

## PLENARY SPEAKERS

### **Oscar Bruno**

California Institute of Technology, Applied & Computational Mathematics, Pasadena, CA 91125

#### ***Fast Spectral Frequency- and Time-domain PDE Solvers for General Domains***

We present fast frequency- and time-domain spectrally accurate solvers for Partial Differential Equations that address some of the main difficulties associated with simulation of realistic engineering systems, including geometric complexity, heterogeneity, high frequencies, geometric singularities, etc. Based on a novel Fourier-Continuation (FC) method for the resolution of the Gibbs phenomenon, associated surface-representation methods and fast high-order methods for evaluation of integral operators, these methodologies give rise to fast and highly accurate frequency- and time-domain solvers for PDEs on general three-dimensional spatial domains. Our fast integral algorithms can solve, with high-order accuracy, problems of electromagnetic and acoustic scattering for complex three-dimensional geometries; our FC-based differential solvers for time-dependent PDEs, in turn, give rise to essentially spectral time evolution, free of pollution or dispersion errors. A variety of applications to linear and nonlinear PDE problems demonstrate the very significant improvements the new algorithms provide over the accuracy and speed resulting from other approaches.

### **Naomi Ehrich Leonard**

Princeton University, Department of Mechanical and Aerospace Engineering, Princeton, NJ 08544

#### ***Information Passing and Collective Animal Motion***

Information passing through social interactions in moving animal groups, such as bird flocks and fish schools, is credited both with improving group responsiveness to external environmental stimuli and with maintaining group cohesiveness in the presence of uncertainty. Agent-based dynamical models with interaction terms that enable information diffusion have been used successfully to reproduce a range of observed collective motions. I will discuss analytic approaches for examining group decision making and exploring group robustness to uncertainty. Of particular interest is the role of the topology of the interconnections among individuals on the emergent outcomes and performance at the level of the group.

### **Joyce McLaughlin**

Rensselaer Polytechnic Institute, Department of Mathematical Sciences, Troy, NY 12180

#### ***Biomechanical Imaging in Tissue - Using Time Dependent Data***

Biomechanical Tissue Imaging is inspired by the doctor's palpation exam where the doctor presses against the skin to feel abnormal stiff regions within the body. This talk about this imaging area will contain a description of inventive technologies that utilize the concept of interior radiation force; an example of one of these technologies is Supersonic Imaging which is developed in Paris. In these technologies low amplitude (tens of microns) propagating wave motion is produced in the body and the technologies output a movie of this motion. We will discuss elastic and viscoelastic mathematical models and the essential properties that must be included so that solutions mimic the data produced by the experiment. Algorithms, that utilize the fundamental features of the model and the time dependent data, will be presented. Images of cancerous tissue, corroborated with ultrasound images, including cancerous inclusions a few millimeters in diameter will be shown.

## **George Papanicolaou**

Stanford University, Department of Mathematics, Stanford, CA 94305

### ***Correlation Based Imaging***

Imaging with passive sensor arrays using ambient noise for illumination is a recent development with some very promising applications in geophysics and elsewhere. I will present an overview of this imaging methodology, pointing out the challenges it poses mathematically for a deeper understanding of why it works and how it can be improved.

## **Jacob White**

Massachusetts Institute of Technology, Department of Electrical Engineering and Computer Science, Cambridge, MA 02139

### ***Surface Absorbers in Fast Integral Equation Solvers***

When fast surface integral equation (SIE) methods are used to solve wave propagation problems, one might presume that absorbers are unnecessary given the infinite exterior domain is resolved exactly. For geometries with infinite surfaces, such as nanophotonics couplers between infinite channels, the problem of absorbers reappears because the channels must be terminated. In this talk we show that the obvious approach to termination, making the volume of the channel mildly conductive outside the domain of interest, causes too much numerical reflection to be practical. We then describe a new method in which the absorber has a gradually increasing surface conductivity; as such an absorber is easily incorporated in fast integral equation solvers. Numerical experiments from a surface-conductivity modified FFT-accelerated PMCHW-based solver are correlated with analytic results, demonstrating that this new method is orders of magnitude more effective than a volume absorber, and that the smoothness of the surface conductivity function determines the performance of the absorber. This work was supported by the Singapore-MIT Alliance Flagship Program in Computational Engineering. Joint work with L. Zhang, J.H. Lee, A. Oskooi, A. Hochman, and S. Johnson.

## MINISYMPOSIUM SPEAKERS

### **David Ambrose**

Drexel University, Department of Mathematics, 3141 Chestnut Street, Philadelphia, PA 19104

#### ***Time-Periodic Solutions of Nonlinear Systems of PDE***

We introduce a numerical method for the computation of time-periodic, spatially periodic solutions of nonlinear systems of partial differential equations. This method is first applied to the Benjamin-Ono equation, finding continua of genuinely time-periodic solutions bifurcating from trivially time-periodic solutions (traveling waves or stationary solutions). We are able to verify, using explicit expressions for time-periodic solutions of Benjamin-Ono, that all of the computed time-periodic solutions correspond to actual time-periodic solutions of the equation. Time-periodic vortex sheets with surface tension will also be discussed.

### **Agis Athanassoulis**

University of Cambridge, DAMTP, Wilberforce Road, Cambridge CB3 0WA, UK

#### ***Semiclassical Limits for Non-smooth Potentials: Quantum Selection Principles for Certain Ill-posed Classical Problems***

One of the main limitations of semiclassical asymptotics in linear problems is the regularity of the potential  $V(x)$ ; indeed ill-posed problems appear for non-regular potentials. Great progress has been achieved recently in the extension of the theory (from the traditional  $V \in C^{\{1,1\}}$ ) to problems with  $\nabla V \in BV$  in great generality, by working with a statistical population of initial data and thus dealing with the loss of uniqueness in a probabilistic sense, by Ambrosio, Figalli and their collaborators. We present a complementary approach, where additional conditions are needed for certain potentials of the BV type, and for the initial data, but under these conditions we can control completely the semiclassical limit for a single initial datum.

This allows the capture of exotic behaviour: a delta in classical phase space possibly splitting into two deltas after some time in our case, as opposed to a cloud of deltas splitting into two clouds of deltas in the more general case.

### **Helene Barucq**

INRIA Bordeaux Sud-Ouest Research Center, Team Project Magique-3D, France

LMA, Université de Pau et des Pays de l'Adour, France

#### ***Enriched Absorbing Boundary Conditions for Acoustic Waves***

The numerical simulation of scattering problems generally involves the truncation of the propagation domain and boundary conditions on the exterior boundary are then required. In some cases such as scattering problems by elongated obstacles, the size of the computational box can be reduced significantly if the external boundary is adapted to the shape of the obstacle. Hence, it is interesting to use boundary conditions which both approximate the behavior of infinity accurately and can be set on arbitrarily shaped surfaces. These conditions are called Absorbing Boundary Conditions (ABCs) when they satisfy the following properties: ABCs correspond to the approximation of a transparent condition, involve local or pseudo-local operators and minimize the reflections generated by the exterior boundary. It is worth noting that there are few works dealing with high-order ABCs for arbitrarily-shaped surfaces and high-order conditions are generally written for piecewise-flat surfaces and corner conditions must be introduced. Now ABCs are generally obtained from the approximation of the Dirichlet-to-Neumann operator in the propagation cone [2]. It is thus possible that the performance of ABCs might be improved by broadening its spectrum to evanescent and/or grazing waves. Recently, a new ABC has been proposed by Hagstrom et al. [4]. It is an Improved Higdon ABC (IHABC) [5] in which a differential operator is included to represent

evanescent waves. The IHABC is efficient when coupled with a standard finite element method, but it seems to hamper the Courant-Friedrichs-Lewy (CFL) condition in particular when using a Discontinuous Galerkin Method (DGM) for the space discretization. Moreover, it is not easy to apply on arbitrarily-shaped boundaries because it requires supplementing conditions at each corner of the polyhedral boundary. In [1], we have designed an ABC which takes into account both propagating and evanescent waves and can be applied on arbitrarily-shaped convex boundaries. Numerical experiments have shown that the CFL condition is preserved. In this work, we present a new ABC that is obtained from the approximation of a complete transparent boundary condition modeling propagating, evanescent and grazing waves. It is pseudo-local since it involves a fractional derivative arising from the grazing part of the solution. However, it is easily included into an Interior Penalty Discontinuous Galerkin (IPDG) formulation of the acoustic wave equation. Moreover, it does not generate large computational costs because the band width of the discrete fractional operator involves a very low number of points. Numerical experiments illustrate the efficiency of the new condition both in the time and harmonic domains. They show that the absorption rate is improved when compared to classical ABCs, in particular for harmonic waves. We also perform long-time simulations to illustrate the robustness of the numerical scheme. Joint work with J. Diaz and V. Duprat.

