FACM '16

FRONTIERS IN APPLIED AND COMPUTATIONAL MATHEMATICS

New Jersey Institute of Technology
Newark, New Jersey
June 3 – 4, 2016

Program Guide and Abstracts

Hosted by
Department of Mathematical Sciences and
Center for Applied Mathematics and Statistics
http://www.math.njit.edu

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NJIT
New Jersey Institute
of Technology

ORGANIZING COMMITTEE

FRONTIERS IN APPLIED AND COMPUTATIONAL MATHEMATICS
NEW JERSEY INSTITUTE OF TECHNOLOGY
NEWARK, NEW JERSEY
JUNE 3 – 4, 2016

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COMMITTEE STAFF

Alison Boldero

Fatima Ejallali

Nickcoy Findlater

Maria Laygo

Eileen Michie

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FRONTIERS IN APPLIED AND COMPUTATIONAL MATHEMATICS

MESSAGE FROM THE ORGANIZING COMMITTEE

Welcome to Frontiers in Applied and Computational Mathematics 2016 (FACM '16). This is the thirteenth in a series of conferences that have been held each year since 2004. The conferences are hosted by the Department of Mathematical Sciences and the Center for Applied Mathematics and Statistics at New Jersey Institute of Technology. Each year, members of the department form a local organizing committee, select a theme or topics for the conference, and in the last few years they then invite colleagues from outside NJIT to augment the committee and help to guide it. Hosting the conference is definitely one of the most enjoyable events of our year, and financial support from the National Science Foundation and NJIT has made it possible.

This year, in applied mathematics the conference themes are mathematical and computational aspects of materials science; wave propagation and scattering; topics in mathematical biology, including the dynamics and neural control of animal locomotion; and biofluids and microscale fluid dynamics. In statistics, the main theme is biostatistics. At the interface between applied mathematics and statistics, the conference features contributions in optical imaging data analysis and the statistical analysis of neural data.

The FACM conferences actively seek and support presentations by early-career researchers. These are selected from applications that are submitted by some of the best young applied mathematicians and statisticians. It is a pleasure for us to give the future leaders of the field an opportunity to present their work among more established colleagues.

The FACM conferences are indicative of the central role that mathematical sciences have at NJIT. We hope that you enjoy the meeting, and that you return again next year to present your most recent work, discuss your new ideas, research and achievements.

We take this opportunity to thank the Administrative Staff of the Department of Mathematical Sciences for the enthusiasm and hard work they bring to the event: Eileen Michie, Fatima Ejallali, Alison Boldero, Nickoy Findlater and Maria Laygo.

FACM '16 Organizing Committee

DMS CHAIR'S MESSAGE

The Department of Mathematical Sciences (DMS), along with the Center for Applied Mathematics and Statistics (CAMS), is very pleased to welcome you to NJIT for our thirteenth conference on Frontiers in Applied and Computational Mathematics (FACM). For 2016, we have embraced a somewhat more diverse range of topics than in previous years. We hope that you will find ideas of interest across this range in presentations that have something of value for both the expert and the novice. Facilitating cross-fertilization among the areas represented is one of our ambitions–the more unexpected the better.

In addition to welcoming you to our campus, we welcome you to the City of Newark. Newark has a number of perhaps unexpected attractions: the New Jersey Performing Arts Center, the Cathedral Basilica of the Sacred Heart, Branch Brook Park (site each April of the Essex County Cherry Blossom Festival featuring over five thousand cherry trees), the Newark Museum (situated very close to the path from NJIT to the Robert Treat Hotel were many participants will stay). Some will be surprised by the diversity of Newark, which includes one of the largest Portuguese-speaking populations in North America. Our banquet this year will take us to an iconic restaurant in Newark's Ironbound District, Iberia Tavern, to experience Newark's culinary offerings. As in any unfamiliar urban environment, we ask that you exercise due caution as you visit with us. But we believe that you will find that Newark possesses its own special charm.

The nature of a conference is to bring people together to share ideas and foster collaborations and new directions. Through FACM, we are pleased to include early-career scientists, statisticians and applied mathematicians in these activities. To see the flourishing careers of so many past participants is immensely gratifying and encourages us to further expand these opportunities. All participants are especially encouraged to attend the poster sessions and minisymposia where early-career participants are presenting and to interact with these rising talents.

Jonathan Luke
Professor and Chair
Department of Mathematical Sciences

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Classic Car Service at 973-484-9494 (or 3344)

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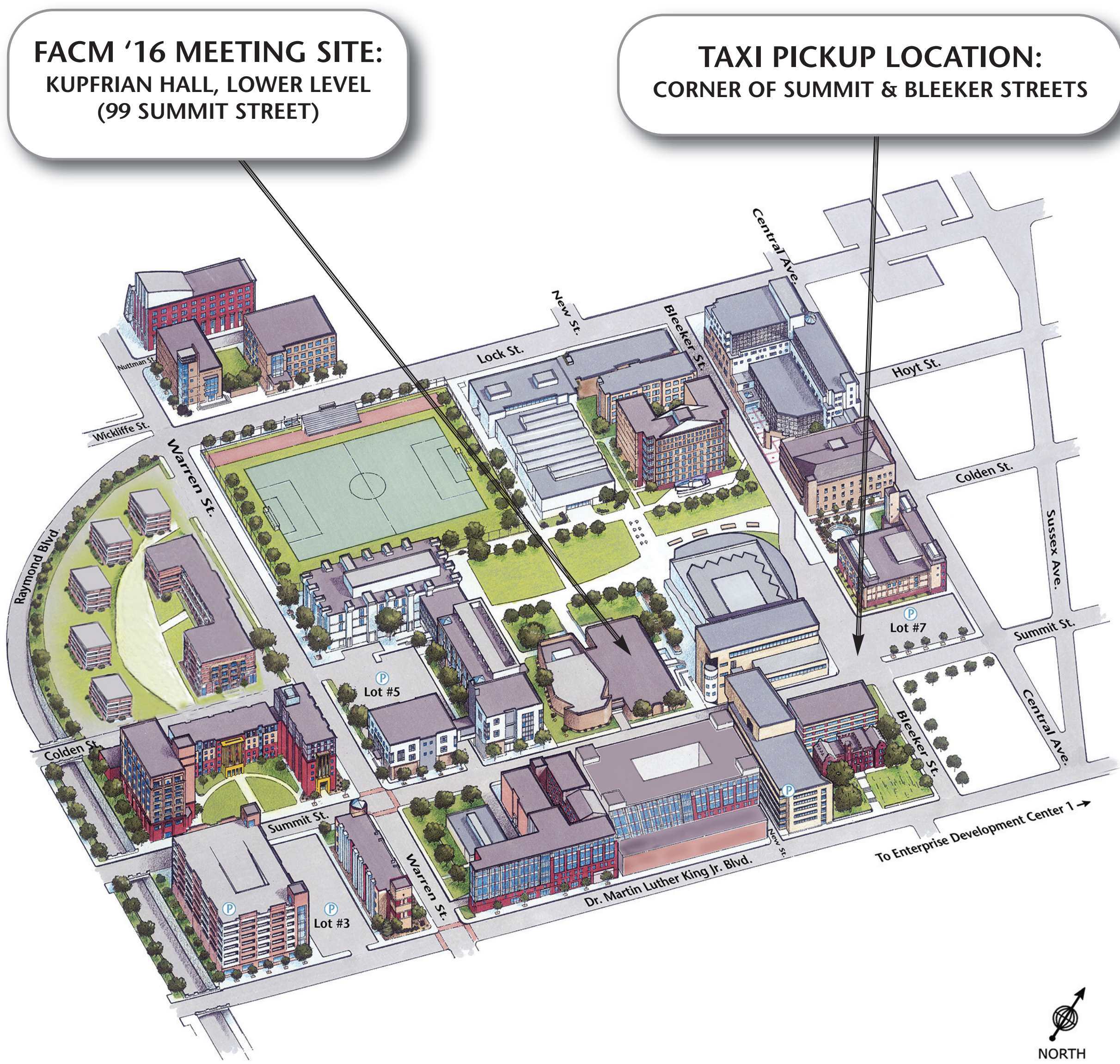
Telephone either one and request pick up at "NJIT campus, corner of Summit and Bleeker Streets." This is near the guard station at Parking Lot 7 by Cullimore Hall. If you plan to pay with a credit card instead of cash, tell them when you call because some drivers only accept cash.



