or may depend on the developmental context. In addition, we verify the experimentally observed robustness of the wild type patterning of the ventral ectoderm and show that negative feedback control through Argos serves to impart this robustness.

Joint work with Rachel Kalifa and Stanislav Y. Shvartsman (Princeton University) and Daryl E. Klein and Mark A. Lemmon (University of Pennsylvania School of Medicine).

**Max Roman**

NJ Institute of Technology, Mechanical Engineering Department, University Heights, Newark, NJ 07102

***Modeling, Design, and Fabrication of Pulsed Micro-Jet Actuators***

The forced vibration of a thin flexible plate or membrane in a sealed cavity with a small opening can cause fluid to be pumped into and out-of the cavity. If the frequency and amplitude of vibration are large enough, a streaming of vortex rings occurs near the orifice. Moving under their own self-induced momentum, downstream of the opening these vortex pairs ultimately break up to form a fully developed jet. This phenomenon has been shown to be effective for a multitude of applications, including mixing, cooling of electronic components, micro-propulsion and flow control, such as the suppression of vortex shedding. Our own preliminary studies measuring the heat dissipation of dense circuitry by direct impingement with a pulsed jet have shown great promise.

Microfabrication (MEMS) offers a platform to build miniaturized inexpensive, reliable, light-weight, and low power actuators and sensors. Such small actuators can have a very unique function in microfluidics, where they can serve as micromixers, pumps, and non-invasive cell manipulators. This work is dedicated to the analysis, design, and fabrication of electrostatically actuated pulsed microjet actuators. This work is unique in that theoretical modeling, computer simulation (CFD-Computational Fluid Dynamics) and experiments are conducted in unison. A low dimensional theoretical model takes into account the coupling between the electrostatic actuation, the solid deformation of the membrane, and the squeeze flow in the cavity. Computational fluid dynamics allows us to better understand the formation of the vortex rings both inside and outside the cavity and how the jet develops. Experiments, aided by the use of PIV (Particle Image Velocimetry) validate both the model and CFD results. It is our goal that by understanding fundamentally the coupled physics of the actuator, the performance, in terms of exiting volume flux and dynamic response, can be precisely controlled and, therefore, applied to many diverse applications. Joint work with Nadine Aubry (NJIT).

**Satrajit Roychoudhury**

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Family of Probability Generating Functions Induced by Shock Model***

The question investigated here can be simply posed as follows: Under what conditions is the function defined by:

$$\int_0^{\infty} \frac{p^z}{Q(dp)},$$

a *probability generating function* (p.g.f) of a non-negative integer valued random variable  $N$ . The answer is clearly affirmative if the support of the mixing distribution  $Q$  is no larger than  $(0; 1]$ . This paper explores necessary conditions for which the function is a p.g.f. The motivation of this problem comes from some nonparametric aging properties of reliability methods. Joint work with M.C. Bhattacharjee (NJIT).

Keywords: Probability generating function, completely monotone functions, Essay Marshall and Proschan (EMP) shock model.

Roman Samulyak

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***MHD of Multiphase Flows at Low Magnetic Reynolds Numbers***

We have developed mathematical models, numerical algorithms, and computational software for the study of magnetohydrodynamics (MHD) at low magnetic Reynolds numbers of multiphase flows with phase transitions and free surfaces. The numerical models are based on the front tracking method for interfaces, a liquid-vapor phase transition and ablation models for phase boundaries, and high performance solvers for coupled hyperbolic - elliptic systems in geometrically complex and moving domains. Numerical simulations of hydro- and MHD processes in liquid mercury targets for future accelerators, and processes associated with the refueling of tokamaks through the injection of frozen deuterium pellets will be discussed.

Tobias Schaefer

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***Impact of Microstructures on Macroscopic Observables in Nonlinear Systems***

We present three approaches to understand the relation of microscopic and macroscopic scales in nonlinear systems. Each approach is discussed with an example that is of its own interest:

- (a) Method of multiple scales: Nonlinear Schroedinger vs. Shortpulse equation
- (b) Coarse-graining randomness in nonlinear systems: Random susceptibility and random dispersion
- (c) Chorin's Optimal Prediction: Averaging of Hamiltonian Systems

Eric Shea-Brown

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***How Architecture Restricts Spiking Patterns in Networks of Phase Oscillators***

We study networks of coupled phase oscillators and show how their architecture shapes their dynamics, forcing subsets to have the same oscillation numbers and interleaving spiking times. Our analysis follows the theory of coupled systems of ODEs developed by Stewart, Golubitsky, Pivato, and Torok, developing surprising new consequences for phase systems.