#### References:

- [1] H. Barucq, J. Diaz, V. Duprat, Micro-differential boundary conditions modelling the absorption of acoustic waves by 2D arbitrarily-shaped convex surfaces, *Comm. in Comp. Phys.*, 2011, in press.
- [2] B. Engquist, A. Majda, Absorbing boundary conditions for the numerical simulation of waves, *Math. Of Comp.*, 31 (1977), 629-651.
- [3] M.J. Grote, A. Schneebeli, D. Schötzau, Discontinuous Galerkin finite element method for the wave equation, *SIAM J. Num. Anal.*, 44 (2006), 2408-2431.
- [4] T. Hagstrom, A. Mar-Or, D. Givoli, High-order local absorbing conditions for the wave equation: extensions and improvements, *J. Comp. Phys.*, 227 (2008), 3322-3357.
- [5] R. Higdon, Numerical absorbing boundary conditions for the wave equation, *Math. Comp.*, 49 (1987), 65-90.

#### **James Bremer**

University of California, Davis, Department of Mathematics, Davis, CA 95616

##### ***An Approach to the Numerical Solution of Integral Equations on Singular Domains***

I will describe an approach to the solution of integral equations on singular domains. It is rather comprehensive in that it applies to many of the integral equations of mathematical physics without modification. Moreover, a priori analytical estimates for solutions are not required. Singularities are instead resolved numerically either on-the-fly while solving the integral equations or in a series of precomputations. Much of this work is joint with Vladimir Rokhlin.

#### **Aloknath Chakrabarti**

Indian Institute of Science, Department of Mathematics, Bangalore-560012, India

##### ***Solution of Three-part Wiener-Hopf Problems Occurring in Scattering Theory***

Three-part Wiener-Hopf problems of special forms, arising in studies involving scattering of electromagnetic and acoustic waves as well as in surface water waves, are examined for their solutions. The method of solution is suitable to problems of scattering by strips and plates.

**Leon Cohen**

City University of New York, Department of Physics and Astronomy, Hunter College, 695 Park Ave, 1225 Hunter North, New York, NY 10065

***Wave Propagation in Phase-Space***

We show an immense simplification occurs if one formulates wave propagation in the phase space of position-wave number or time-frequency. The simplification is not only conceptual but leads to a simple approximation scheme. We show that each phase space point propagates at constant velocity given by the group velocity at the phase space point. The approximation obtained is very accurate and particularly so in comparison to the stationary phase approximation. We show that the reason for the high accuracy of the approximation is that the important low order moments are exactly given by the approximation and that these low order moments preserve very well the basic shape of the pulse. A number of concrete examples, such as propagation in acoustic wave guides, are worked out exactly and approximately to show the validity of the approximation. We use the Wigner distribution and other time-frequency distributions to define the phase space of position and wave number and we also show that it leads naturally to a particle view of wave propagation.

**Laurent Demanet**

Massachusetts Institute of Technology, Department of Mathematics, Cambridge, MA 02139

***Matrix Probing: Fitting Preconditioners from Applications to Random Vectors***

What can be determined about the inverse  $A^{-1}$  of a matrix  $A$  from one application of  $A$  to a vector of random entries? If the  $n$ -by- $n$  inverse  $A^{-1}$  belongs to a specified linear subspace of dimension  $p$ , then come to the talk to hear which assumptions on this subspace,  $p$ , and  $n$  guarantee an accurate recovery of  $A^{-1}$  with high probability. This randomized fitting method provides a compelling preconditioner for the wave-equation Hessian (normal operator) in seismic imaging. Joint work with Pierre-David Letourneau (Stanford) and Jiawei Chiu (MIT).

**Thomas Erneux**

Universite Libre de Bruxelles, CP231, boulevard du Triomphe, 1050 Bruxelles, Belgium

***Fronts and Pulses Controlled by Time-delayed Feedbacks***

We first examine the stability of a steady-state front subject to a time-delayed feedback control (TDFC). TDFC is based on the use of the difference between system variables at the current moment of time and their values at some time in the past. The problem is motivated by recent studies on the control of optical cavity solitons [Tlidi et al, Phys. Rev. Lett. 103, 103904 (2009); Erneux et al. Phil. Trans. R. Soc. A 368, 483–493 (2010)]. We show that the delayed feedback induces a bifurcation to a stable moving front. We next examine the effect of delay on pulse propagation in excitable media and analyze the conditions for pulse suppression. The problem is motivated by recent investigations in neuroscience [Schneider et al. Chaos 19, 015110 (2009)].

**Stefanos Folias**

University of Pittsburgh, Department of Mathematics, Pittsburgh, PA 15260

***Spatially-localized Synchronous Oscillations in Neuronal Networks***

We study the qualitative behavior of synchronous oscillations localized in space and organized by inhibitory synaptic interactions in two types of spatially-extended, conductance-based neuronal network models that are driven by a localized constant input. Typically such equations generate complex spatiotemporal behavior; however, with strong inhibitory coupling, the response of the network is a single band of neurons firing nearly synchronous action potentials (spikes) almost periodically. The boundary of the band of spikes evolves with time and exhibit both stationary and dynamic long term behavior. Subsequently, we derive heuristic one- and two-dimensional discrete maps that track the evolution of the width of the band of action potentials and show that the low-dimensional discrete maps can capture the qualitative behavior and bifurcations of solutions in the full spatial model.

**Murthy Guddati**

North Carolina State University, Department of Civil, Construction and Environmental Engineering, Raleigh, NC 27695

***Modeling Wave Propagation in Unbounded Domains: Links Between Various Absorbing Boundary Conditions and Perfectly Matched Layers***

Wave propagation in unbounded domains is typically modeled by truncating the domain around the region of importance and applying so called absorbing boundary conditions (ABCs) that mimic the effect of wave absorption by the truncated exterior. Many ABCs developed over the past four decades are based on (a) directly using the Dirichlet-to-Neumann (DtN) map of the exterior that renders the computation global and expensive, and (b) approximating the wave absorption into the exterior, leading to local ABCs that are computationally efficient. Most of the existing local ABCs, for polygonal interiors with straight computational boundaries, are developed based on three different ideas: (a) rational approximation of the DtN maps (rational ABCs, e.g. by Engquist and Majda, 1977); (b) explicitly constructing operators that absorb waves propagating in different directions (multi-directional ABCs by Higdon, 1986); and (c) introduction of artificial attenuation in the exterior while preserving impedance at the interior-exterior interface (perfectly matched layers, PML, by Berenger, 1994). While these three ABCs appear to be completely disparate, we show that they are closely linked and in some sense equivalent. While the link between rational ABCs and multi-directional ABCs has been recognized before, we have recently shown that there is also a close link between PML and other ABCs. In this talk, I will highlight the links between the three ABCs, and present a unifying boundary condition named perfectly matched discrete layers (PMDL) that inherits the respective advantages of these three ABCs.

**Huaxiong Huang**

York University, Department of Mathematics and Statistics, 4700 Keele Street, Toronto, Ontario, Canada

***A Neuronal Model for the Instigation and Propagation of Cortical Spreading Depression***

Cortical spreading depression (CSD) is a slow wave phenomenon in the cortex of the brain that is associated with the spread of depression of the electroencephalogram signal. Functionally, it is associated with migraine with aura. In this talk, we present a mathematical model for the instigation and propagation of CSD. Our model is a simplification and extension of a single neuron model proposed by Kager et al. (2000, 2002) for studying the instigation of CSD.

The main mechanisms in our model for the transport of ions into and out of neurons are cross-membrane ionic currents and (active) pumps, coupled with diffusion in the extracellular space. To demonstrate the applicability of our model, we have carried out extensive numerical simulations under different initial conditions and inclusion of various mechanisms. Our results show that CSD waves can be instigated by injecting cross-membrane ionic currents or by applying KCl in the extracellular space. Furthermore, the estimated speeds of CSD waves are within the experimentally observed range. Effects of specific ion channels, background ion concentrations, extracellular volume fractions, and cell swelling on the propagation speed of CSD are also investigated. This is joint work with R.M. Miura and W. Yao.

**Jingfang Huang**

University of North Carolina, Chapel Hill, Department of Mathematics, CB # 3250, Phillips Hall, Chapel Hill, NC 27599

***On the Order and Stiffness of Gauss Collocation Methods for Time Dependent PDEs***

Existing analysis shows that when the Gaussian Runge-Kutta (GRK) (also called Gauss Collocation or Gauss) formulation with  $s$  Gaussian nodes is applied to ODE initial value problems, the discretization is order  $2s$  (super-convergent). For time dependent PDEs with boundary conditions, however, super-convergence can only be observed for periodic boundary conditions in our numerical experiments, and the numerical scheme's order is only  $s$  for general boundary conditions. In this talk, we analyze these order behaviors and validate the theoretical results using numerical experiments. We also show the "controlled

stiffness" in the elliptic equation system resulting from the GRK formulation for PDEs. When coupled with the Krylov deferred correction (KDC) methods and fast elliptic equation solvers, the GRK discretization of a wide class of time dependent PDEs can be solved efficiently and accurately.

**Chiu-Yen Kao**

The Ohio State University, Department of Mathematics, 410 Math Tower, 231 West 18th Avenue, Columbus, OH 43210

***Numerical Study of the KP Equation for Non-periodic Waves***

The Kadomtsev-Petviashvili (KP) equation describes weakly dispersive and small amplitude waves propagating in a quasi-two dimensional situation. Recently a large variety of exact soliton solutions of the KP equation has been found and classified. Those soliton solutions are localized along certain lines in a two-dimensional plane and decay exponentially everywhere else, and they are called line-soliton solutions. The classification is based on the far-field patterns of the solutions which consist of a finite number of line-solitons. We study the initial value problem of the KP equation with V- and X-shape initial waves consisting of two distinct line-solitons by means of the direct numerical simulation. We then show that the solution converges asymptotically to some of those exact soliton solutions. The convergence is in a locally defined L<sup>2</sup>-sense. The initial wave patterns considered in this paper are related to the rogue waves generated by nonlinear wave interactions in shallow water wave problem.