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GUEST ACCESS TO THE NJIT NETWORK

JUNE 3 - 4, 2016

Welcome to NJIT. Please make use of the wired and wireless connections available in the meeting area. To do so please follow these three steps:

1. *CONNECT* using either a wireless or wired connection. Addresses are assigned automatically.
   - **Wired:** Most wall plates are active in the meeting area and noted by a RED or YELLOW port on the wall plate.
   - **Wireless:** Connect to the Site ID (SSID) of "NJIT" (all upper case, no quotes), which should appear in your list of available wireless networks.

2. *AUTHENTICATE* by visiting any website: http://www.njit.edu/ for example. When prompted, enter the following authentication credentials:

User name (UCID):	**guest274**
Password:	**thrush43**

If the "Please enter your UCID and Password" prompt reappears, verify that you have entered the correct UCID and Password, this means you have provided an incorrect username and password combination.

3. *ACCESS* to the NJIT network should now be available. Your guest account will give you access for 12 hours, or until your wireless device goes to sleep. If you have lost connection open a web browser and repeat step 2.

Please note: these access credentials are only good until midnight of June 5, 2016.

PROGRAM SCHEDULE

FRIDAY, JUNE 3

Time	Event	Location
8:15 – 8:45 a.m.	Registration + Coffee/ Pastries	Kupfrian 1st Floor Lobby
	Set Up Posters	Kupfrian 2nd Floor Rotunda
8:45 – 9:00 a.m.	**Introductory Remarks** Jonathan Luke, Chairperson, Department of Mathematical Sciences **Welcoming Remarks** Kevin Belfield, Dean, College of Science and Liberal Arts	Jim Wise Theater, Kupfrian Hall
9:00 – 10:00 a.m.	**Plenary Lecture I**	
	Robert Kass, Carnegie Mellon University *Oscillations and Synchrony in Spike Trains: A Statistical Perspective*	Jim Wise Theater, Kupfrian Hall
10:00 – 10:30 a.m.	Coffee Break	Kupfrian 1st Floor Lobby
10:30 – 1:00 p.m.	**Minisymposia I, II and III**	Kupfrian 1st Floor
1:00 – 2:15 p.m.	Lunch	Kupfrian 1st Floor Lobby
	Poster Session	Kupfrian 2nd Floor Rotunda
2:15 – 3:15 p.m.	**Plenary Lecture II** Laura Miller, University of North Carolina at Chapel Hill *The Flight of the Smallest Insects*	Jim Wise Theater, Kupfrian Hall
3:15 – 3:45 p.m.	Coffee Break	Kupfrian 1st Floor Lobby
3:45 – 6:15 p.m.	**Minisymposia IV, V, and VI**	Kupfrian 1st Floor
6:15 – 9:00 p.m.	**Banquet**	**Iberia Tavern** 80-84 Ferry St. Newark, NJ 07105

PROGRAM SCHEDULE

SATURDAY, JUNE 4

Time	Event	Location
8:30 – 9:00 a.m.	Registration + Coffee/ Pastries	Kupfrian 1st Floor Lobby
	Set Up Posters	Kupfrian 2nd Floor Rotunda
9:00 – 10:00 a.m.	**Plenary Lecture III** Mitchell Luskin, University of Minnesota *Mathematical Modeling of Incommensurate 2D Materials*	Jim Wise Theater, Kupfrian Hall
10:00 – 10:30 a.m.	Coffee Break	Kupfrian 1st Floor Lobby
10:30 – 1:00 p.m.	**Minisymposia VII, VIII, and IX**	Kupfrian 1st Floor
1:00 – 2:00 p.m.	Lunch	Kupfrian 1st Floor Lobby
	Poster Session	Kupfrian 2nd Floor Rotunda
2:00 – 3:00 p.m.	**Plenary Lecture IV** André Nachbin, IMPA, Brazil *The Uncertain Trajectory of a Pilot-Wave*	Jim Wise Theater, Kupfrian Hall
3:00 – 3:15 p.m.	Coffee Break	Kupfrian 1st Floor Lobby
3:15 – 5:30 p.m.	**Minisymposia X, XI, and XII**	Kupfrian 1st Floor

PROGRAM EVENTS

FRIDAY MORNING

PLENARY LECTURE I

9:00 – 10:00 a.m.	**Robert Kass,** Carnegie Mellon University *Oscillations and Synchrony in Spike Trains: A Statistical Perspective* Location: Jim Wise Theater, Kupfrian Hall

MINISYMPOSIA I, II, AND III

	Minisymposium I Biofluids Location: Kupfrian 117 Chair: Sarah Olson	**Minisymposium II** Waves I Location: Kupfrian 118 Chair: Catalin Turc	**Minisymposium III** Optical Imaging Data Analysis Location: Kupfrian 104 Chair: Mark Reimers
10:30 – 11:00 a.m.	**Isaac Klapper** Temple University *Transport in Biofilms*	**Carlos Borges** NYU - CIMS *Inverse Medium Scattering with Multiple Frequency Data and Multiple Angles of Incidence*	**Mark Reimers** Michigan State University *Optical Imaging Data: Analysis Challenges for the Next Decade*
11:00 – 11:30 a.m.	**Wanda Strychalski** Case Western Reserve University *Computational Challenges in Simulating Models with Intracellular Flow*	**Feruza Amirkulova** Western New England University *Multiple Scattering Effects Using Recursive and Iterative Techniques*	**Eftychios Pnevmatikakis** Simons Foundation *Demixing and Deconvolution of Calcium Imaging Data*
11:30 – 12:00 a.m.	**Sookkyung Lim** University of Cincinnati *Polymorphic Transformation of Bacterial Flagella During Locomotion*	**Carlos Jerez-Hanckes** Pontificia Universidad Católica de Chile *Multiple Traces Formulation: Preconditioning Strategies*	**Behtash Babadi** University of Maryland *State-Space Models for Mapping Functional Neural Circuitry at High Spatiotemporal Resolutions*

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FRIDAY MORNING

MINISYMPOSIA I, II, AND III

12:00-12:30 p.m.	**Boyce Griffith** UNC Chapel Hill *Towards Validated Models of In Vitro Cardiac Fluid Dynamics*	**Carlos Perez-Arancibia** California Institute of Technology *Windowed Green Function Method: An Efficient High-Order Integral Equation Method for Scattering in Layered Media*	**Andrew Leifer** Princeton University *Whole Brain Neural Dynamics and Behavior in C. Elegans*
12:30-1:00 p.m.	**Said Antonio Kas-Danouche** Universidad de Oriente *Non-Linear Stability of Core-Annular Flows in Pulmonary Airways with an Electrical Field*	**Stephen Shipman** Louisiana State University *Bound States and Resonance in Perturbed Periodic Quantum Graphs*	**Nathan Danielson** Columbia University *Optical Imaging of Neuronal Population Dynamics During Learning* *(12:30 - 12:45 p.m.)* **Pengcheng Zhou** Carnegie Mellon University *A Hybrid Model for Source Extraction of Microendoscope Calcium Imaging Data* *(12:45 - 1:00 p.m.)*

FRIDAY AFTERNOON

PLENARY LECTURE II

2:15 – 3:15 p.m **Laura Miller,** University of North Carolina at Chapel Hill
The Flight of the Smallest Insects
Location: Jim Wise Theater, Kupfrian Hall

MINISYMPOSIA IV, V, AND VI

	Minisymposium IV	Minisymposium V	Minisymposium VI
	Materials Science I Location: Kupfrian Hall, 117 Chair: Gideon Simpson	Stochastic Neuronal Dynamics Location: Kupfrian Hall, 118 Chair: Victor Matveev	Biostatistics I Location: Kupfrian Hall, 104 Chair: Antai Wang
3:45 – 4:15 p.m.	**Maria Cameron** University of Maryland *A Graph-Algorithmic Approach for Analysis of Complex Networks with Exponentially Small Transition Rates*	**Deena Schmidt** University of Nevada, Reno *Dimension Reduction for Stochastic Conductance Based Neural Models with Time Scale Separation*	**Judith Lok** Harvard T.H. Chan School of Public Health *Defining and Estimating Causal Direct and Indirect Effects When Setting the Mediator to Specific Values is Not Feasible*
4:15 – 4:45 p.m.	**Jonathan Weare** University of Chicago *Understanding Umbrella Sampling Approaches to Rare Event Simulation*	**Hye-Won Kang** University of Maryland *A Stochastic Model of the Melanopsin Phototransduction Cascade*	**Ao Yuan** Georgetown University *U-Statistics for Some Missing Data Models with Conditional Kernel*
4:45 – 5:15 p.m.	**Petr Plechac** University of Delaware *Information-Theoretic Tools for Uncertainty Quantification of High Dimensional Stochastic Models*	**Christoph Kirst** The Rockefeller University *Dynamic Function and Functional Dynamics in Neuronal Networks*	**Takumi Saegusa** University of Maryland *Statistical Methods for a Stratified Sample*