We say that two oscillators coevolve if the space on which their phases are equal is dynamically invariant and prove the results about oscillation numbers and spike times for these pairs. We then introduce a partition of oscillators in a network into 'collections' with closely related dynamics. We illustrate all of our results using the well-known 'theta neuron' model; implications for integrate and fire neurons are also discussed. Joint work with Martin Golubitsky and Kresimir Josic (University of Houston).

Asya Shpiro

New York University, Center for Neural Science, 4 Washington Place, New York, NY 10003

***Dynamics of Neuronal Competition Models for Binocular Rivalry***

We consider several reduced population firing rate models to describe oscillation dynamics during neuronal competition, in particular, during binocular rivalry - an alternation of percepts when different steady images are presented to the two eyes. These models, by Laing and Chow

(2002) and Wilson (2003), involve two neuronal populations, that correspond to the neural representations of competing percepts. They include recurrent excitation, cross-inhibition, and a slow negative feedback process. We focus on examining the effect of the input strength (e.g., contrast) to the two populations on the rate (and existence) of oscillations. In all models considered, there is a range of parameters when five distinct regimes of behavior are observed: as

the stimulus strength, common to both populations, decreases, the system's dynamics changes from both populations being highly active (fusion regime) to oscillations with the period increasing with decreasing input, followed by a winner-take-all regime, then by the oscillatory regime again, but with the period of oscillations decreasing as input decreases, and, finally, by the fusion at low activity level.

This result contradicts the classical view, based on many psychophysics experiments, in which the oscillation's period increases with decreasing input (this constitutes Levelt's Proposition I, 1968). We use phase plane methods to analyze the system's dynamics in a particular case of a Laing-Chow-like model with spike frequency adaptation, and show that different period vs. stimulus strength dependencies correspond to different mechanisms of establishing the alternating behavior: "release" and "escape" (Wang and Rinzal, 1992). We calculate the values of the input where the transitions between regimes occur, as functions of the model's parameters. Finally, we use phase plane arguments to analyze Levelt's Proposition II, which states



that if the stimulus strength to one population is changed, it is the dominance duration of the other population will be affected. We show that satisfaction of Levelt's Proposition II depends on whether the Levelt's Proposition I is satisfied or not. Joint work with Rodica Curtu (Transylvania University of Brasov, Romania), Nava Rubin (New York University), and John Rinzel (Courant Institute of Mathematical Sciences and Center for Neural Science).

Michael Siegel

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Steady Deformation and Tip-Streaming of a Slender Bubble with Surfactant in an Extensional Flow***

We consider steady-state deformation and time-dependent evolution of an inviscid, axisymmetric bubble in zero-Reynolds-number extensional flow when an insoluble and immobile surfactant is present on the bubble surface. Asymptotic solutions of slender-body theory show (i) steady ellipsoidal bubbles covered with surfactant, and (ii), at sufficiently large deformation, bubbles with a cylindrical surfactant-free central part and ellipsoidal surfactant-covered end caps. These bubble shapes are rounded at their end-points, in contrast to the non-rounded shapes found for entirely surfactant-free bubbles.

Simple expressions are found that relate the capillary number to the bubble slenderness ratio, and these show a critical capillary number above which steady solutions cease to exist. Beyond the critical capillary number, slender-body model equations show time-dependent spindle shapes at the bubble end-points with tip-streaming filaments. Joint work with M.R. Booty (NJIT).

Linda Smolka

Bucknell University, Department of Mathematics, Lewisburg, PA 17837

***Getting Your Hands Wet in Mathematics***

In recent years there has been increasing interest and support for physical labs in mathematics departments. The newest of these labs is being built at Bucknell University. Bucknell is a liberal arts college of 3,350 undergraduate and 150 graduate students. Bucknell is distinct among liberal arts colleges in that it has several professional programs including an engineering school.