**William Kath**

Northwestern University, Engineering Sciences and Applied Mathematics, 2145 Sheridan Road, Evanston, IL 60208

***Methods to Determine Large Deviations and Rare Events in Optical Pulses***

In optical systems, amplified spontaneous emission noise causes signal fluctuations that lead to errors in those rare cases when the noise-induced changes are large. We discuss methods capable of determining large deviations induced by noise in such systems. First, large deviations are found using a constrained optimization problem that exploits the mathematical structure of the governing equations and a numerical implementation of the singular value decomposition. The results of the optimization problem then guide importance-sampled Monte-Carlo simulations to determine the events' probabilities. We show that the method works for a general class of intensity-based optical detectors and for arbitrarily shaped pulses.

**Andreas Kloeckner**

New York University, Courant Institute of Mathematical Sciences, Department of Mathematics, 251 Mercer Street, New York, NY 10012

***Generalized Debye Sources: Computational Aspects on Arbitrary Surfaces***

After a brief introduction to the theory of generalized Debye sources and the problems they address in the solution of the time-harmonic Maxwell equations, I will report initial experience with these representations as a computational tool for the solution of electromagnetic boundary value problems, such as scattering from a perfect conductor. Starting from the abstract idea of the representation, I will present a variety of reformulations that improve implementability and numerical conditioning given an algebra of layer potential operators on triangulated surfaces embedded in  $\mathbb{R}^3$ . I will further discuss a number of computational prerequisites such as the computation of curvatures and a representation of the Laplace-Beltrami operator within the context of our solver. I will close by presenting a complement of numerical results illustrating convergence properties in simple and various corner cases.

**Mary-Catherine Kropinski**

Simon Fraser University, Department of Mathematics, 8888 University Drive, Burnaby, BC V5A 1S6, Canada

***Fast Integral Equation Methods for the Laplace-Beltrami Equation on the Sphere***

Integral equation methods for solving the Laplace-Beltrami equation on the unit sphere in the presence of multiple "islands" are presented. The surface of the sphere is first mapped to a multiply-connected region in the complex plane via a stereographic projection. After discretizing the integral equation, the resulting dense linear system is solved iteratively using the fast multipole method for the 2D Coulomb potential in order to calculate the matrix-vector products. This numerical scheme requires only  $O(N)$  operations, where  $N$  is the number of nodes in the discretization of the boundary. The performance of the method is demonstrated on several examples, including the motion of several point vortices on the sphere.

**Paul Martin**

Colorado School of Mines, Department of Mathematical and Computer Sciences, Golden, CO 80401

***Internal Gravity Waves and Hyperbolic Boundary-value Problems***

Waves are generated by an oscillating object surrounded by an incompressible fluid in which the density is an increasing function of depth. After removing the dependence on time, a boundary-value problem for a hyperbolic PDE remains. Such problems are unfamiliar to (most) mathematicians. Some of the following aspects will be discussed: energy production and characteristic wave beams; radiation conditions; boundary integral equations. Comparisons with the more familiar acoustic problems will also be made.

**Govind Menon**

Brown University, Division of Applied Mathematics, 182 George Street, Providence, RI 02912

***Complete Integrability of Shock Clustering and Burgers Turbulence***

The emergence of structure from disorder is interesting in several physical models such as galaxy formation in astrophysics, vortex coalescence in 2d flows, and domain growth in materials science. One mathematical model for such phenomena is to study the equations of continuum physics with random initial data. We show that this problem has a very rich structure even for the simplest nonlinear equations. Our main result is that the evolution of shock statistics for scalar conservation laws with convex flux and suitable random data is completely integrable. These results sit at an interesting junction of kinetic theory, integrable systems, and probability theory. Little background will be presumed in any of these areas. Joint work with Ravi Srinivasan (UT, Austin).

**Shari Moskow**

Drexel University, Department of Mathematics, 3141 Chestnut Street, Philadelphia, PA 19104

***Inverse Born Series for the Calderon Problem***

We propose a direct reconstruction method for the Calderon problem based on inversion of the Born series. We characterize the convergence, stability and approximation error of the method and illustrate its use in numerical reconstructions. Joint work with Simon Arridge and John Schotland.

**Michael O'Neil**

New York University, Courant Institute of Mathematical Sciences, Department of Mathematics, 251 Mercer Street, New York, NY 10012

***A Robust Axisymmetric Electromagnetic Scattering Solver using Generalized Debye Sources***

Many existing surface integral equation methods for the solution to electromagnetic scattering problems exhibit numerical instability in several regimes (low-frequencies, non-simply connected geometries, etc.) However, when formulated using generalized Debye sources, as recently introduced by Epstein and Greengard, well conditioned surface integral equations for the solution to the time-harmonic Maxwell equations can be constructed which are valid on arbitrary geometries and at any frequency.



Using the framework that generalized Debye sources provides, we have developed a high-order numerical solver for the solution to electromagnetic scattering problems on bodies of revolution of genus 1. In this talk we will detail the generalized Debye source formulation for scattering from a perfect electrical conductor and from a dielectric with piecewise constant material properties, as well as provide numerical examples for each. Depending on the boundary conditions, these methods involve the careful construction of non-physical electric and magnetic surface currents in the form of a Hodge decomposition.

Additionally, in the course of implementing our numerical scheme, we discovered what appear to be new boundary conditions on the electric field and the vector potential for non-simply connected geometries. These new boundary conditions are not specific to the generalized Debye source formulation, and should be relevant in many other electromagnetic scattering applications, both analytical and computational.

This is joint work with Charles Epstein and Leslie Greengard.

### **John Pearson**

Los Alamos National Laboratory, Applied Theoretical and Computational Physics, XCM, MS F645, Los Alamos, NM 87545

#### ***A Data-driven Model of a Modal Gated Ion Channel: The Inositol 1,4,5-Trisphosphate Receptor in Insect Sf9 Cells***

The inositol 1,4,5-trisphosphate (IP<sub>3</sub>) receptor calcium channel plays a central role in the generation and modulation of intracellular calcium signals in animal cells. To gain insight into the complex mechanisms regulating this ubiquitous channel, we developed iteratively a quantitative continuous time Markov chain model to account for all experimentally observed gating behaviors of single native IP<sub>3</sub> channels from insect Sf9 cells. Ligand (calcium and IP<sub>3</sub>) dependencies of channel open probability ( $P_o$ ) established six main ligand-bound channel complexes. Channel gating in three distinct modes added one additional complex and indicated that three of the complexes can gate in two different modes. This also restricted the connectivity between channel complexes. Finally, channel responses to abrupt ligand concentration changes defined a model with 9 closed states and 3 open states, and its network topology. The model with 24 parameters can closely reproduce the equilibrium  $P_o$  and channel gating statistics for all three gating modes for a broad range of ligand concentrations. It also captures the major features of channel response latency distributions. Global fit to the latency distributions is significantly improved in a modified model with 28 parameters. The models can generate falsifiable predictions of IP<sub>3</sub> channel gating behaviors not yet explored, provide insights to improve  $\text{IP}_3$  channel gating analysis and guide future experiment development. Our approach demonstrates a transparent approach to construct the simplest model that accounts for complex observed behaviors of a system, which can be adopted to Markov chain models in general. We believe our data-driven physics based approach for learning Markov chains is generally applicable for learning the binding kinetics of other complex biologically interesting single molecules.

### **Jianliang Qian**

Michigan State University, Department of Mathematics, East Lansing, MI 48824

#### ***Fast Multiscale Gaussian Wavepacket Transforms and Multiscale Gaussian Beams for the Wave Equation***

We introduce a new multiscale Gaussian beam method for the numerical solution of the wave equation with smooth variable coefficients. The first computational question addressed in this paper is how to generate a Gaussian beam representation from general initial conditions for the wave equation. We propose fast multiscale Gaussian wavepacket transforms and introduce a highly efficient algorithm for generating the multiscale beam representation for a general initial condition. Starting from this multiscale decomposition of initial data, we propose the multiscale Gaussian beam method for solving the wave equation. The second question is how to perform long time propagation. Based on this new initialization algorithm, we utilize a simple reinitialization procedure that regenerates the beam representation when the beams become too wide. Numerical results in one, two, and three dimensions are provided to illustrate the

properties of the proposed algorithm. The methodology can be readily generalized to treat other wave propagation problems.

**Koby Rubinstein**

Technion, Israel, Department of Mathematics, Haifa 32000, Israel

***Introduction to Mathematical Optometry***

We introduce basic notions in optometry. We then review some of the main concepts in modern spectacle lens design. Finally we present a few innovative ideas and a few open problems on ophthalmic lens design, supervision and more.