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FRIDAY AFTERNOON

MINISYMPOSIA IV, V AND VI

5:15 – 5:45 p.m.	**Miranda Holmes-Cerfon** NYU - CIMS *Statistical Mechanics of Singular Sphere Packings*	**Robert Rosenbaum** University of Notre Dame *Statistical Dynamics of Balanced Cortical Circuits*	**Yuping Zhang** University of Connecticut *Leveraging Diverse Omics Data to Infer Regulations in Complex Diseases*
5:45 – 6:15 p.m.	**Emilio Zappa** NYU - CIMS *Computational Methods for the Study of Self-Assembly of Sticky-Spheres Clusters* *(5:45 - 6:00 p.m.)*	**Christopher Ebsch** University of Notre Dame *Correlated Variability, Surround Suppression and Amplification in Balanced Network Models of Visual Cortical Circuits* *(5:45 - 6:00 p.m.)*	**Zhengqing Ouyang** The Jackson Laboratory for Genomic Medicine *Statistical Modeling of Hi-C Data for 3D Genome Structure Reconstruction*
	Brittan Farmer Drexel University *Crystallization for a Brenner-like Potential* *(6:00 - 6:15 p.m.)*	**Frederik Ziebell** Heidelberg University *Revealing the Dynamics of Neural Stem Cells in the Adult Hippocampus* *(6:00 - 6:15 p.m.)*	

PROGRAM EVENTS

SATURDAY MORNING

PLENARY LECTURE III

9:00 – 10:00 a.m.	**Mitchell Luskin,** University of Minnesota *Mathematical Modeling of Incommensurate 2D Materials* Location: Jim Wise Theater, Kupfrian Hall

MINISYMPOSIA VII, VIII, AND IX

	Minisymposium VII Micro and Bio Fluids Location: Kupfrian Hall, 117 Chair: Yuan-Nan Young	**Minisymposium VIII** Waves II Location: Kupfrian Hall, 118 Chair: Yassine Boubendir	**Minisymposium IX** Biostatistics II Location: Kupfrian Hall, 104 Chair: Sunil Dhar
10:30 – 11:00 a.m.	**M. Yvonne Ou** University of Delaware *On Dynamic Tortuosity of Poroelastic Materials*	**Fatih Ecevit** Boğaziçi University *Frequency-Adapted Boundary Element Methods for Single-Scattering Problems*	**Somnath Datta** University of Florida *Multi-Sample Adjusted U-Statistics that Account for Confounding Covariates*
11:00 – 11:30 a.m.	**Nguyenho Ho** Worcester Polytechnic Institute *Swimming Filaments in a Viscous Fluid with Resistance*	**Ibrahim Fatkullin** University of Arizona *A Model of Aggregation: Limit Shapes of Young Diagrams and Applications to Liquid Crystals*	**Susmita Datta** University of Florida *Differential Network Analysis with Multiply Imputed Lipidomic Data*
11:30 – 12:00 p.m.	**Michael Miksis** Northwestern University *Simulations of Particle Structuring Driven by Electric Fields*	**Panayotis Panayotaros** Universidad Nacional Autónoma de México *Breathers and Shelf-Type Solutions in a Nonlocal Discrete NLS Equation*	**Dipankar Bandyopadhyay** Virginia Commonwealth University *A Two-Stage Model for Dental Caries Assessment Using Non-Gaussian Markov Random Fields*

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MINISYMPOSIA VII, VIII, AND IX

12:00 – 12:30 p.m.	**David Rumschitzki** City College of New York *The Evolution of Tumor Populations Due to Mitosis, Treatment and Metastasis*	**Aloknath Chakrabarti** Indian Institute of Science *Approximate Solutions of the Integral Equations of a Class of Water Wave Scattering Problems*	**Suddhasatta Acharyya** Novartis Pharmaceuticals Corporation *Combining Efficacy, Safety, and Patient Reported Outcomes in Cancer Drug Development – A Late Phase Example*
12:30 – 1:00 p.m.	**Carlos Colosqui** Stony Brook University *Wetting Dynamics and Kinetics in Colloidal Systems*	**Michael Pedneault** NJIT *Schur Complement Domain Decomposition Methods for the Solution of Multiple Scattering Problems*	**Joe Bible** NICHD *Cluster Adjusted Regression (12:30 - 12:45 p.m.)* **Sinjini Sikdar** University of Florida *An Integrative Exploratory Analysis of -Omics Data from the ICGC Cancer Genomes Lung Adenocarcinoma Study (12:45 - 1:00 p.m.)*

SATURDAY AFTERNOON

PLENARY LECTURE IV

2:00 – 3:00 p.m.	**André Nachbin**, IMPA, Brazil The Uncertain Trajectory of a Pilot-Wave Location: Jim Wise Theater, Kupfrian Hall

MINISYMPOSIA X, XI, AND XII

	Minisymposium X	Minisymposium XI	Minisymposium XII
	Materials Science II Location: Kupfrian Hall, 117 Chair: David Shirokoff	Dynamics and Neural Control of Animal Locomotion Location: Kupfrian Hall, 118 Chair: Gal Haspel	Biostatistics III Location: Kupfrian Hall, 104 Chair: Ji Meng Loh
3:15 – 3:45 p.m.	**Margetis Dionisios** University of Maryland *A Three-Scale Perspective of Epitaxy: From Atomistic Dynamics to PDEs*	**Melanie Falgairolle** NIH, NINDS *Role of Spinal V1 Interneurons in Fictive Locomotion in the Isolated Neonatal Mouse Spinal Cord: An Optogenetic Study*	**Pei Wang** Icahn School of Medicine at Mount Sinai *A New Method for Joint Network Analysis Reveals Common and Different Co-Expression Patterns Among Genes and Proteins in Breast Cancer*
3:45 – 4:15 p.m.	**Gideon Simpson** Drexel University *Stochastic Processes and Diffusive Molecular Dynamics*	**Megan Leftwich** George Washington University *An Investigation into Sea Lion Locomotion*	**Xiang Li** Columbia University *Efficient Method to Optimally Identify Important Biomarkers for Disease Outcomes with High-Dimensional Data*
4:15 – 4:45 p .m.	**Xiaochuan Tian** Columbia University *Trace Theorems for Some Nonlocal Function Spaces*	**Andrew Spence** Temple University *Modeling Gait Regulation to Understand the Control of, and Constraints Shaping, Locomotion*	**Adam Ciarleglio** Columbia University *Flexible Functional Regression Methods for Estimating Individualized Treatment Regimes*

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SATURDAY AFTERNOON

MINISYMPOSIA X, XI, AND XII

4:45 – 5:15 p .m.	**Rolf Ryham** Fordham University *Calculating Energy Barriers and Activation States for Steps of Fusion*	**Eli Shlizerman** University of Washington *Dynamics of Caenorhabditis Elegans Worm Neuronal Network*	**Yang Feng** Columbia University *Neyman-Pearson Classification under High-Dimensional Settings*
5:15 – 5:30 p.m.	**Emanuel Lazar** University of Pennsylvania *Voronoi Topology for Atomistic Simulation Analysis*	**Gal Haspel** NJIT *A Model of the C. Elegans Locomotion Network Demonstrates Multiple Solutions for the Distribution of Oscillators that Produce Coherent Undulatory Motor Output*	**Yilong Zhang** New York University *Concordance Probability in Survival Models*

ROBERT KASS

Carnegie Mellon University

Oscillations and Synchrony in Spike Trains: A Statistical Perspective

As a potential mechanism for communication across areas in the brain, it has been suggested that coherent network oscillations drive many neurons to fire nearly synchronously, inducing a gain in downstream activity. As we try to establish statistical evidence for such a mechanism, several questions arise. How should we go about demonstrating a relationship between spiking activity and an oscillatory local field potential (LFP)? What if we are uncertain of the relevance of the LFP to the spiking activity? How do we assess the link between oscillation and synchrony? And, in this context, how should we deal with the multiplicity of possible interactions when the data involve large numbers of neurons? Based on work with several collaborators, I will provide some answers.

MITCHELL LUSKIN

University of Minnesota

Mathematical Modeling of Incommensurate 2D Materials

Incommensurate materials are found in crystals, liquid crystals, and quasi-crystals. Stacking a few layers of 2D materials such as graphene and molybdenum disulfide, for example, opens the possibility to tune the elastic, electronic, and optical properties of these materials. One of the main issues encountered in the mathematical modeling of layered 2D materials is that lattice mismatch and rotations between the layers destroys the periodic character of the system. This leads to complex commensurate-incommensurate transitions and pattern formation.