I'll explain the role and goals of the lab at Bucknell within the context of the mathematics department, the university, and my own research program. I'll also discuss the process of designing a lab; including issues of funding, renovating, and selecting/purchasing equipment for the lab.

Seongho Song

University of Connecticut, Department of Statistics, 215 Glenbrook Rd. U-4120, Storrs, CT 06269-4120

***Genetic Diversity of Microsatellite Loci in Hierarchically Structured Populations***

Patterns of genetic variation within and among populations are determined by population sizes, migration rates, and mutation rates. We provide exact expressions for the first two moments of a stochastic model with hierarchically structured migration, mutation, and drift. Specifically, we consider the symmetric stepwise mutation model for microsatellite evolution under the assumption that the number of repeats is finite in Wright's finite island model. Further, we suggest two measures,  $\theta^{(I)}$  and  $\theta^{(II)}$ , as an analogue of Wright's  $F$ -Statistics and compared them to  $R_{ST}$  as discussed in Slatkin(1995). As a result,  $\theta$ 's and  $R_{ST}$  have the same properties under some conditions. Through numerical study we observe that  $R_{ST}$  measure is quite robust for the stepwise mutation model and the two-phase mutation model (Di Rienzo et al, 1994).

Keywords:  $F$ -statistics, Finite Island Model, Genetic Drift, Hierarchical Population Structure, Microsatellite Loci, Migration, Mutation, Singular Value Decomposition, Stepwise Mutation Model. Joint work with Dipak K. Dey and Kent E. Holsinger (University of Connecticut).

David Stickler

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Layered Media***

Ray theoretic methods are very useful in determining high frequency solutions to the scalar Helmholtz wave equation. This poster concerns the solution of the eiconal equation for an almost stratified medium. For a stratified medium the index of refraction depends only on  $Z$ , i.e.,  $n = n(Z)$ . For an almost stratified medium  $n = n(Z - E h(xy))$  where  $E$  is a small parameter and  $h(xy)$  are given. With minor assumptions on  $n(Z)$  and  $h(xy)$ , a solution to the eiconal equation to order  $E^2$  is obtained which is uniform in  $E$ , i.e., it contains no secular terms.

Louis Tao

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

***Visual Cortical Orientation Selectivity by Fluctuation-Controlled Criticality***

We examine how synaptic fluctuations modify the effects of strong recurrent network amplification to produce orientation selectivity in a large-scale neuronal network model of the macaque primary visual cortex. Typically, strong cortical amplification leads to network instabilities and unrealistically high firing rates even in the presence of strong cortical inhibition. In this poster, we show that large fluctuations in the cortico-cortical conductances can stabilize the network, allowing strong cortical gain and the emergence of orientation selective neurons. By increasing the strength of synaptic fluctuations, say, through sparsifying the network connectivity, we identify a transition between two types of dynamics, mean- and fluctuation-driven. In a network with strong recurrent excitation, this fluctuation-controlled transition is signified by a near hysteretic behavior and a rapid rise of network firing rates as the synaptic drive or stimulus input is increased. Finally, we demonstrate that network sparsity leads naturally to a recently observed invariance of orientation selectivity across the cortical network, even in the presence of orientation hypercolumns.

Burt S. Tilley

Franklin W. Olin College of Engineering, Department of Mathematics, 1000 Olin Way, Needham, MA 02492-1200

#### ***Electrokinetic Instabilities in Thin Microchannels***

An important class of electrokinetic, microfluidic devices aims to pump and control electrolyte working liquids that have spatial gradients in conductivity. These high-gradient flows can become unstable under the application of a sufficiently strong electric field. In many of these designs, flow channels are thin in the direction orthogonal to the main flow and the conductivity gradient. Viscous stresses due to the presence of these walls introduce a stabilizing force that plays a major role in determining the overall instability. A thin channel model for fluid flow is developed and shown to provide good agreement with a complete three-dimensional model for channel aspect ratio less than approximately one-tenth. Joint work with Brian D. Storey (Franklin W. Olin College of Engineering) and Hao Lin and Juan G. Santiago (Stanford University).