**Bjorn Sandstede**

Brown University, Division of Applied Mathematics, 182 George Street, Providence, RI 02912

***Nonlinear Stability of Defects***

Defects are interfaces that mediate between two wave trains with possibly different wave numbers. Of particular interest in applications are sources for which the group velocities of the wave trains to either side of the defect point away from the interface. While sources are ubiquitous in experiments and can be found easily in numerical simulations of appropriate models, their analysis still presents many challenges. One difficulty is that sources are not travelling waves but are time-periodic in an appropriate moving coordinate frame. A second difficulty is that perturbations are transported towards infinity, so that weighted norms cannot be used. In this talk, I discuss a different approach that relies on pointwise estimates. I will focus on preliminary nonlinear-stability results for a toy problem that captures the essential features of general sources and for the Nozaki-Bekki holes of the complex Ginzburg-Landau equation.

**Francisco-Javier Sayas**

University of Delaware, Department of Mathematical Sciences, 532 Ewing Hall, Newark, DE 19716

***Energy Estimates in Semidiscrete Time-domain Boundary Integral Equations***

Boundary integral operators in the time domain offer competitive ways to solve exterior scattering problems for different kind of transient (acoustic, elastic, visco-elastic, electromagnetic, ...) waves. They also provide exact absorbing boundary conditions that can be placed arbitrarily close to the support of source terms or inhomogeneities. In this talk I will address the problem of how space discretization with Galerkin BEM redistributes the energy, leaking energy to the interior of the scatterer. In the case of transmission problems, BEM--FEM space discretization creates a ghost wave in the interior domain. This effect can be shown by considering abstract wave equations with exotic transmission condition that are exactly satisfied by the semidiscrete equations. This novel energy analysis can be used to better understand the correct balance of energy of Boundary Integral Methods and might lead to evidence for or against the possibility of using non--symmetric BEM-FEM coupled methods in the time domain. Because of its generality, the conclusions are valid both for Galerkin or Convolution Quadrature discretizations in time.

**Eli Shlizerman**

University of Washington, Department of Applied Mathematics, Seattle, WA 98195

***Neural Activity Measures and Their Dynamics***

The collective behavior of a finite size neural population is often determined by the individual dynamics. The interactions within the population effectively modify the individual dynamics even in the presence of synchrony.

In this talk I will present a framework that we have developed to resolve the asymptotic dynamics of a projection (Activity Measure Evolution Equations - AMEE) that expresses the functionality of a network. In the presence of synchrony, we show that the AMEE shadow the activity measure of the network that is composed of neurons governed by continuous conductance based equations, i.e. Hodgkin-Huxley equations or their reductions, and general interactions. Effectively, these equations serve as a dimension reduction for the complex network.

Such an approach allows to construct low dimensional models that retain the dynamics of coherent structures in a neural network and identify responsible mechanisms for decoherence. Computational results comparing the full network dynamics with the AMEE model and examples of neural networks in which low-dimensionality is observed will be presented.

### **Stephen Shipman**

Louisiana State University, Department of Mathematics, Baton Rouge, LA 70803

#### ***An Exactly Solvable Model for Nonlinear Resonant Scattering***

The interaction of plane waves and guided modes of an open periodic waveguide causes resonance that is manifest as sharp scattering anomalies. In the linear problem, the frequency of a guided mode can be viewed as an embedded eigenvalue of a pseudo-periodic differential operator, and it is the instability of this eigenvalue that lies behind the resonance. Strong amplitude enhancement at resonance magnifies the effects of any material nonlinearities in the waveguide, no matter how weak, giving rise to non-uniqueness of scattering solutions. We present an exactly solvable model that incorporates the essential features of nonlinear resonance: (1) a transmission line that models the ambient space, (2) a point mass acting as the scatter, (3) a resonator serving as an unstable mode, providing an embedded eigenvalue in the linear case that is unstable under small coupling to the transmission line, (4) cubic nonlinearity in the resonator. We analyze regimes of weak coupling and small nonlinearity, in which nonlinear resonance effects are most pronounced. The frequency continuum is partitioned into intervals of unique and stable solutions and intervals of nonunique solutions exhibiting bistability. We establish asymptotic power relations between the coupling and nonlinearity parameters at which these frequency intervals are destroyed and created. Joint work with Stephanos Venakides.

### **William Troy**

University of Pittsburgh, Mathematics Department, Pittsburgh, PA 15260

#### ***The Lowest Possible Temperature of an Einstein Solid is Strictly Positive***

In 1907 Einstein derived a formula for the specific heat,  $C_V$ , of a solid. This widely acclaimed formula, which depends on the temperature,  $T$ , of the solid, predicts that  $C_V \rightarrow 0$  as  $T \rightarrow 0$ . Upon examination of the derivation of  $C_V$ , we have discovered that this theoretical conclusion is false. Instead, we will show that (i) the temperature of the solid must remain above a positive minimal value, and (ii) the specific heat  $C$  must also remain above a positive minimal value.

### **Chrysoula Tsogka**

University of Crete, Heraklion, Department of Applied Mathematics, GR-71409 Heraklion, Crete, Greece

#### ***Adaptive Time-Frequency Detection and Filtering for Imaging in Heavy Clutter***

We consider the problem of detecting and imaging the location of compactly supported reflectors embedded in strongly heterogeneous background media (heavy clutter). Imaging in such regimes is quite challenging as the incoherent wave field that is produced from reflections by the background medium overwhelms the scattered field from the object that wish to image. To detect the presence of a reflector in such regimes we introduce an adaptive time-frequency representation of the array response matrix followed by a Singular Value Decomposition (SVD). The detection is adaptive because the time windows that contain the primary echoes from the reflector are not determined in advance. Their location and width is determined by searching through the time-frequency binary tree of the LCT. After detecting the presence of the reflector we filter the array response matrix to retain information only in the time windows that have been selected. We also project the filtered array response matrix to the subspace associated with the top singular value and then image using travel time migration. We show with extensive numerical simulations that this approach to detection and imaging works well in heavy clutter.

**Catalin Turc**

Case Western Reserve University, Department of Mathematics, 216 Yost, Cleveland, OH 44106

***Efficient Solution of Three-Dimensional Problems of Acoustic and Electromagnetic Scattering by Closed and Open Surfaces with Edges and Corners***

We present a computational methodology (a novel Nystrom approach based on use of a non-overlapping-patch technique and Chebyshev discretizations) for efficient solution of problems of acoustic and electromagnetic scattering by closed and open surfaces with edges and corners. In the case of acoustic scattering problems by closed surfaces with edges and corners we use well-conditioned integral equation formulations whose solutions are Holder continuous. In the case of scattering problems by open surfaces, our integral equation formulations (1) Incorporate, as ansatz, the singular nature of open-surface integral-equation solutions, and (2) For the Electric Field Integral Equation (EFIE), use analytical regularizers that effectively reduce the number of iterations required by iterative linear-algebra solution based on Krylov-subspace iterative solvers. Joint work with A. Anand (IIT Kanpur, India), O. Bruno (ACM Caltech), and J. Chaubell (JPL Caltech).

**J. Douglas Wright**

Drexel University Department of Mathematics, 3141 Chestnut Street, Philadelphia, PA 19104

***Well-posedness Issues for Degenerate Dispersive Equations***

Linear dispersion plays a fundamental role in the study of a large number of physical scenarios and has been the subject of intense theoretical development in recent years. Consequently there has been an explosion of results concerning nonlinear dispersive equations. Nevertheless there are situations in which the mechanism which creates dispersion is itself nonlinear and degenerate. Examples can be found in the study of sedimentation, magma dynamics, granular media, numerical analysis and elasticity. Little is understood about general well-posedness issues for such equations. In this talk we will discuss some recent results which show that degenerate dispersive effects can result in catastrophic instability akin to a backwards heat equation.

**Jack Xin**

University of California, Irvine, Department of Mathematics, Irvine, CA 92697

***Asymptotic Properties of Flame Speeds in Turbulent Combustion Models***

Turbulent combustion is a complex nonlinear multiscale phenomenon. Analyzing and computing the turbulent flame speed is a fundamental problem in turbulent combustion theory. Several simplified models have been proposed to study the turbulent flame speed, such as Hamilton-Jacobi equations (HJ), and reaction-diffusion-advection equations. A popular HJ model is G-equation describing the front motion law in the form of local normal velocity equal to a constant (laminar speed) plus the normal projection of fluid velocity. In level set formulation, G-equation is an HJ with convex (L1 type) but non-coercive Hamiltonian. We shall use homogenization theory and analysis of cell problems to show how the front speed asymptotics (growth rates) depend on viscosity and strain terms of the G-equation in the regime of strong advection. In particular, we shall consider periodic flows such as compressible flows, shear flows, cellular and cat's eye flows. We also compare with front speed growth asymptotics in reaction-diffusion models, and give a dynamic criterion on front speed bending phenomenon (sublinear growth) in terms of periodic orbits and rotation vectors of the underlying advective flow fields. Joint work with Y. Yu and Y-Y Liu.

**Linghai Zhang**

Lehigh University, Department of Mathematics, Bethlehem, PA 18015

***Traveling Wave Solutions of Integral Differential Equations Arising from Synaptically Coupled Neuronal Networks***

We study traveling wave solutions to a general nonlinear singularly perturbed system of integral differential equations arising from synaptically coupled neuronal networks. We accomplish the existence and stability of traveling wave solutions by constructing speed index functions and stability index functions for the

system of integral differential equations. We also investigate the influence of biological mechanisms on the wave speeds. More specifically, we derive lower bound and upper bound of wave speed. We also compare speeds of traveling wave solutions for various integral differential equations.