Even basic concepts like the Cauchy-Born strain energy density, the electronic density of states, and the Kubo-Greenwood formulas for transport properties have not been given a rigorous analysis in the incommensurate setting. New approximate approaches will be discussed and the validity and efficiency of these approximations will be examined from mathematical and numerical analysis perspectives.

LAURA MILLER

University of North Carolina at Chapel Hill

The Flight of the Smallest Insects

A vast body of research has described the complexity of flight in insects ranging from the fruit fly, Drosophila melanogaster, to the hawk moth, Manduca sexta. The smallest flying insects have received far less attention, although previous work has shown that flight kinematics and aerodynamics can be significantly different. In this presentation, three-dimensional direct numerical simulations and experiments with dynamically scaled robotic insects are used to compute the lift and drag forces generated by flexible and/or bristled wings to reveal the aerodynamics of these tiny fliers. An adaptive version of the immersed boundary method is used to simulate simplified flexible wings in pure translation, rotation, and performing a 'clap and fling' maneuver. Results are validated against dynamically scaled physical models using particle image velocimetry. At the lowest Reynolds numbers relevant to tiny insect flight, the ratio of lift to drag forces decreases. For Reynolds numbers below 10, the relative forces required to rotate the wings and perform 'clap and fling' become substantially greater. Wing flexibility and bristles can reduce the drag forces necessary to fling the wings apart while increasing the peak and average lift forces produced during the stroke.

ANDRÉ NACHBIN

IMPA, Brazil

The Uncertain Trajectory of a Pilot-Wave

This talk addresses a new dynamical system for a wave-particle pair. Yves Couder (Paris 7) and coworkers reported on walking droplets on the surface of a vibrating bath and discussed their properties previously thought to be peculiar to the microscopic, quantum realm. John Bush (MIT) and coworkers have also produced laboratory experiments which were compared to theoretical predictions. In this presentation I will briefly review some of their work and introduce our recent hydrodynamic pilot-wave model. Our model considers a trajectory equation for the walking droplet/particle coupled to a wave equation for the pilot-wave which guides the droplet. The wave dynamics starts from rest while the fluid domain is vibrated according to the Faraday theory. The dynamical properties of this wave-particle pair depends on a memory parameter. When the pilot-wave is confined to bounded domains in the high memory regime interesting random dynamics arise. When two cavities are separated by a barrier our model displays the unpredictable tunneling of this classical wave-particle association.

SUDDHASATTA ACHARYYA

Novartis Pharmaceuticals Corporation

Combining Efficacy, Safety, and Patient Reported Outcomes in Cancer Drug Development – A Late Phase Example

The critical question, in the context of confirmatory oncology drug trials is whether we have a clear answer on the risk-benefit ratio. A comprehensive metric that combines both efficacy and safety endpoints, as well as, patient-reported quality of life endpoints could be very useful in this context. A popular approach is to use a modified overall survival type analysis, where, instead of the usual survival time, a 'quality-adjusted' version of it is analyzed. One such measure is the Q-TWiST, which may be described as the 'quality-adjusted time without symptoms and toxicity'. Originally, QTWiST was developed for the adjuvant setting but has since been extended in several directions. Here, we adapt the QTWiST methodology to our specific situation, which is a two-arm randomized phase III oncology study, in multiple myeloma. The application of this methodology to specific clinical trials often brings up analytical issues, some of which will be discussed, as they apply to our study.

FERUZA AMIRKULOVA

Western New England University

Multiple Scattering Effects Using Recursive and Iterative Techniques

Multiple scattering (MS) of waves by a system of scatterers is of great theoretical and practical importance and is required in a wide variety of physical contexts such as the implementation of "invisibility" cloaks, the effective parameter characterization, and the fabrication of dynamically tunable structures, superlenses, etc. Here we develop fast, rapidly convergent iterative techniques to expedite the solution of acoustic MS problems. The formulation of MS problems reduces to a system of linear algebraic equations using Graf's theorem and separation of variables. The iterative and recursive techniques are developed using Neumann expansion and Block Toeplitz structure of the linear system; they are very general, and suitable for parallel computations and a large number of MS problems, i.e. acoustic, elastic, electromagnetic, etc. The theory is implemented in Matlab and FORTRAN, and the theoretical predictions are compared to computations obtained by COMSOL.

BEHTASH BABADI

University of Maryland

State-Space Models for Mapping Functional Neural Circuitry at High Spatiotemporal Resolutions

We consider the problem of inferring functional circuitry of multiple cortical areas from spike recordings and two-photon imaging data. Assuming that the neurons in each area influence the others through a cross-history dependent point process model with sparse and time-varying parameters, we perform adaptive system identification using sparse point process filters. We then apply a novel filtering and smoothing algorithm for estimating the parameters of a state-space model accounting for the Granger causality among the neurons in the ensemble with high temporal resolution and with recursively computed statistical confidence intervals. In addition, we develop a state-space model for capturing the covariance dynamics of the underlying networks. We apply the proposed algorithms to simultaneous multi-unit recordings from the ferret's primary auditory (A1) and prefrontal (PFC) cortices under behavioral auditory tasks as well as spontaneous two-photon recordings from the mouse's auditory cortex. Our analyses reveal the temporal details of the functional interaction between A1 and PFC under attentive behavior as well as among the A1 neurons under spontaneous activity at unprecedented spatiotemporal resolutions.

Joint work with: Alireza Sheikhattar, Sahar Akram, Ji Liu, Jonathan B. Fritz, Shihab Shamma, and Patrick Kanold

DIPANKAR BANDYOPADHYAY

Virginia Commonwealth University

A Two-Stage Model for Dental Caries Assessment Using No-Gaussian Markov Random Fields

In dental caries research, the data generated reveal two levels of hierarchy: a tooth-level and a surface-level. Assessments at the tooth level yield binary outcomes (presence/absence of teeth), and at the surface level yield trinary outcomes, indicating the healthy, decayed, or filled surfaces. Furthermore, the caries outcomes exhibit spatial referencing among neighboring teeth and surfaces (i.e. the disease/decay status of proximal tooth or surfaces are similar than those located further apart).Under a Bayesian paradigm, we develop a two-stage spatial (random effects) model that accommodates the hierarchy from tooth-level to surface-level of the (mixed) discrete responses. At the first stage, we focus on estimating the degree of spatial association between existing and missing teeth using an autologistic model. At the second stage (conditioned on a tooth being non-missing), we analyze the extent of spatial-referencing for the non-missing tooth using a Potts model. Computational difficulty in the Bayesian estimation scheme due to the intractable normalizing constant is tackled using a double Metropolis-Hastings sampler, which approximates the popular exchange algorithms leading to a significant improvement in the computational efficiency. Using data from a clinical study on dental caries conducted at the Medical University of South Carolina, we compare our model to alternative models to demonstrate the improvement in predictions, and to assess the effect of important covariates on caries experience.

This is joint work with Ick-Hoon Jin of the University of Norte Dame and Ying Yuan of the University of Texas.

JOE BIBLE

NICHD

Cluster Adjusted Regression

Ignorance of the mechanisms responsible for the availability of information presents an unusual problem for analysts. It is often the case that the availability of information is dependent on the outcome. In the analysis of cluster data we say that a condition for informative cluster size (ICS) exists when the inference drawn from analysis of hypothetical balanced data varies from that of inference drawn on observed data. Much work has been done in order to address the analysis of clustered data with informative cluster size; IPW, CWGEE and DWGEE. However, when dealing with longitudinal data with displaced cluster members, that is, when data possess temporally varying cluster sizes (TVCS), these methods may not produce unbiased inference for the underlying marginal distribution of interest. We propose a new marginalization that may be appropriate for TVCS.

CARLOS BORGES

NYU - CIMS

Inverse Medium Scattering with Multiple Frequency Data and Multiple Angles of Incidence

We consider the problem of reconstructing the medium from scattering measurements. The input data is assumed to be the far-field generated when a plane wave impinges on an unknown medium from multiple directions and at multiple frequencies. It is well known that this inverse scattering problem is both ill posed and nonlinear. We will use the recursive linearization algorithm of Chen to turn this problem in a sequence of well-posed problems. During the course of solving the inverse problem, we need to compute the solution to a large number of forward scattering problems. For this, we use high-order accurate PDE solver coupled with a fast direct solver.

MARIA CAMERON

University of Maryland

A Graph-Algorithmic Approach for Analysis of Complex Networks with Exponentially Small Transition Rates

Large stochastic networks a.k.a. continuous-time discrete-space Markov chains arise in modeling complex physical systems. I will introduce a greedy graph algorithm for analysis of such networks. It finds the sequence of characteristic time scales at which the dynamics of the systems undergoes qualitative changes. It gives an effective description of the dynamics for each time scale and extracts quasi-invariant and metastable sets of states. Under a certain genericness assumption, it gives asymptotic estimates for eigenvalues of the generator matrix of the Markov chain.