Natalia Toporikova

Florida State University, Department of Biological Science and Mathematics and Institute of Molecular Biophysics, Tallahassee, FL 32306

#### ***Mathematical Model of Neuronal Network Regulating Prolactin Release in Rats***

The mating stimulus of the rat uterine cervix (CS) induces two daily surges of the anterior pituitary hormone prolactin (PRL), which lasts for 12 days. PRL secretion occurs in response to relief from hypothalamic dopaminergic (DA) inhibition and stimulation by releasing oxytocin (OT). We have proposed a mathematical model to explain the origin of rhythmic PRL secretion. The model consists of a system of delay differential equations (DDE) and includes variables for the activity level of OT, PRL and DA cell populations. The oscillatory mechanism in the model is the mutual interaction between DA neurons and lactotrophs. Prior to CS, the system is in a stable state with a low basal level of PRL and a high level of DA. Following CS or injection of OT, PRL and the DA levels start to oscillate. The rhythm termination factors (PL or some other uterus factors) are modeled as an increasing function of time with a positive connection to the DA neurons. After 12 days this factor suppresses the oscillation by stimulation DA neurons and the system returns to the steady state. Joint work with M. Egli (Florida State University and Space Biology Group, ETH Zurich, Switzerland), and R. Bertram and M. E. Freeman (Florida State University).

A. David Trubatch

United States Military Academy, Department of Mathematical Sciences, West Point, NY 10996

#### ***Soliton Dynamics in the Integrable Discrete Vector Nonlinear Schrödinger Equation***

The fundamental solitons of the integrable discrete vector nonlinear Schrödinger equation (IDV-NLS) retain many of the interesting properties of their continuous counterpart (i.e., the solitons of Vector NLS, also known as the Manakov equation). In particular, the collision-induced phase shifts of the vector solitons can be described by fractional linear transformations and constitute a solution of the set-theoretical Yang-Baxter equation. Moreover, as in the continuous case, logical operations can be encoded in the vector-soliton interaction such that it is possible to carry out general computations with the discrete vector solitons. On the other hand, the discrete system contains composite soliton states that have no counterpart in the Manakov system. These traveling breathers are related to a class of traveling breathers of the scalar integrable discrete NLS (also known as the Ablowitz-Ladik equation). However, unlike their scalar, discrete counterparts the composite solitons have a minimal nonlinear spectrum as solutions of the vector system.

Dmitri Tseluiko

NJ Institute of Technology, Mathematical Sciences Department, University Heights, Newark, NJ 07102

#### ***Nonlinear Stability of the Solutions of Modified Kuramoto-Sivashinsky Equations***

We study equations that arise in the modelling of the wave motion in a perfectly conducting viscous thin film falling down an inclined plane under gravity in the presence of an electric field which is uniform in its undisturbed state, and normal to the plate at infinity. These are modified Kuramoto-Sivashinsky equations with an additional non-local term due to the Maxwell stresses exerted at the interface by the electric field. The numerical results show that the solutions of these equations are nonlinearly stable

and exhibit a complicated behavior including chaotic oscillations as in the case of the usual Kuramoto-Sivashinsky equation; the basins of attraction of chaotic dynamics is significantly affected by the presence of the electric field, however, and this is seen as significantly larger windows in phase space where the global attracting solutions exhibit complicated dynamics. The nonlinear stability of the solutions is also proved analytically. The proof also leads to an upper bound estimate of the 2-norm of the solution in terms of the length of the system and the electric field intensity parameter. Joint work with Demetrios T. Papageorgiou (NJIT).