**Denis Zorin**

New York University, Computer Science Department, 719 Broadway, 12th floor New York, NY 10003

***Large Scale Simulation of Vesicle Flows***

Vesicles are locally-inextensible fluid membranes that can sustain bending. We consider the dynamics of flows of vesicles suspended in Stokesian fluids. We use a boundary integral formulation for the fluid that results in a set of nonlinear integro-differential equations for the vesicle dynamics. The motion of the vesicles is determined by balancing the nonlocal hydrodynamic forces with the elastic forces due to bending and tension. Numerical simulations of such vesicle motions are quite challenging. On one hand, explicit time-stepping schemes suffer from a severe stability constraint due to the stiffness related to high-order spatial derivatives and a milder constraint due to a transport-like stability condition. On the other hand, an implicit scheme can be expensive because it requires the solution of a set of nonlinear equations at each time step. We present a set of numerical techniques for efficient simulation of vesicle flows. The distinctive features of these numerical methods include (1) using boundary integral method accelerated with the fast multipole method (2) spectral (spherical harmonic) discretization of deforming surfaces in space (3) an algorithm for surface reparameterization ensuring stability of the time-stepping scheme and spectral filtering accuracy while minimizing computational costs. By introducing these algorithmic components, we obtain a time-stepping scheme that experimentally is unconditionally stable and has a low cost per time step. We present numerical results to analyze the cost and convergence rates of the scheme.

## CONTRIBUTED TALKS

### **Lyudmyla Barannyk**

University of Idaho

#### ***Regularized Deconvolution Closure Method for Spatially Averaged Dynamics of Particle Chains***

We study the closure problem for continuum balance equations that model mesoscale dynamics of large ODE systems. The underlying microscale model consists of classical Newton equations of particle dynamics. As a mesoscale model we use the balance equations for spatial averages obtained earlier by a number of authors: Murdoch and Bedeaux, Hardy, Noll and others. The momentum balance equation contains a flux (stress), which is given by an exact function of particle positions and velocities. We propose a method for approximating this function by applying regularized deconvolution operators to average density and momentum. The resulting approximate mesoscopic models are systems in closed form. The closed form property allows one to work directly with the mesoscale equations without the need to calculate underlying particle trajectories, which is useful for modeling and simulation of large particle systems. The proposed closure method utilizes the theory of ill-posed problems, in particular regularization methods for solving first order linear integral equations. The closed form approximations are obtained in two steps. First, we use Tikhonov regularization to (approximately) reconstruct the interpolants of relevant microscale quantities from the average density and momentum. Second, these reconstructions are substituted into the exact formulas for stress. The developed general theory is then applied to non-linear oscillator chains. Joint work with Alex Panchenko (Washington State University).

### **Matthew Causley**

New Jersey Institute of Technology

#### ***Wave Propagation in Dielectric Media that Exhibit Fractional Relaxation***

In this talk I will address asymptotic and numerical results for pulse propagation through fractionally relaxing dielectrics. The Havriliak-Negami (H-N) model is an empirical model which captures the non-exponential nature of such dielectric relaxation phenomena. The resulting dielectric polarization field is given by a fractional operator, which is defined by a convolution in the time domain. The development and analysis of a robust method for wave propagation through an H-N medium is presented using the finite difference time domain (FD-TD) method. The FD-TD methods are validated by evaluating the electric field using the Green's function for the medium; in addition, the behavior of pulse propagation is studied asymptotically using the Green's function.

### **Jiawei Chiu**

Massachusetts Institute of Technology

#### ***Matrix Probing and its Conditioning***

When a matrix  $A$  with  $n$  columns is known to be well approximated by a linear combination of basis matrices  $B_1, \dots, B_p$ , we can apply  $A$  to a random vector and solve a linear system to recover this linear combination. The same technique can be used to recover an approximation to  $A^{-1}$ . A basic question is whether this linear system is invertible and well-conditioned. In this paper, we show that if the Gram matrix of the  $B_j$ 's is sufficiently well-conditioned and each  $B_j$  has a high numerical rank, then  $n - p \log^2 p$  will ensure that the linear system is well-conditioned with high probability. Our main application is probing linear operators with smooth pseudo-differential symbols such as the wave equation Hessian in seismic imaging [6]. We demonstrate numerically that matrix probing can also produce good preconditioners for inverting elliptic operators in variable media. Joint work with Laurent Demanet.

**Elodie Estecahandy**

INRIA Bordeaux Sud-Ouest Research Center, Universite de Pau et des Pays de l'Adour, France

***Analysis of the Fréchet Differentiability with Respect to Lipschitz Domains for an Elasto-Acoustic Scattering Problem***

The determination of the shape of an obstacle from its effects on known acoustic or electromagnetic waves is an important problem in many technologies such as sonar, radar, geophysical exploration, medical imaging and nondestructive testing. This inverse scattering problem is difficult to solve, especially from a numerical viewpoint, because it is ill-posed and nonlinear. Its investigation requires as a prerequisite the fundamental understanding of the theory for the associated direct scattering problem, and the mastery of the corresponding numerical solution methods. Moreover, ensuring the stability, fast convergence, and computational efficiency of the regularized Newton method applied to the solution of this class of inverse obstacle problems calls for computing the Fréchet derivatives arising during the Newton iterations with a greater robustness and a higher level of accuracy than possible with finite differences. To this effect, it is noted that the Fréchet derivative of the acoustic scattered field with respect to the shape of a rigid obstacle can be characterized as the solution of a direct acoustic scattering problem which differs from the direct acoustic scattering problem only in the boundary conditions [1,2].

We propose to extend this result to the case of elastic scatterers [3]. Our proof is based on the implicit function theorem and the standard trace theorems. It assumes the boundary of the considered elastic scatterer to be only Lipschitzian, and therefore can include sharp corners. We prove that the Fréchet derivative of the elasto-acoustic scattered field satisfies the same direct elasto-acoustic scattering problem but with different transmission conditions at the boundary of the considered scatterer. The computational implication of this theoretical characterization is as follows. If the sought-after shape is represented by  $N$  parameters, then, at each regularized Newton iteration, the  $N$  directional derivatives needed for constructing the Jacobians can be computed by solving  $N$  direct elasto-acoustic scattering problems that differ only by their boundary conditions — or in algebraic terms after FEM discretization, by solving a single system of equations with  $N$  right-hand sides. In contrast, evaluating the same  $N$  directional derivatives by a central differencing scheme would require first choosing an arbitrary small parameter, then solving  $2N + 1$  distinct direct elasto-acoustic scattering problems.

This result has the potential to advance the state-of-the-art of the solution of inverse elasto-acoustic scattering problems. Moreover, the methodology described above for characterizing the Fréchet derivative of the scattered field with respect to the shape of an elastic scatterer can also be applied to analyze the Fréchet differentiability of such a scatterer with respect to its material properties. This is relevant to many inverse obstacle problems where not only the shape of an obstacle is of interest, but also, and often more importantly, its structure. Joint work with H. Barucq (INRIA) and R. Djellouli (California State University Northridge).

**Sathishkumar Gurupatham**

New Jersey Institute of Technology

***Breaking Up of Particle Clumps on Liquid Surfaces***

The aim of this paper is to study the mechanism by which clumps of some powdered materials breakup and disperse on a liquid surface to form a monolayer of particles. We show that a clump breaks up because when particles on its outer periphery come in contact with the liquid surface they are pulled into the interface by the vertical component of capillary force overcoming the cohesive forces which keep them attached, and then these particles move away from the clump. In some cases, the clump itself is broken into smaller pieces and then these smaller pieces break apart by the aforementioned mechanism. The newly-adsorbed particles move away from the clump, and each other, because when particles are adsorbed on a liquid surface they cause a flow on the interface away from themselves. This flow may also cause particles newly-exposed on the outer periphery of the clump to break away. Interestingly, when many particles asymmetrically break away from a clump, the clump itself is pushed in the opposite direction by the flow caused by the newly-adsorbed particles. Since millimeter-sized clumps can breakup and spread on a liquid

surface within a few seconds, their behavior appears to be similar to that of some liquid drops which can spontaneously disperse on solid surfaces. However, if the capillary force is not large enough to overcome the cohesive force holding the clump together, the clump may not breakup. Joint work with M. Hossain, B. Dalal, I.S. Fischer, P. Singh (all NJIT), and D.D. Joseph (Univ. of Minn.).

### **Dongdong He**

York University

#### ***On the Motion of a Conducting Drop on an Electrowetting Device***

In this work, an immersed boundary/level set method is proposed for simulating the motion of a conducting drop on an electrowetting device (EWD) in 2D. The model for the two-phase moving contact line is based on the effective slip boundary conditions developed by Weiqing Ren and Weinan E et al. (Physics of Fluids, 19, 022101, 2007). A modified version of the standard MAC method is developed for the two-phase flow solver, while a level set method is used to capture the interface. Convergence analysis shows that the method is first order accurate. Numerical results on the spreading and recoiling without applied electrical field are consistent with those in literature. For the motion of a conducting drop on EWD, good agreements are also obtained with both experimental observations and electrowetting theory. Joint work with Huaxiong Huang.