ALOKNATH CHAKRABARTI

Indian Institute of Science

Approximate Solutions of the Integral Equations of a Class of Water Wave Scattering Problems

A class of problems of scattering of surface water waves is examined for their approximate solutions. The original physical problems under consideration are transformed to certain singular integral equations whose approximate solutions are determined by utilizing expansions in terms of Chebyshev polynomials. The Reflection and Transmission Coefficients are evaluated for certain special scattering problems involving vertical barriers and the results are found to be in good agreement with the known ones, obtained analytically, by previous workers.

ADAM CIARLEGLIO

Columbia University

Flexible Functional Regression Methods for Estimating Individualized Treatment Regimes

A major focus of personalized medicine is on the development of individualized treatment rules that depend upon baseline measures. Good decision rules have the potential to significantly advance patient care and reduce the burden of a host of diseases. Statistical methods for developing such rules are progressing rapidly, but few methods have considered the use of pre-treatment functional data to guide decision-making. Furthermore, those methods that do allow for the incorporation of functional pre-treatment covariates typically make strong assumptions about the relationships between the functional covariates and the response of interest. We propose two approaches for using functional data to select an optimal treatment that address some of the shortcomings of previously developed methods. Specifically, we combine the flexibility of functional additive regression models with Q-learning or A-learning in order to obtain treatment decision rules. Properties of the corresponding estimators are discussed. Our approaches are evaluated in several realistic settings using synthetic data and are applied to data arising from a clinical trial comparing two treatments for major depressive disorder in which baseline imaging data are available for subjects who are subsequently treated.

CARLOS COLOSQUI

SUNY Stony Brook University

Wetting Dynamics and Kinetics in Colloidal Systems

A comprehensive understanding of wetting phenomena in colloidal systems with micro- and nanoscale characteristic dimensions is essential to fully exploit the potential of novel applications ranging from colloidal self-assembly to drug delivery and water treatment. Our fundamental understanding of wetting phenomena is embodied in classical mathematical models such as the Young-Dupre, Young-Laplace, and Lucas-Washburn equations, derived in the framework of continuum thermodynamics under the assumption of perfectly smooth and homogeneous surfaces. Such models predict dynamic behaviors that are governed by deterministic forces (e.g., capillary and hydrodynamic forces) and do not consider the effects of stochastic forces due to random thermal fluctuations. An increasing volume of experimental evidence indicates that the interplay between thermal motion and the nanoscale surface structure produces nontrivial phenomena that can be exploited for diverse technical applications. I will present experimental, theoretical, and computational (Molecular Dynamics/Langevin Dynamics) studies of colloidal systems where wetting processes exhibit a remarkable transition from “dynamic” regimes, dominated by hydrodynamic and capillary forces, to “kinetic” regimes governed by thermally-activated processes. These studies indicate possible directions to extend current models for wetting dynamics and specific pathways to control wetting processes through combinations of system-level geometry and nanoscale surface structure.

NATHAN DANIELSON

Columbia University

Optical Imaging of Neuronal Population Dynamics During Learning

In this talk I will discuss an experimental paradigm for the recording of calcium activity in large populations of identified hippocampal neurons at subcellular resolution in the awake, behaving mouse. I will present issues related to the acquisition and analysis of the resulting datasets, and I will discuss the advantages and limitations of current approaches. In addition, I will motivate the challenge by presenting data resulting from the application of these techniques to the assessment of functional heterogeneity in hippocampal microcircuits.

SOMNATH DATTA

University of Florida

Multi-Sample Adjusted U-Statistics that Account for Confounding Covariates

Multi-sample U-statistics encompass a wide class of test statistics that allow the comparison of two or more distributions. U-statistics are especially powerful because they can be applied to both numeric and non-numeric (e.g., textual) data. However, when comparing the distribution of a variable across two or more groups, observed differences may be due to confounding covariates. For example, in a case-control study, the distribution of exposure in cases may differ from that in controls entirely because of variables that are related to both exposure and case status and are distributed differently among case and control participants. We propose to use individually reweighted data (using the propensity score for prospective data or the stratification score for retrospective data) to construct adjusted U-statistics that can test the equality of distributions across two (or more) groups in the presence of confounding covariates. Asymptotic normality of our adjusted U-statistics is established and a closed form expression of their asymptotic variance is presented. The utility of our procedures is demonstrated through simulation studies as well as an analysis of genetic data.

SUSMITA DATTA

University of Florida

Differential Network Analysis with Multiply Imputed Lipidomic Data

Lipidomics analyses are characterized by large yet not a huge number of mutually correlated variables measured and their associations to outcomes are potentially of a complex nature. Differential network analysis provides a formal statistical method capable of inferential analysis to examine differences in network structures of the lipids under two biological conditions. It also guides us to identify potential relationships requiring further biological investigation. We provide a recipe to conduct permutation test on association scores resulted from partial least square regression with multiple imputed lipidomic data from the LUdwigshafen RIsk and Cardiovascular Health (LURIC) study, particularly paying attention to the left-censored missing values typical for a wide range of data sets in life sciences.

MARGETIS DIONISIOS

University of Maryland, College Park

A Three-Scale Perspective of Epitaxy: From Atomistic Dynamics to PDEs

The evolution of crystal surfaces involves the synergy of three length scales, from the atomistic to the continuum. In this talk, I will discuss progress and challenges in seamlessly connecting these scales. At the atomistic scale, the starting point is a master equation for the motion of adsorbed atoms. This description is connected to a mesoscale model for line defects in 1+1 dimensions. This model is in turn linked to a Partial Differential Equation for the continuum-scale height profile of the crystal surface.

CHRISTOPHER EBSCH

University of Notre Dame

Correlated Variability, Surround Suppression and Amplification in Balanced Network Models of Visual Cortical Circuits

In the primary visual cortex (V1), synaptic connection probabilities depend on location and functionality. Connectivity structure in V1 is well-studied, but the relationship between connectivity, network dynamics and visual coding remains an open problem. A clue to understanding visual cortical coding comes from the observation that V1 circuits operate in an inhibitory-stabilized or balanced regime in which strong recurrent excitation is balanced by strong inhibition.

We study the implications of balanced excitation and inhibition on visual coding using spatially extended models of visual cortical circuits. We extend the mean-field theory of balanced networks to account for arbitrary spatial structure. We find that, in the balanced state, firing rate profiles are determined by the solution to a linear Fredholm integral equation. Modeling the spatial structure of V1 circuits reveals that excitatory-inhibitory balance promotes the sharpening of orientation tuning curves and produces surround-suppression dynamics even when inhibitory neurons project more locally than excitatory neurons. We supplement our mean field analysis with simulations of integrate-and-fire network with biologically realistic parameters.

FATIH ECEVIT

Boğaziçi University

Frequency-Adapted Boundary Element Methods for Single-Scattering Problems

We introduce a class of hybrid boundary element methods for the solution of sound soft scattering problems. To facilitate the applicability of our algorithms throughout the entire frequency spectrum, we have enriched our Galerkin approximation spaces, through incorporation of oscillations in the incident field of radiation, into the algebraic and trigonometric polynomial approximation spaces. The resulting methodologies have three distinctive properties. Indeed, from a theoretical point of view, they can be tuned to demand only an O(k^a) increase (for any a > 0) in the number of degrees of freedom to maintain a fixed accuracy with increasing wavenumber k. Perhaps more importantly, from a practical point of view, they give rise to linear systems with significantly enhanced condition numbers and this, in turn, allows for more accurate solutions if desired.

MELANIE FALGAIROLLE

NIH, NINDS

Role of Spinal V1 Interneurons in Fictive Locomotion in the Isolated Neonatal Mouse Spinal Cord: An Optogenetic Study

V1 interneurons are a class of inhibitory, ipsilaterally-projecting neurons, located in the ventral part of the spinal cord, that express the transcription factor Engrailed-1. In this study, we investigated the role of V1 interneurons by expressing the light-gated proteins Archaerhodopsin-3 or channelrhodopsin-2 in engrailed-1::Cre mice. This allowed us to monitor the effects of optically silencing or activating (respectively) the V1 interneurons during fictive locomotion. Experiments were performed on the isolated superfused spinal cords of neonatal mice.

Hyperpolarizing V1 interneurons slowed and improved the quality of drug-induced fictive locomotion. In some striking cases, before the drugs were added and only tonic activity was present, silencing V1 interneurons induced the emergence of fictive locomotion. Performing the corollary experiment of depolarizing V1 neurons, produced a profound disruption of the locomotor rhythm. Calcium imaging of the cut surface of the cord revealed that the rhythmic activity of spinal interneurons was similarly disrupted.