A. Kerem Uguz

University of Florida, Chemical Engineering Department, Gainesville, FL 32611

***An Experimental Study on the Stability of Elliptical Liquid Bridges***

The break-up point of an elliptical liquid bridge was investigated in a Plateau chamber using two density-matched liquids. The objective was to show that an elliptical liquid bridge is more stable than a companion circular bridge where the elliptical end plates are slight deviations from the circular end plates. The semi-major axis of the ellipse was roughly 20% larger than the radius of the circle yet maintaining the areas the same for both geometries. The volume in the elliptical liquid bridge was fixed to be the same as the volume of the companion cylindrical bridge at its critical point and the end plates were parallel and oriented so that they were not twisted with respect to one another. In this study, two different sizes of circular end plates were used to confirm our results. The distortion amount, which was roughly 20%, was kept constant for both cases and elliptical liquid bridge experiments were performed. It was found that the elliptical liquid bridge break-up point is about 3% longer than its corresponding cylindrical liquid bridge demonstrating that an elliptical liquid bridge is more stable than its companion circular liquid bridge. A theory showing that the elliptical end plates do not break the classical bifurcation is presented. This supports the view that the elliptical liquid bridge ought to be more stable than its circular counterpart. Joint work with N. J. Alvarez and R. Narayanan (University of Florida).

A. Kerem Uguz

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***Rayleigh-Taylor Instability with Shear-Induced Flow***

It is known in the Rayleigh Taylor problem that there is a decrease in stability when the liquid is sheared with a constant stress. This decrease in the stability limit has been explained with the symmetry breaking effect of the shear. In this study, we prove that the fluid mechanics of the light fluid (vapor or liquid) is important and it changes the characteristics of the problem. Shear induced Rayleigh-Taylor instability in an open-channel flow and in a closed container is studied in this paper. For both cases, at the base state, we satisfied the conditions for a flat interface between the two liquids and studied the stability of this base state to small disturbances via linear stability analysis. In the open channel flow, the critical point remained unchanged compared to the classical Rayleigh-Taylor instability, but the critical point exhibits oscillations and the frequency of the oscillations depends on the wall speed. On the other hand, in a closed geometry, moving the wall stabilizes the classical Rayleigh-Taylor instability and it does not show any oscillation at the onset of break-up. We also applied weakly nonlinear analysis to study the nature of the bifurcation via a dominant balance method and concluded that the problem shows a backward pitchfork bifurcation, as does the classical Rayleigh-Taylor instability problem. Joint work with Ranga Narayanan (University of Florida).

Suleyman Ulusoy

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***An Entropy Dissipation-Entropy Estimate for a Thin Film Type of Equation***

We prove a lower bound on the rate of relaxation to equilibrium in the  $H^1$  norm for a thin film equation. We find a two stage relaxation, with power law decay in an initial interval, followed by exponential decay, at an essentially optimal rate, for large times. The waiting time until the exponential decay sets in is explicitly estimated. Joint work with E.A. Carlen. Keywords: thin film, Lyapunov functional, entropy dissipation.

Vianey Villamizar

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***Grid Generation with Curve Control and Its Application in Acoustic Scattering***

A new algorithm to automatically generate two-dimensional boundary conforming coordinates, with grid curve control, on multiply connected regions, is devised. The technique is based on the numerical solution of the widely used Poisson grid generation equations. The physical domain  $D$  is transformed into a topologically equivalent connected rectangular domain  $D'$  by defining a branch cut inside  $D$ . Grid curve control over the multiply connected regions with one or more interior holes is established by appropriately distributing grid points with the desired spacing on the branch cut, and on other boundary curves. From this initial distribution of points, control functions present in the Poisson system are defined, creating a natural link between clustering properties and the control functions. An iterative smoothing process relocating the branch cut is described. As a result, a smooth grid retaining the spacing of the non-smooth initial grid is obtained.

Tested hole shapes include a rose, an epicycloid, an astroid, and a pacman. These grids are used to numerically solve acoustic scattering problems. Approximations of the pressure field and the scattered cross section for arbitrary shape obstacles are obtained. Joint work with Joseph Mabey (Brigham Young University).