### **Michael Higley**

New Jersey Institute of Technology

#### ***Tank-treading, Bursting and Cusping: Capsule Response at Large Deformation***

We consider the deformation of a two-dimensional elastic capsule with an inviscid interior, which allows for a much greater degree of analysis than is possible in the three-dimensional case. In particular, we give analytic results for the steady-state behavior of the capsule over a large range of deformation in some canonical flows. We show that, in a linear shear flow, a capsule reaches a steady-state tank-treading motion regardless of the imposed shear rate. Alternatively, a capsule in strain flow is shown to either burst or form cusps after a critical strain rate. Joint work with Michael Siegel and Michael Booty.

### **Mridula Kanoria and Sukla Banik**

University of Calcutta

#### ***Two Temperature Generalized Thermo-piezoelastic Problem with Three-phase-lag Effect under Different Types of Thermal Loading***

This paper deals with the thermoelastic interaction in a piezoelastic half-space body with stress free and in the presence of thermal loading on the boundary. The three-phase-lag (3P) thermoelastic model, GN model III (TEWED) and LS model are employed to study the thermophysical quantities. In the theory of 3P lag heat conduction equation leads to a hyperbolic partial differential equation with a fourth order derivative with respect to time. The basic equations have been written in the form of vector-matrix differential equation in Laplace-transform domain which is then solved by state-space approach. The numerical inversion of the transform is carried out by a method based on Fourier-series expansion techniques. The numerical estimates of the conductive temperature, the thermodynamic temperature, the stress and the strain distributions are obtained and are shown graphically. The effect of two-temperature and the 3P lag are studied and the comparisons of the results for different thermoelastic models are made. Keywords: Generalized thermopiezo-elasticity, vector-matrix differential equation, Three-phase-lag thermoelastic model, Fourier series expansion techniques

### **Alan Lindsay**

University of Arizona

#### ***Quenching Solutions of a Fourth Order Nonlinear Parabolic PDE Modeling a MEMS Capacitor***

Finite time singularity formation in a fourth order nonlinear parabolic partial differential equation (PDE) is analyzed. The PDE is a variant of a ubiquitous model found in the field of Micro-Electro



Mechanical System (MEMS) and is studied on a one-dimensional (1D) strip and the unit disc. The solution itself remains continuous at the point of singularity while its higher derivatives diverge, a phenomenon known as quenching. For certain parameter regimes it is shown numerically that the singularity will form at multiple isolated points in the 1D strip case and along a ring of points in the radially symmetric 2D case. The location of these touchdown points is accurately predicted by means of asymptotic expansions. The solution itself is shown to converge to a stable self-similar profile at the singularity point. Analytical calculations are verified by use of adaptive numerical methods which take advantage of symmetries exhibited by the underlying PDE to accurately resolve solutions very close to the singularity.

### **Yu-Yu Liu**

University of California, Irvine

#### ***Turbulent Flame Speed for G-equations***

In combustion theory various models have been proposed in modeling of the flame propagation. By level curve formulation, G-equation describes the motion of the flame front by a constant normal velocity (called laminar flame speed) and the advection of the fluid. If the initial flame is planar in some direction, the front will be wrinkled by the advection in time and becomes very complicated in time. Eventually the front will evolve into an asymptotic state propagating at a constant speed (called turbulent flame speed). Consider the G-equation with 2D cellular flow. We are interested in the turbulent flame speed parameterized by the intensity of the cellular flow. For the basic G-equation model, the turbulent flame speed is enhanced by the cellular flow with marginally linear growth rate. If a dissipation term is added into G-equation, however, the growth rate will be drastically altered and becomes uniformly bounded. Correction terms may be also added to laminar flame speed to take account of the effects of the curvature of the level curve and the strain of the advection. We will discuss numerical methods in computing the turbulent flame speed. The numerical results support the laboratory observation that flame front may be quenched by the turbulence.

### **Mike Nicholas**

Tulane University

#### ***A Spectral Method for Periodic Scattering***

We develop a highly accurate numerical method for scattering of 3D electromagnetic waves by doubly periodic structures. We approximate scattered fields using the Mueller boundary integral formulation of Maxwell's equations. The Green's functions are accelerated through Ewald splitting, and accuracy on these functions is achieved as singularities are isolated through the use of partitions of unity, leaving smooth, periodic integrands that can be evaluated with high accuracy using trapezoid sums. The removed singularities are resolved through a transformation to polar coordinates. The method relies on the ideas used in the free-space scattering algorithm of Bruno and Kunyansky.

### **Filippo Posta**

University of California, Los Angeles

#### ***Mathematical Modeling of Epithelial Wound Healing***

Recent experiments monitoring the healing process of wounded epithelial monolayers have demonstrated the necessity of MAPK activation for coordinated cell movement after damage. This MAPK activity is characterized by two wave-like phenomena. One MAPK "wave" that originates immediately after injury, propagates deep into the cell sheet, away from the edge, and then rebounds back to the wound interface. After this initial MAPK activity has largely disappeared, a second MAPK front propagates slowly from the wound interface and also continues into the cell sheet, maintaining a sustained level of MAPK activity throughout the cell sheet. It has been suggested that the first wave is initiated by Reactive Oxygen Species (ROS) generated at the time of injury. In this work, we develop a minimal mathematical model that reproduces the observed behavior. The main ingredients of our model are a competition between ligand (e.g., Epithelial Growth Factor) and ROS for the activation of Epithelial Growth Factor Receptor, and a

feedback loop between receptor occupancy and MAPK activation. We explore the mathematical properties of the model and look for traveling wave solutions consistent with the experimentally observed MAPK activity patterns. Joint work with Tom Chou.

### **Trevor Potter**

University of California-Berkeley

#### ***Effective Dynamics for N-solitons of the Gross-Pitaevskii Equation***

We consider several solitons moving in a slowly varying external field. We show that the effective dynamics obtained by restricting the full Hamiltonian to the finite dimensional manifold of N-solitons (constructed when no external field is present) provides a remarkably good approximation to the actual soliton dynamics. That is quantified as an error of size  $h^2$  where  $h$  is the parameter describing the slowly varying nature of the potential. This also indicates that previous mathematical results of Holmer-Zworski for one soliton are optimal. For potentials with unstable equilibria the Ehrenfest time,  $\log(1/h)/h$ , appears to be the natural limiting time for these effective dynamics.

### **Bryan Quaife**

Simon Fraser University

#### ***Integral Equation Methods for the Modified Biharmonic Equation***

When solving the two dimensional Navier-Stokes equations, it is advantageous to reformulate the system of PDEs in terms of a streamfunction. The advantages are clear: the number of unknowns drops from four to one and incompressibility is automatically satisfied. However, the governing PDE is fourth-order. One can split this equation using a streamfunction-vorticity formulation, but this introduces the need to specify artificial boundary conditions. We take an alternative approach which is to first discretize in time, and then solve a modified biharmonic equation at each time step. The solution of the modified biharmonic is written as the sum of a volume integral and two layer potentials. Once the volume integral is computed, the no-slip boundary conditions are satisfied by adding the layer potentials with unknown densities. This presentation will focus on integral equation methods to determine these layer potentials in an arbitrary geometry. The layer densities satisfy a system of Fredholm integral equations of the second kind which are preconditioned and then discretized with high-order quadrature rules and solved iteratively. Progress on solving this system of integral equations and future direction will be discussed. This is joint work with Shidong Jiang and Mary-Catherine Kropinski.

### **Siddarth Savadatti**

North Carolina State University

#### ***Absorbing Boundary Conditions for Anisotropic Acoustic and Elastic Media***

We investigate the accuracy aspects of local absorbing boundary conditions (ABCs) designed for homogeneous anisotropic acoustic and elastic media in the frequency domain. These media support wavemodes with opposing signs of group and phase velocities that have long posed a formidable challenge in designing accurate local ABCs. This work presents the design of two local ABCs - one for acoustic waves and another for elasticity - that are accurate in absorbing all outgoing waves (including those with opposing signs of group and phase velocities). The ABCs utilized here are based on perfectly matched discrete layers (PMDLs) that can be viewed as particularly efficient versions of popular local ABCs like rational ABCs and perfectly matched layers (PMLs). PMDL combines the accuracy of rational ABCs along with the versatility of PML and is thus used for the present study; moreover, the underlying links make the results of this work applicable to other rational ABCs and PML in general. For acoustic waves, we show that the reflection coefficient of PMDL can be expressed in terms of group velocities and not phase velocities. This allows us to design PMDLs that are accurate for all wavemodes with positive group velocities - even those with negative phase velocities. Elastic waves however, do not lend themselves to a similar solution; a new variant of PMDL based on an unconventional mesh stretching is presented to tackle the absorption of elastic wavemodes with opposing group and phase velocity signs. The validity of the above assertions is

demonstrated through a series of slowness diagrams and frequency domain simulations. Joint work with M. N. Guddati.