Collectively these findings suggest that V1 interneurons modulate the locomotor central pattern generator by targeting the rhythm generator. Therefore, identifying the synaptic targets of subsets of V1 interneurons may provide insight into the nature of spinal locomotor rhythm generator.

BRITTAN FARMER

Drexel University

Crystallization for a Brenner-like Potential

Graphene is a carbon molecule with the structure of a honeycomb lattice. We show how this structure can arise in two dimensions as the minimizer of an interaction energy with two-body and three-body terms. In the engineering literature, the Brenner potential is commonly used to describe the interactions between carbon atoms. We consider a potential of Stillinger-Weber type that incorporates certain characteristics of the Brenner potential: the preferred bond angles are 180 degrees and all interactions have a cutoff radius. We show that the thermodynamic limit of the ground state energy per particle is the same as that of a honeycomb lattice. We also prove that, subject to periodic boundary conditions, the minimizers are translated versions of the honeycomb lattice.

IBRAHIM FATKULLIN

University of Arizona

A Model of Aggregation: Limit Shapes of Young Diagrams and Applications to Liquid Crystals

I will discuss a few statistical mechanical aggregation/polymerization models and their relation to measures on integer partitions and limit shapes of Young diagrams. I will derive explicit formulas for distribution of aggregate sizes for several ensembles and use these results to study critical phenomena in polydisperse nematic liquid crystals.

YANG FENG

Columbia University

Neyman-Pearson Classification under High-Dimensional Settings

Most existing binary classification methods target on the optimization of the overall classification risk and may fail to serve some real-world applications such as cancer diagnosis, where users are more concerned with the risk of misclassifying one specific class than the other. Neyman-Pearson (NP) paradigm was introduced in this context as a novel statistical framework for handling asymmetric type I/II error priorities. It seeks classifiers with a minimal type II error and a constrained type I error under a user specified level. This article is the first attempt to construct classifiers with guaranteed theoretical performance under the NP paradigm in high-dimensional settings. Based on the fundamental Neyman-Pearson Lemma, we used a plug-in approach to construct NP-type classifiers for Naive Bayes models. The proposed classifiers satisfy the NP oracle inequalities, which are natural NP paradigm counterparts of the oracle inequalities in classical binary classification. Besides their desirable theoretical properties, we also demonstrated their numerical advantages in prioritized error control via both simulation and real data studies.

BOYCE GRIFFITH

University of North Carolina at Chapel Hill

Towards Validated Models of In Vitro Cardiac Fluid Dynamics

Approximately 250,000 heart valve procedures are performed annually in the United States, including 50,000 surgeries for aortic valve replacement. Computational platforms for simulating prosthetic valves promise to improve prosthetic valve design and to assist in treatment planning. This talk will describe ongoing work to develop a dynamic model of an experimental pulse duplicator widely used by academic and industrial research labs as well as the Food and Drug Administration for designing, testing, and validating the design of heart valve prostheses. Our computational model is based on a version of the immersed boundary (IB) method that employs a finite strain continuum mechanics description of the immersed structure. Versions of this numerical framework have been developed to treat both rigid mechanical heart valve prostheses as well as flexible bioprosthetic heart valves. Extensions of these models can be used with medical image data from patients to enable patient-specific device selection.

NGUYENHO HO

Worcester Polytechnic Institute

Swimming Filaments in a Viscous Fluid with Resistance

We study propulsion of an infinite cylinder in a fluid with a sparse, stationary network of obstructions governed by the Brinkman equation. For fixed bending kinematics, we find that swimming speeds are enhanced due to the resistance from the obstacles. The limit for the Stokes case is recovered as the resistance goes to zero. We compare the asymptotic solutions with the numerical solutions obtained from the Method of Regularized Brinkmanlets.

MIRANDA HOLMES-CERFON

NYU - CIMS

Statistical Mechanics of Singular Sphere Packings

What are all the ways to arrange N hard spheres to form a rigid cluster? The answer brings insight to a number of phenomena in materials science, from nucleation, to emergence, to self-assembly. We enumerate packings of $N \leq 19$ spheres using a deterministic numerical algorithm, whose completeness could be addressed using geometrical methods.

We next ask: what is the free energy of the clusters when the spheres interact with a very short-range potential? For all so-called ``regular' clusters, this can be evaluated using a harmonic approximation for the energy. However, the list contains a great many ``singular' clusters, which correspond to singular solutions to a set of algebraic equations. These are also the clusters one sees with unusually high probability in experiments. We show how to compute the leading-order contribution to their free energy, and discuss implications for problems in materials science.

CARLOS JEREZ-HANCKES

Pontificia Universidad Católica de Chile

Multiple Traces Formulation: Preconditioning Strategies

Multiple Traces Formulations (MTFs) were developed in recent years to tackle wave scattering by heterogeneous obstacles via boundary integral methods. For first kind MTFs, Galerkin discretization yields ill-conditioned matrices which require preconditioning to achieve convergence of iterative schemes with Calder\'on-type techniques being proved optimal. Still, the underlying use of dual meshes becomes prohibitively expensive very quickly. In this work, we introduce preconditioning alternatives based on more algebraic approaches while considering the properties of the boundary integral operators. We discuss their numerical efficiency and further improvements.

HYE-WON KANG

University of Maryland, Baltimore County

A Stochastic Model of the Melanopsin Phototransduction Cascade

Melanopsin is a photopigment expressed in a small subset of intrinsically photosensitive ganglion cells (ipRGCs). Melanopsin signaling is involved in non-image forming vision, and controls circadian rhythms, pupillary light reflex, and sleep. The biochemical cascade underlying the light response in ipRGCs has not been fully understood. We suggest a hypothesized melanopsin phototransduction cascade and develop a stochastic model for the cascade using a continuous-time Markov jump process. Parameter values in the signaling pathway under several different environments are estimated based on the experimental results. Comparing the simulation results to the experimental data, our stochastic model can qualitatively reproduce experimental results. We perform parameter sensitivity analysis using a method of partial rank correlation coefficient (PRCC), which suggests that the melanopsin phototransduction pathway is robust as the one in Drosophila photoreceptors.

This is joint work with R.L. Brown, E. Camacho, E.G. Cameron, C. Hamlet, K.A. Hoffman, P.R. Robinson, K.S. Williams, and G.R. Wyrick.

SAID ANTONIO KAS-DANOUCHE

Universidad de Oriente

Non-Linear Stability of Core-Annular Flows in Pulmonary Airways with an Electrical Field

The study of core-annular flows confined in tubes with flexible walls has its major motivation on pulmonary fluid dynamics. In this case, there is no pressure gradient in the system and we impose a radial electrical field on the tube walls, and going into it. We assume that the system is axisymmetric and the annulus is thin compared with the core radius. Using asymptotic analysis, we derived a mathematical model for the evolution of the interface and the evolution of the airway walls under the effects of the electrical field applied.

CHRISTOPH KIRST

The Rockefeller University

Dynamic Function and Functional Dynamics in Neuronal Networks

Facing the highly parallel and distributed processes in the brain it is astonishing how it sub-parts co-act to generate coherent behaviour. Here we study mechanism that coordinate information processing and communication between different sub-parts of complex networks.

In classical approaches to neuronal computation the structure of a network is designed in order to perform a specific function and the collective dynamics of the network follow. Here we invert this view: When information is encoded in the deviations around a collective dynamical reference state that is intrinsically generated by the network the propagation of the fluctuations strongly depends on precisely this underlying reference. Information then 'surfs' on top of the collective reference dynamics and switching between states enables fast and flexible rerouting of information. The collective dynamics become functional by determining the systems information routing pattern and by switching between collective states the network can dynamically change its function.

In modular networks, local changes within a sub-network, e.g. as a result of a local computation, are capable of influencing the network's global collective dynamics. In turn, these global states determine the effective communication pattern and thereby will influence local processing. In this loop, the network while performing a function is thus also dynamically updating its own function continuously and in a self-organized way. We show that this naturally enables context dependent processing and flexible multi-modal integration.

We demonstrate the power of this approach in oscillatory Hopfield that perform self-organized contextual multi-modal pattern recognition and discuss applications of our results in the analysis of neuronal population activity.