## X. Sheldon Wang

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### ***From Immersed Boundary Method to Immersed Continuum Method***

In this talk, a new modeling method, the immersed continuum method (ICM), is proposed for the coupling of different continua (fluid-fluid, fluid-solid, or solid-solid). This new method retains the same strategies employed in the immersed boundary (IB) method [1] and the recent extensions, namely, the extended immersed boundary method (EIBM) [2] and the immersed finite element method (IFEM) [3]. The immersed continuum method deals with submerged continua (compressible or incompressible) which occupy finite volumes within the surrounding fluid (or solid) medium. In the context of fluid-solid interactions [4] [5], like EIBM and IFEM, in ICM, an independent solid mesh moves on top of a fixed or prescribed arbitrary Lagrangian-Eulerian (ALE) background fluid mesh. The procedure of constructing an entire fluid domain over both fluid and solid domains is similar to that of the fictitious domain method [6]. However, unlike the fictitious domain method which is designed for immersed rigid bodies; ICM handles arbitrary immersed deformable solids/structures. Furthermore, in order to handle submerged compressible continua and to circumvent the stringent requirement for the time step size as demanded in the explicit time marching schemes in the IB method, EIBM, and IFEM, we introduce in ICM an implicit formulation along with the combination of the Newton-Raphson and GMRES iterations. The new attributes in ICM enable a wide variety of applications in aerospace, mechanical, civil, and in particular bio-engineering fields. Several numerical examples in micro- and capillary vessel hemodynamics are also presented for illustrative purposes.

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## Xinli Wang

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### ***Influence of Surfactant on Air Entrainment at a Contact Line***

We present a model for the rolling motion of a viscous fluid onto a rigid substrate, in the case when insoluble surfactant is present at the fluid interface. The model is used to examine the influence of surfactant on air entrainment at the line where the fluid contacts the wall. In the absence of surfactant, an analytical solution has been obtained by Benney and Timson (*Stud. Appl. Math* 1980) for the local flow field near the point of steady attachment. They find that a steady local solution exists for all capillary numbers. In the presence of surfactant, we find that there is a critical capillary above which steady shapes no longer exist. This suggests that the presence of surfactant can lead to air entrainment for large enough capillary number. Joint work with Michael Siegel (NJIT).

## Wonsuk Yoo

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### ***Model Selection Method using Reversible Jump MCMC Algorithm for Longitudinal Biomarkers***

Markov chain Monte Carlo (MCMC) methods provide a very effective sampling base by generating from extremely complex distributions but they can be used only within fixed dimensions. We consider a model within a fully Bayesian framework which postulates a mixture for longitudinal data, for which one component contains a change point and the other does not. While MCMC methods cannot be used in this trans-dimensional situation which needs to move between different states or dimensions, the reversible jump Markov chain Monte Carlo (Green 1995) allows a Markov transition between models with parameter spaces of different dimensions, but holds the aperiodicity, irreducibility, and detailed balance conditions necessary for MCMC convergence. It is particularly useful in the model selection procedure within the Bayesian context. This paper focuses developing the algorithms of the reversible jump MCMC, and evaluating them on the basis of the early detection. This paper can be valuable in Bayesian model determination using reversible jump method since the algorithms are proposed based on usage of various auxiliary variables for dimension-matching. The results from these proposed algorithms can be more reasonable because they allow various

and realistic situation on the relationship between parameters of both models. We provide following steps: birth, death, update and move steps on each iteration. We apply this reversible jump algorithm to Nutritional prevention of Cancer Trial (Clark 1996).

Yun Yoo

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***Periodic Orbits Near a Saddle-Focus in Systems with Strong Contraction***

We study a one-parameter family of three-dimensional flows near an Andronov-Hopf bifurcation (AHB). We specify conditions on the global vector field that guarantee the existence of a rich family of multimodal periodic orbits passing close to a saddle-focus. We identify two bifurcation scenarios for periodic orbits depending on the character of the AHB and analyze the properties of the periodic orbits using asymptotic techniques for ordinary differential equations. This work is motivated by the numerical results for a finite-dimensional approximation of a free boundary problem modeling solid combustion.

Yuan-Nan Young

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***Effect of Capillary Network Hemodynamics on Tumor Growth***

A two-dimensional model of tumor necrosis, neo-vascularization and tissue invasion was recently developed by Zheng, Wise and Cristini. This model describes the angiogenesis and vascular nutrient delivery that occur during tumor growth; however, blood flow and other physiological details of transport in the capillary network are not included. To improve this model, a two-phase (red cells and plasma) continuum model of blood flow is used to estimate the local capacity for nutrient delivery within the network. This model includes empirical relations describing known nonlinear effects (Fahraeus, Fahraeus-Lindqvist, and plasma skimming) and allows calculation of the steady-state blood flow distribution within the network. Using calculated capillary network blood flows to modulate nutrient delivery, it is shown how tumor growth and steady-state patterns differ from those obtained assuming constant nutrient delivery throughout the network. Currently, blood flows are calculated only at selected times during tumor growth, however in the future the blood flow pattern will be updated simultaneously with tumor evolution. This is a joint collaboration with Daniel Goldman (NJIT), and V. Cristini and X. Zhang (UC Irvine).