**Melissa Stoner**

Lehigh University

***Existence and Stability of Standing Wave Solutions Arising from Synaptically Coupled Neuronal Networks***

There have been many models of neuronal networks developed and analyzed to determine the wave and speed of the wave in a nerve pulse. The goal of this research is to investigate the existence and stability of standing wave solutions of the system of integral differential equations incorporating two types of delay in the neuronal network. These model equations generalize many important integral differential equations used in most recent related papers when modeling neuronal networks. For the system of integral differential equations, if the sodium current function is linear or cubic and conditions on the constants and kernel functions are satisfied then there exist two standing wave solutions to the system. Additionally, the stability of the standing wave is dependent on the network's parameters. The results for the system are surprisingly interesting in mathematical neuroscience, especially this change in stability. Joint work with Linghai Zhang.

**Qiming Wang**

New Jersey Institute of Technology

***Numerical Simulations of Drop Dynamics with Soluble Surfactant***

The effect of insoluble or soluble surfactant on the deformation of a viscous drop surrounded by another viscous fluid in an imposed flow is studied numerically. The effect of bulk surfactant solubility is considered in the physically representative limit of large bulk Peclet number by a novel 'hybrid' numerical method, which solves boundary layer equation for the bulk concentration. Effect of various parameters on drop deformation is presented when steady state is obtained. In addition, similar to the case of insoluble surfactant, above some critical capillary number, tip streaming can occur when the drop is relatively inviscid.

**Xinli Wang**

University of Virginia

***Transport of Brownian Particles Confined to a Channel by a Periodic Potential***

Recent progress in microfluidic devices has led to the development of novel separation strategies that take advantage of the unprecedented control on geometry and chemistry of the stationary phase at scales that are comparable to the size of the transported species. Here we consider the transport of Brownian particles confined to a channel of periodically varying cross section, but the confinement is induced by a potential energy landscape instead of the solid boundaries of a channel. Asymptotic analysis and Brownian dynamics simulation are used to study two important transport properties: average velocity and effective diffusivity in a narrow channel or weakly corrugated channel. Our results show that leading order solution is equivalent to that obtained from the Fick-Jacobs approximation. The analytical results agree well with Brownian Dynamics simulations for transport properties over a wide a range of Peclet numbers.

**Ying Wang**

University of Minnesota

***The Modified Buckley-Leverett Equation***

The focus of the present study is the modified Buckley-Leverett (MBL) equation describing two-phase flow in porous media. The MBL equation differs from the classical Buckley-Leverett (BL) equation by including a balanced diffusive-dispersive combination. The dispersive term is a third order mixed derivatives term, which models the dynamic effects in the pressure difference between the two phases. The classical BL equation gives a monotone water saturation profile for any Riemann problem; on the contrast, when the

dispersive parameter is large enough, the MBL equation delivers non-monotone water saturation profile for certain Riemann problems as suggested by the experimental observations. In this talk, we first show that the solution of the finite interval  $[0,L]$  boundary value problem converges to that of the half-line  $[0,+\infty)$  boundary value problem for the MBL equation as  $L \rightarrow +\infty$ . This result provides a justification for the use of the finite interval boundary value problem in numerical studies for the half line problem. Furthermore, we extend the classical central schemes for the hyperbolic conservation laws to solve the MBL equation which is of pseudo-parabolic type. Numerical results confirm the existence of non-monotone water saturation profiles consisting of constant states separated by shocks. (Joint work with Chiu-Yen Kao)

## POSTERS

### **Shuchi Agrawal**

New Jersey Institute of Technology

#### ***Heating of a Thin Ceramic Slab in a Multimode Microwave Cavity***

Two-dimensional reaction diffusion equations, which contain a functional and an inhomogeneous source term, are good models for describing microwave heating of thin ceramic slabs in a multi mode, highly resonant cavity. A thin ceramic slab situated in a  $TE_{N03}$  rectangular cavity modeled in the small Biot number limit is studied to gain insight into the dynamics of the heating process. The evolution of temperature is governed by a two-dimensional reaction diffusion equation and a spatially non-homogeneous reaction term. Numerical methods are applied to accurately approximate the steady state leading order temperature of this equation and to determine the stability of solutions for Neumann boundary conditions. The choices of parameters in the equation that lead to uniform heating of the ceramic slab have been characterized.

### **Todd Caskey, Albi Kavo, Mandeep Singh, and David J. Horntrop**

New Jersey Institute of Technology

#### ***Variance Reduction Techniques for Stochastic Differential Equations***

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

### **J. Champanerkar and A. Eladdadi**

William Paterson University

#### ***Mathematical Modeling of Cancer***

Cancer cells can be thought of as competitors for resources in the normal tissue where they harbor and also as preying upon the normal host tissue. We investigate the behavior of cancer cells as described in ecology by modified predator-prey systems. We use differential equations to model this behavior and numerically solve them for various values of parameters.

### **Milena Chermisi**

New Jersey Institute of Technology

#### ***Singular Perturbation Models in Phase Transitions for Second Order Materials***

A variational model proposed in the physics literature to describe the onset of pattern formation in two-component bilayer membranes and amphiphilic monolayers leads to the analysis of a second order Ginzburg-Landau type energy where the free energy depends not only on the concentration and its first derivatives but also on the second gradient. In addition, the singular perturbation term involving the gradient is multiplied by a stiffness coefficient  $-q$ . When  $q > 0$ , that is, the singular perturbation containing the gradient is negative, one expects curvature instabilities of the membrane which, in turn, generate a pattern of domains that differ both in composition and in local curvature. Motivated by the theory of Gamma-convergence, we scaled the energy by a small parameter  $\epsilon$  in such a way all the terms have the same order and we studied the asymptotic behavior, as  $\epsilon$  goes to zero, of the rescaled families of energies using Gamma-convergence techniques. In particular, compactness results and an integral representation of the limit energy are obtained. At a macroscopic scale, stable patterns of the system under analysis are described as minimizers (global or local) of the limit energy. This is a joint work with G. Dal Maso (SISSA), I. Fonseca (CMU), and G. Leoni (CMU).

### **Bhavin Dalal**

New Jersey Institute of Technology

#### ***The Role of Particle Inertia in its Motion in the Direction Normal to a Fluid-liquid Interface***

It is shown that the inertia of a particle plays an important role in its motion in the direction normal to a fluid-liquid interface, and in determining its adsorption trajectory and orientation in the adsorbed state. Although the importance of inertia diminishes with decreasing particle size, on an air-water interface the inertia continues to be important even when the size is as small as a few nanometers. Furthermore, similar to an underdamped system, an adsorbed particle has characteristic linear and rotational frequencies that can be excited by an external forcing. Joint work with P. Singh and I. S. Fischer (NJIT), and D. D. Joseph (Univ. of Minnesota).

### **Arnaud Goulet**

New Jersey Institute of Technology

#### ***Characterization of Two Dimensional Granular System under Isotropic Compression***

We consider a two dimensional granular system subject to an isotropic compression until 90% of the maximum volume fraction is attained. As compression occurs, force chains appear and reorganize themselves throughout the granular material. These force chains have been observed experimentally using photoelastic particles. The optical properties of these particles change as a function of the force applied, allowing direct visualization of the force chains. Rather than studying individual force chains, we are interested in a quantitative description of the system as a whole. Going beyond the traditional statistical quantities, we apply some tools used in algebraic topology to describe the two dimensional granular system, namely the Betti numbers. We will present the effect of friction model and polydispersity on the Betti numbers as well as other interesting quantities such as the percolation threshold of the force chains and cluster sizes. Joint work with Michel Tsukahara and Lou Kondic.

### **Muhammad Hameed**

University of South Carolina Upstate

#### ***Breakup and Deformation of a Liquid Jet Containing Solid Particles***

The phenomenon of liquid jet breakup is studied for the case of a very viscous jet containing one or more solid particles. A mathematical model is derived which represents the complex dynamics as a combination of two relatively simpler problems. Governing equations for the dynamics are derived for Stokes flow using long wavelength assumptions for the capillarity-driven flow, and the influence of the force-free particle is represented by a symmetric hydrodynamic force dipole, also termed a stresslet. The total flow field is the

combination of the outer long wavelength approximated, combined with the inner flow induced by the force dipole representation of a particle. Imposing the standard stress balance and kinematic condition at the jet surface to the combined flow leads to a well-posed problem for the evolution of the jet shape. The model equations are solved numerically by an implicit finite difference scheme. The theoretical calculations based on this hybrid long wavelength and singularity approach yield qualitatively accurate and encouraging agreement with experimental observations. Results of calculations for one particle centered or off-center and for two particles are presented. Results showing the influence of varying particle size are also presented. Joint work with J. Morris.

**Md. Shahadat Hossain**

New Jersey Institute of Technology

***Modeling of Cerebral Blood Flow in the Human Brain***

The non-Newtonian properties of blood, i.e., shear thinning and viscoelasticity, can have a significant influence on the distribution of Cerebral Blood Flow (CBF) in the human brain. The aim of this work is to quantify the role played by the non-Newtonian nature of the blood. Under normal conditions, CBF is autoregulated to maintain baseline levels of flow and oxygen to the brain. However, in patients suffering from heart failure (HF), Stroke, or Arteriovenous malformation (AVM), the pressure in afferent vessels varies from the normal range within which the regulatory mechanisms can ensure a constant cerebral flow rate, leading to impaired cerebration in patients. It has been reported that the change in the flow rate is more significant in certain regions of the brain than others, and that this might be relevant to the pathophysiological symptoms exhibited in these patients. We have developed mathematical models of CBF under normal and the above disease conditions that use direct numerical simulations (DNS) for the individual capillaries along with experimental data in a one-dimensional model to determine the flow rate and the methods for regulating CBF. The model also allows us to determine which regions of the brain would be affected relatively more severely under these conditions. Joint work with Bhavin Dalal, Ian S. Fischer, Pushpendra Singh (all NJIT), and Nadine Aubry (Carnegie Mellon University).