ISAAC KLAPPER

Temple University

Transport in Biofilms

Biofilms are collections of microbes anchored together into sessile communities by self -secreted polymers. As such the realities of biofilms as physical materials are important to their function. In particular, function is often constrained by transport of soluble quantities, such as substrates and signals, into or out of the community. However, the combination of transport with reaction can lead to spatial heterogeneity and pattern formation within the biofilm structure, even without direct biological control. Examples include formation of active layers, formation of "external" structure (like mushrooms), and formation of "internal" structure (like lumps). Conversely, such pattern formation can impact biofilm function, particularly through transport but also through mechanics. Examples include formation of microenvironments and impacts on community level transport efficiency. Relatively simple mathematical models of biofilms, coupling growth with transport, will be used to illustrate the importance of physics in biofilm form and function.

EMANUEL LAZAR

University of Pennsylvania

Voronoi Topology for Atomistic Simulation Analysis

Atomic systems are routinely studied as large sets of point-like particles, and so understanding how particles are arranged in these systems is a very natural problem. However, aside from perfect crystals and ideal gases, describing this "structure" in an insightful yet tractable manner can be extremely challenging. Analysis of the configuration space of local arrangements of neighbors helps explain fundamental limitations of continuous metric approaches to this problem, and motivates the use of Voronoi cell topology in their stead. Examples from computational materials research help illustrate strengths of this approach, especially for studying high-temperature systems.

MEGAN LEFTWICH

George Washington University

An Investigation into Sea Lion Locomotion

California Sea Lions are highly maneuverable swimmers, capable of generating high thrust and agile turns. Their main propulsive surfaces, the fore flippers, feature multiple degrees of freedom, allowing their use for thrust production (through a downward, sweeping motion referred to as a "clap"), turning, stability and station holding (underwater "hovering"). To determine the two-dimensional kinematics of the California sea lion fore flipper during thrust generation, digital, high definition video is obtained using the specimen at the Smithsonian National Zoo in Washington, DC. Single camera videos are analyzed to digitize the flipper during the motions, using 10 points spanning root to tip in each frame. Digitized shapes were then fitted with an empirical function that quantitatively allows for both comparison between different claps and for extracting kinematic data. The resulting function shows a high degree of curvature (with a camber of up to 32%). Analysis of sea lion acceleration from rest shows thrust production in the range of 150-680 N and maximum flipper angular velocity (for rotation about the shoulder joint) as high as 20 rad/s. Analysis of turning maneuvers indicate extreme agility and precision of movement driven by the fore flipper surfaces.

ANDREW LEIFER

Princeton University

Whole Brain Neural Dynamics and Behavior in C. Elegans

How does a nervous system control an animal's behavior? We are investigating this question by manipulating and monitoring neural activity of populations of neurons in the brain of a simple transparent organism and correlating the observed neural dynamics with behavior. I will present a suite of optical tools to control and record activity in the nematode C. elegans as it moves, including the first instrument to perform whole-brain calcium imaging with cellular resolution in an awake and unrestrained behaving animal. We have used these techniques to gain insight into the underlying neural mechanisms behind mechanosensation, forward locomotion, and the C. elegans escape response. Now we are beginning to expand our investigation to reveal how collective neural dynamics generates any behavior in the C. elegans behavioral repertoire. These measurements reveal a need for new conceptual frameworks to explore how brain-wide population neural dynamics relate to animal behavior and nervous system structure.

XIANG LI

Columbia University

Efficient Method to Optimally Identify Important Biomarkers for Disease Outcomes with High-dimensional Data

Advances in high-throughput technologies in genomics and imaging yield unprecedentedly large numbers of prognostic biomarkers. The ideal variable selection procedure would search for the best subset of predictors, which is equivalent to imposing an L0-penalty on the regression coefficients. Since this optimization is a NP-hard problem, we propose a two-stage procedure for L0-penalty variable selection based on an alternating direction method of multipliers (ADMM) algorithm with an augmented penalization (ADMM-L0). Our method iterates between a convex regularized regression and a simple hard-thresholding estimation. We propose to simultaneously select regularization tuning parameter and thresholding parameter based on cross-validation. A one-step coordinate descent algorithm is used in the first stage to significantly improve computational efficiency. Through extensive simulation studies and real data application in Huntington's disease, we demonstrate superior performance of the proposed method in terms of selection accuracy and computational speed as compared to existing methods. The ADMM-L0 procedure outlined here is implemented in the R-package ADMMnet.

SOOKKYUNG LIM

University of Cincinnati

Polymorphic Transformation of Bacterial Flagella During Locomotion

E. coli swims in an aqueous environment by utilizing the rotation of flagellar motors and alternates two modes of motility, runs and tumbles. Runs are steady forward swimming driven by bundles of flagellar filaments turning CCW; tumbles involve a reorientation of the direction of swimming triggered by motor reversals. During tumbling, the helical flagellum undergoes polymorphic transformation, which is a local change in helical pitch and helical radius. In this work, we investigate the underlying mechanism of structural conformation and how this polymorphic transition plays a role in bacterial swimming.

This work is in collaboration with B. Griffith, Y. Kim, C.S. Peskin, H. Berg, W. Ko, and W. Lee.

JUDITH LOK

Harvard T.H. Chan School of Public Health

Defining and Estimating Causal Direct and Indirect Effects When Setting the Mediator to Specific Values is Not Feasible

Natural direct and indirect effects decompose the effect of a treatment into the part that is mediated by a covariate (the mediator) and the part that is not. Their definitions rely on the concept of outcomes under treatment with the mediator "set" to its value without treatment. Typically, the mechanism through which the mediator is set to this value is left unspecified, and in many applications it may be challenging to fix the mediator to particular values for each unit or patient. Moreover, how one sets the mediator may affect the distribution of the outcome. This article introduces "organic" direct and indirect effects, which can be defined and estimated without relying on setting the mediator to specific values. Organic direct and indirect effects can be applied for example to estimate how much of the effect of some treatments for HIV/AIDS on mother-to-child transmission of HIV infection is mediated by the effect of the treatment on the HIV viral load in the blood of the mother.

MICHAEL MIKSIS

Northwestern University

Simulations of Particle Structuring Driven by Electric Fields

Recent experiments show intriguing surface patterns when a uniform electric field is applied to a droplet covered with colloidal particles. Depending on the particle properties and the electric field intensity, particles organize into an equatorial belt, pole-to-pole chains, or dynamic vortices. Here we present 3D simulations of the collective particle dynamics, which account for electrohydrodynamic and dielectrophoresis of particles. In stronger electric fields, particles are expected to undergo Quincke rotation and impose disturbance to the ambient flow. Transition from ribbon-shaped belt to rotating clusters is observed in the presence of the rotation-induced hydrodynamical interactions. Our results provide insight into the various particle assemblies discovered in the experiments.

M. YVONNE OU

University of Delaware

On Dynamic Tortuosity of Poroelastic Materials

Dynamic tortuosity is the Fourier transform of the kernel in the memory term of poroelastic wave equations. It plays an important role in the quantifying energy dissipation of wave propagating through prelatic materials. In this talk, the theory and algorithm for reconstructing the dynamic tortuosity from finite data set at distinct frequencies will be presented. Mathematical quantification of its dependence on the pore space geometry will also be explained. A new numerical method for handling the memory term in solving the wave equation will be proposed.

ZHENGQING OUYANG

The Jackson Laboratory for Genomic Medicine

Statistical Modeling of Hi-C Data for 3D Genome Structure Reconstruction

Genome-wide chromosome conformation capture (Hi-C) is a powerful technology that has recently generated massive, complex data sets for exploring the 3D structure of the genome. However, few computational and statistical approaches are existing to quantitatively analyze Hi-C data, thus hindering the investigation of the structure and function of the genome. Here, we introduce a novel statistical model for reconstructing 3D genome structure from Hi-C data. It describes a chromosome as a Markov chain under a generalized linear model framework, and uses simulated annealing to globally search for the latent 3D structure. We demonstrate that the model is more accurate and robust than existing approaches via extensive simulations and real data applications.

PANAYOTIS PANAYOTAROS

Universidad Nacional Autónoma de México (UNAM)

Breathers and Shelf-Type Solutions in a Nonlocal Discrete NLS Equation

We study properties of some breather type solutions of a nonlocal discrete NLS equation modeling propagation in waveguide arrays built from a nematic liquid crystal substratum. The nonlocality leads to some new effects, such as internal modes in orbitally stable breathers, and nonmonotonic profiles in solutions with interfaces. We present some new theoretical results explaining some of these features. In particular we discuss symmetry, monotonicity, and spectral properties of energy minimizers, and some spectral properties of shelf-type solutions.