Yuan-Nan Young

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***Effect of Surfactant on Bubble Deformation***

The effect of surfactant on bubble deformation is investigated using direct numerical simulations. In particular we focus on the formation of long, thin thread due to the surfactant effect, and investigate the possibility of local similarity solution that leads to pinch-off of the thin thread in the presence of insoluble surfactant. In the second part of this investigation we include soluble surfactant and report how the formation of the thin thread can be altered. This is a joint work with Jie Li (Cambridge University), and Michael Siegel and Demetrios T. Papageorgiou (NJIT).

Hui Zhang

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***Adaptive Level Set Method for Droplet Dynamics and Solidification in Sprayed Coating Applications***

Sprayed coatings are formed by injecting a powder feedstock through a thermal plasma or combustion flame, where the powder is melted. The resulting molten droplets are accelerated to high velocity and impact on a substrate. The droplets spread into disk-like pancake shapes called splats and rapidly solidified. Agglomerating splats form a thick film coating with a distinctive lamellar microstructure, characterized by the splat interfaces or interphases. In this presentation, current status of thermal spray research will be reviewed. An advanced numerical model based on the adaptive level set method is developed that is capable of solving the deformation of the free surface, fluid instability, and evolution of solidification interface simultaneously. In the new model conservation of mass is guaranteed and the solution domain can be adaptively deformed depending on the solution process. Theoretical and numerical analyses are performed to predict the splat-flattening ratio and related the splat geometry with the droplet Reynolds, Weber, Jakob numbers and substrate conditions. The numerical predictions are in good agreement with the experimental data. Through studies, good understanding has been achieved on the single splat formation and the roles of kinetic, dissipation and surface energies on the droplet spreading and solidification process. Numerical and experimental studies are also performed to study the splashing phenomena. Different splashing mechanisms are proposed and confirmed with the experimental data. The fragmentation degree is related to surface wetting, rapid solidification, substrate roughness and surface chemistry. The ability to control and manipulate the splat formation will significantly advance the spray coating technology.

Kai Zhang

### **TIMDA: A Toolkit for Integrated Genotyping Microarray Data Analysis**

Background: TIMDA (Toolkit for Integrated Genotyping Microarray Data Analysis) is designed for integrated data analysis for spotted single nucleotide polymorphism (SNP) genotyping microarrays.

Results: We have implemented TIMDA using Matlab, a powerful and popular engineering computing programming language which integrates seamlessly the mathematical computation, analysis, visualization and algorithm development. The framework of TIMDA consists of several function modules for microarray image processing which implements precise gridding and robust segmentation techniques, data preprocessing, genotype-calling which implements novel machine learning-based algorithms and Loss-of-Heterozygosity which is used to study the genetic basis of certain diseases, Graphical User Interface and text and graphical outputs. Each individual module works seamlessly with each other. Some modules, such as the image-processing module, can also be singled out to work on their own. A user can also bypass some modules by supplying with information generated from other software, which makes TIMDA a flexible framework.

Conclusions: We have done extensive testing of TIMDA, which shows that TIMDA is a powerful framework for performing robust data analysis in genotyping microarrays.

Joint work with Li Jia, Marc Ma, Frank Shih, Yu Wang, and I-Jen Yeh (NJIT), Honghua Li and Hui-Yun Wang (UMDNJ, Robert Wood Johnson Medical School), Tongsheng Wang (NJIT and Public Health Research Institute), and Patricia Soteropoulous (Public Health Research Institute).