**Xinxian Huang, Farzan Nadim, and Amitabha Bose**

New Jersey Institute of Technology

***Using Feed-forward Networks to Infer the Activity of Feed-back Neuronal Networks***

In a network of two reciprocally inhibitory neurons, the firing time of each neuron affects the period of the other one. When these inputs are strong, an alternate method to using phase response curves is required to determine the steady state behavior. We derive a new method using two different feed-forward maps to determine existence and stability of phase-locked solutions. The method involves showing how these maps affect one another prior to composing them to find phase-locking.

**Kimberly Kilgore**

Drexel University

***Inverse Born Series for Diffuse and Propagating Waves***

This poster is concerned with the study of the inverse scattering problems for both diffuse and propagating waves. These problems consist of using boundary measurements to recover the values of the absorption coefficient and refractive index, respectively, within the domain. These values can be found through inversion of the Born series. We will present results on the convergence of the inverse Born series, and considering a radially symmetric medium, summarize and compare numerical simulations for both the diffuse and propagating cases in two and three dimensions.

**Dongwook Kim**

New Jersey Institute of Technology

***Firing Rate (Super-Threshold) Frequency Preferences in a Persistent Sodium / h-current Medial Entorhinal Cortex Layer II Stellate Cell Model***

Various neuron types exhibit sub-threshold and firing frequency resonance in which the sub-threshold membrane potential or firing frequency responses to periodic inputs (such as sinusoidal) peak at a preferred frequency (or frequencies). Previous experimental work has shown that medial entorhinal cortex layer II stellate cells (SCs) exhibit sub-threshold and firing frequency resonance in the theta frequency band (4 - 10 Hz). In this project we seek to understand the biophysical and dynamic mechanism underlying these phenomena, and how sub-threshold and firing frequency resonance are related. We studied the effects of sinusoidal current and synaptic conductance inputs at various frequencies, at various noise levels, on the supra-threshold dynamics on a SC model. For current inputs, our results show that while the SC model exhibits a single frequency preference peak (in the theta band) for low sinusoidal input levels, it exhibits three preferred frequency peaks for larger input levels. These additional peaks occur at frequencies that are roughly a multiple of the "theta" one. For synaptic conductance inputs, we observe an additional peak in the signal gain which occurs at a much higher frequency (in the high gamma band). These findings depart from the linear prediction. Joint work with Horacio Rotstein.

**Yuwen Liang and Karen Rappaport**

New Jersey Institute of Technology

***A Study of Implied Volatility using Historical Data and the Black Scholes Formula***

The Black Scholes Formula is a tool used to price financial derivatives. Imbedded in the formula is a volatility variable. However volatility is very hard to measure and is difficult to calculate using this formula. Using Historical Data and numerical methods, a program was written to compute implied volatility over various time periods. The results were validated and analysed in the context of actual corporate activities.

**Zhi Liang**

New Jersey Institute of Technology

***Fast Algorithms for Generating Random Numbers with Certain Spatial Correlation***

In the Brownian dynamics of  $N$  particles with the hydrodynamic interactions, the particles follow a diffusion tensor. The square root of diffusion matrix always need to be calculated many times in the simulation. The Cholesky decomposition is commonly used, and takes  $O(N^3)$  arithmetic operations. In this paper, we combine fast multipole method(FMM) with Fixman's Chebyshev approximation to get an  $O(N)$  algorithm for calculating the matrix square root. The algorithm can be applied to arbitrary positive definite hydrodynamic tensor and the corresponding particle configurations. And this allows to include hydrodynamic interactions into large number particle Brownian dynamics simulations, should be useful for simulation studies of diffusion limited reactions, polymer dynamics, protein folding, particle coagulation, and other phenomena. Joint work with Shidong Jiang.

**Te-Sheng Lin**

New Jersey Institute Technology

***Modeling Spreading of Nematic Droplets***

Experiments by Poulard & Cazabat on spreading droplets of nematic liquid crystal reveal a surprisingly rich variety of behavior, including at least two different emerging lengthscales resulting from a contact line instability. In earlier work we modified a lubrication model for nematic liquid crystals due to Ben Amar and Cummings, and showed that, in a qualitative sense, it can account for 2D version of the observed behavior. In the present work we propose a new approach that allows us to explore the effect of anchoring variations on the substrate. This in turn gives a simple way to model the presence of defects, which are always present during such liquid crystal flows. The new model leads to additional terms in the governing

equation. We explore the influence of these additional terms for some simple flow scenarios to gain a basic understanding of their influence.

**Yi Mao**

University of Tennessee, National Institute for Mathematical and Biological Synthesis

***Discover the “Hot-spot” Residues of Peroxidase via Elastic Network Modeling: in Comparison with Directed Evolution Experiments***

Directed evolution has revolutionized the field of protein engineering and become the method of choice for tailoring the properties of enzymes. The method involves the construction of library of protein variants, and despite technical advances normally only tens of the residues can be targeted to build up the library. Here I use elastic network modeling of proteins to identify the “hot-spot” residues of horseradish peroxidase. Horseradish peroxidase is a well-studied enzyme by directed evolution experiments, and the majority of the experimentally discovered selection sites have been reproduced by the modeling. The study supports the robustness of the network model as a potential predictive tool for preselecting residues for directed evolution experiments.

**Myongkeun Oh<sup>1</sup>, Hua-an Tseng<sup>2</sup>, Farzan Nadim<sup>1,2</sup>**

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***Modeling of Synapses Showing a Preferred Frequency in an Oscillatory Neuronal Network***

Experimental and theoretical analysis suggest that a synapse capable of exhibiting both short-term facilitation and depression acts as band-pass filter—where efficacy is maximal at an input frequency referred to as the preferred (resonance) frequency. Recent data from our lab indicates that inhibitory synapses in the crab pyloric central pattern generator (freq ~ 1 Hz) have preferred frequencies. The synapses from the pyloric pacemaker neurons AB/PD to the lateral pyloric (LP) follower neuron and the feedback LP to PD both have a preferred frequency of ~0.5Hz. However the preferred frequency of the LP to PD synapse is sensitive to the voltage range of presynaptic waveform whereas that of the AB/PD to LP synapse is not. We have built mechanistic models of synaptic release to show that the existence of preferred synaptic frequency can be captured using a single presynaptic voltage-dependent transient calcium current. We demonstrate that the preferred frequency is affected by the activation and inactivation time constants of the calcium current as well as the slopes of the steady-state of activation and inactivation curves. In particular, the distinction in the voltage-dependence of the preferred frequencies of the AB/PD to LP and the LP to PD synapse can be due to different activation and inactivation time constants in their respective presynaptic calcium current.

**Anthony D. Rosato, David J. Horntrop, Oleksandr Dybenko, Vishagan Ratnaswamy, and Lou Kondic**  
New Jersey Institute of Technology

***The Evolution of the Microstructure in Density Relaxation by Tapping***

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

**Jacek Wrobel**

New Jersey Institute of Technology

***High-order Adaptive Method for Computing Two-dimensional Invariant Manifolds of Maps***

The authors present efficient and accurate numerical methods for computing invariant manifolds of maps which arise in the study of dynamical systems. In order to decrease the number of points needed to compute a given surface, we propose using higher-order approximation techniques from geometric



modeling. We use Bezier curves and triangles, fundamental objects in surface design, to create adaptive method. The method is based on tolerance conditions derived from properties of Bezier triangles. We develop and test the method for an ordinary parametric surface; then we adapt this method to invariant manifolds of three-dimensional maps.

**Li Yang**

Michigan State University

***Existence of Homoclinic Solutions of the Functionalized Cahn-Hilliard Energy***

We introduce the functionalized Cahn-Hilliard (FCH) energy, a negative multiple of the Cahn-Hilliard energy balanced against the square of its own variational derivative, as a finite width regularization of the sharp-interface Canham-Helfrich energy. We show the existence of the homoclinic solutions for the functionalized Cahn-Hilliard Energy.

**Xing Zhong**

New Jersey Institute of Technology

***Threshold Phenomena in Reaction-Diffusion Equations***

We study the Cauchy problems for bistable nonlinearity reaction-diffusion equations by using energy argument. We prove the one to one relation between long time behavior of solution and the time limit of energy. Moreover, for a suitable monotone one-parameter family of initial data, there exists a sharp threshold between extinction and propagation. Supervised by Prof. C. B. Muratov.

**Ivan Zorych**

Columbia University

***Statistical Methods for Active Surveillance on Medical Observational Databases***

Post-marketing drug safety surveillance can be enhanced by utilizing large health records databases. Application of statistical methods to such longitudinal medical data is a novel and challenging task. We consider a set of statistical methods and their operational characteristics on several real databases. The evaluations are carried out on a set of selected drugs and selected outcomes of interest. Joint work with David Madigan.