Yili Zhang

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### **Modeling Recovery of Rhythmic Activity: Hypothesis for the Role of a Calcium Pump**

The rhythmic activity produced by the pyloric network of crustaceans depends on the release of neuromodulatory substances by axon terminals from adjacent ganglia. After these terminals are destroyed or action potential transmission along these axons is inhibited (decentralization), the rhythmic pyloric activity recovers spontaneously, but the process of activity recovery follows a very complex temporal dynamics that involves the alternating turning on and off of the pyloric rhythm (that we term 'bouts'). This bouting period lasts several hours after which a stable pyloric rhythm emerges.

We have built a model of the activity of a pyloric neuron to study the recovery of rhythmic activity after decentralization. Our model is based on a dynamic oscillation of intracellular  $Ca^{2+}$  due to the interaction of  $Ca^{2+}$  influx,  $Ca^{2+}$  diffusion,  $Ca^{2+}$  pump activity, and IP3 receptor activity at the endoplasmic reticulum (ER). The model assumes that activity is monitored by sensors of intracellular  $Ca^{2+}$  concentration changes. The three  $Ca^{2+}$  sensors represent biochemical pathways sensitive tuned to different frequencies of  $Ca^{2+}$  change. They act as feedback regulators of  $Ca^{2+}$  and  $K^{+}$  conductances, and of  $Ca^{2+}$  pump activity. Our model reproduces qualitatively accurately the dynamics of recovery after decentralization, particularly the transition to a stable rhythm after a period of bouting. We observe that the regulation of the activity of the ER  $Ca^{2+}$  pump is key in the generation of this rich dynamics. Supported by NIH grant MH-64711 (J.G.). Joint work with Jorge Golowasch (NJIT and Rutgers University).

Yongmin Zhang

SUNY at Stony Brook, Applied Mathematics and Statistics, Stony Brook, NY 11794

### **Modeling and Simulation of Fluid Mixing for Laser Experiments and Supernova**

Recently, laboratory astrophysics has been playing an important role in the study of astrophysical systems, especially in the case of supernova explosions through the creation of scaled reproductions of astrophysical systems in the laboratory. In collaboration with a team centered at U. Michigan and LLNL, we have conducted front tracking simulations for axisymmetrically perturbed spherical explosions relevant to supernovae as performed on NOVA laser experiments, with excellent agreement with experiments [1]. We have extended the algorithm and its physical basis for preshock interface evolution due to radiation preheat [2]. The preheat simulations motivate direct experimental measurements of preheat as part of any complete study of shock-driven instabilities by such experimental methods.

Our second focus is to study turbulent combustion in a type Ia supernova (SN Ia) which is driven by Rayleigh-Taylor mixing. We have extended our front tracking to allow modeling of a reactive front in SN Ia. Our 2d axisymmetric simulations show a successful level of burning [3]. Our front model contains no adjustable parameters so that variations of the explosion outcome can be linked directly to changes in the initial conditions.

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Joint work with James Glimm, Paul Drake, Srabasti Dutta, John W. Grove, and David H. Sharp (State University of New York, Stony Brook).

Lin Zhou

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***Complete Transmission Through a Periodically Perforated Solid Slab***

The propagation of a normal incident plane acoustic wave through a 3-dimensional rigid solid slab with periodically placed holes is modeled and analyzed. The period of the structure  $S$ , the wavelength and the thickness of the slab  $L$  are order one parameters compared to the characteristic size of the holes  $R$ , which is a small quantity. Scattering matrix techniques are used to derive expressions for the transmission and reflection coefficients of the lowest mode. These expressions depend on only the transmission coefficient of an infinitely long slab with the same configuration. An infinite system of algebraic equations of the transmission coefficients is derived and solved approximately by exploiting the small parameter  $R/S$ . It turns out that the structure is transparent at certain frequencies which could prove useful in narrow band filters and resonators. Joint work with Gregory A. Kriegsmann (NJIT).

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***Bayesian Models for Location Estimation in Wireless Networks***

The Bayesian modeling approach is used to study location problems in wireless networks using Markov Chain Monte Carlo methods in DAGs (directed acyclic graphs). Nonhierarchical and hierarchical Bayesian models are investigated, as well as penalized Bayesian splines and bivariate splines in combination with a particle approach. Two different data sets are used to illustrate proposed models. (Joint work with D. Madigan, Rutgers University.)