CARLOS PEREZ-ARANCIBIA

California Institute of Technology

Windowed Green Function Method: An Efficient High-Order Integral Equation Method for Scattering in Layered Media

In this talk we present a novel boundary integral equation method for the numerical solution of problems of scattering by obstacles and defects in the presence of layered media. This new approach, that we refer to as the windowed Green function method (WGFM), is based on use of smooth windowing functions and integral kernels that can be expressed directly in terms of the free-space Green function. The WGFM is fast, accurate, flexible and easy to implement. In particular straightforward modifications of existing (accelerated or unaccelerated) solvers suffice to incorporate the WGF capability. The mathematical basis of the method is simple: the method relies on a certain integral equation that is smoothly windowed by means of a low-rise windowing function, and is thus supported on the union of the obstacle and a small flat section of the interface between the two penetrable media. Various numerical experiments demonstrate that both the near- and far-field errors resulting from the proposed approach, decrease faster than any negative power of the window size. In some of those examples the proposed method is up to thousands of times faster, for a given accuracy, than an integral equation method based on use of the layer Green function and the numerical approximation of Sommerfeld integrals. Generalizations of the WGFM to problems of scattering by obstacles in layered media composed by any finite number of layers as well as wave propagation and radiation in open dielectric waveguides are also included in this presentation.

PETR PLECHAC

University of Delaware

Information-theoretic tools for uncertainty quantification of high dimensional stochastic models

We present mathematical tools for deriving optimal, computable bounds on sensitivity indices of observables for complex stochastic models arising in biology, reaction kinetics and materials science. The presented technique allows for deriving bounds also for path-dependent functionals and risk sensitive functionals. Using the rate of relative entropy the sensitivity of a wide class of observables can be bounded by Fisher information and quantities that characterize the statistics (variance, autocorrelation) of observables. The use of variational representation of relative entropy also allows for error estimation and uncertainty quantification in coarse-grained models.

EFTYCHIOS PNEVMATIKAKIS

Simons Foundation

Demixing and Deconvolution of Calcium Imaging Data

We present a modular approach for analyzing calcium imaging recordings of large neuronal ensembles. Our goal is to simultaneously identify the locations of the neurons, demix spatially overlapping components, and denoise and deconvolve the spiking activity from the slow dynamics of the calcium indicator. Our approach relies on a constrained nonnegative matrix factorization that expresses the spatiotemporal fluorescence activity as the product of a spatial matrix that encodes the spatial footprint of each neuron in the optical field and a temporal matrix that characterizes the calcium concentration of each neuron over time. This framework is combined with a novel constrained deconvolution approach that extracts estimates of neural activity from fluorescence traces, to create a spatiotemporal processing algorithm that requires minimal parameter tuning. We demonstrate the general applicability of our method by applying it to in vitro and in vivo multi-neuronal imaging data, whole-brain light-sheet imaging data, and dendritic imaging data.

MARK REIMERS

Michigan State University

Optical Imaging Data: Analysis Challenges for the Next Decade

The BRAIN initiative is one of the biggest scientific programs explicitly aimed at gathering data, specifically aiming to measure functional activity in living brains at high resolution. Although several technologies are being developed for this program, the most promising technologies are the high-throughput optical imaging technologies, which generate high-resolution stacks of images of brain activity, up to terabytes of data per experiment. However the statistical methods and computational infrastructure to analyze and interpret these data are largely undeveloped.

I will summarize current issues and ongoing challenges in optical data analysis, under three main headings: i) pre-processing issues to remove artifacts and reduce noise; ii) dimension reduction and characterizing state-space dynamics, where models and data may most readily be compared right now; iii) inference of network connections and communication. Then I will consider emerging issues that may arise over the next decade, and sketch some approaches that may be fruitful.

ROBERT ROSENBAUM

University of Notre Dame

Statistical Dynamics of Balanced Cortical Circuits

Balanced networks offer an appealing theoretical framework for studying neural variability since they produce intrinsically noisy dynamics with some statistical features similar to those observed in cortical recordings. However, previous balanced network models face two critical shortcomings. First, they produce extremely weak spike train correlations, whereas cortical circuits exhibit both moderate and weak correlations depending on cortical area, layer and state. Second, balanced networks exhibit simple mean-field dynamics in which firing rates linearly track feedforward input. Cortical networks implement non-linear functions and produce non-trivial dynamics.

We propose that these shortcomings of balanced networks are overcome by accounting for the distance dependence of connection probabilities observed in cortex. We extend the mean-field theory of balanced networks to account for distance-dependent connection probabilities and show that, under this extension, balanced networks can exhibit either weak or moderate spike train correlations and also produce high-dimensional spatiotemporal firing rate dynamics.

DAVID RUMSCHITZKI

City College of New York

The Evolution of Tumor Populations Due to Mitosis, Treatment and Metastasis

We propose a new mathematical model for tumor growth, shrinkage and metastasis and two experimental (zebrafish melanoma and BALB/c mouse breast cancer) models to test it. Unlike previous mathematical models that try to describe the dynamics of a typical or mean tumor and generally do not include immunity or therapy, our model describes an entire tumor population's evolution, where each tumor is subject to mitosis, immunity, chemo/immunotherapy and metastasis. The individual terms in our model naturally (and surprisingly) combine to generate a qualitatively new type of behavior – a diffusive process in tumor-size space. This diffusion turns a collection of tumors of similar sizes into one whose sizes are more spread apart, without changing their mean size. When coupled with terms that either grow or shrink all tumors, and noting evidence that patients with small tumors respond to therapy better than patients with larger ones, it can predict the emergence of a tumor that suddenly grows rapidly after a long period of stable tumor load. This is reminiscent of certain patient cohorts, whose members persist with apparently stationary tumors for long periods of time until suddenly one or more tumors begin to grow rapidly.

ROLF RYHAM

Fordham University

Calculating Energy Barriers and Activation States for Steps of Fusion

Fusion between biological membranes is a widespread cellular process, responsible for events as varied as secretion of neurotransmitters and fertilization of egg by sperm. Molecularly, fusion is the merger of two lipid bilayer membranes, and this merger proceeds through several key intermediates states. But the transition energy barriers that separate these intermediates have not been determined. Using the simplified string method, we calculate a least energy pathway and the activation states between intermediates for the entire fusion process. The bilayer energetics are based on a modified Helfrich Hamiltonian that accounts for long range interactions between bilayers, and a novel field theoretic treatment of hydrophobic potentials. Through the energetic analysis, we conclude that lipid de-mixing is required for the transition from a stalk to a hemifusion diaphragm, and that complete fusion is possible provided pore formation is initiated while the diaphragm is small. The calculations provide a movie of individual lipid deformations, as the membrane geometry and topology evolve over time.

TAKUMI SAEGUSA

University of Maryland

Statistical Methods for a Stratified Sample

Two-phase stratified sampling is a sampling technique for cost reduction and improving efficiency. Examples includes stratified case control study and exposure-stratified case cohort study. A main theoretical challenge is a dependent and biased sample due to sampling without replacement in each stratum. A biostatistical approach to this issue is to approximate design by stratified Bernoulli sampling and focus on few specific models including the Cox model, resulting in paucity of research in general methodology such as bootstrap. An approach from sampling theory is to impose general conditions regardless of designs, leading to implicit asymptotic distributions and inefficient statistical methods applicable for any design. Our approach, which extends empirical process theory to two-phase stratified sampling, explicitly obtains asymptotic distributions, and yields general methodology tailored to two-phase stratified sampling. In this talk, we consider three statistical problems, model selection, improving efficiency and variance estimation, arising from the RV144 case control study. Our approach illustrates inadequacy of existing methods in these problems, and naturally introduces our proposed methods. Finite sample properties are investigated in simulation studies using the logistic regression model and the Cox model.

DEENA SCHMIDT

University of Nevada, Reno

Dimension Reduction for Stochastic Conductance Based Neural Models with Time Scale Separation

The Stochastic Shielding Approximation (SSA) is a fast, accurate simplification of randomly gated ion channel models (Schmandt and Galan 2012, Schmidt and Thomas 2014). Viewing the channel as a discrete process on a directed graph, driven by an independent noise source for each edge, the SSA accurately represents the process using independent noise sources for only a small subset of the edges. This approximation preserves the mean field behavior while selectively incorporating only the underlying noise sources that contribute the most significantly to observable system behavior. Thus the stochastic shielding approximation provides an analytically tractable example of incorporating noise in a manner relevant to the network's physiological function. Here we investigate the limits of the SSA by studying its accuracy for systems exhibiting large separation of time scales, including ion channel models with "bursty" dynamics.

STEPHEN SHIPMAN

Louisiana State University

Bound States and Resonance in Perturbed Periodic Quantum Graphs

I will present a class of periodic Schrödinger operators on metric graphs (quantum graphs) for which an appropriately chosen localized defect can engender a bound state at any desired frequency within the continuous spectrum. The dispersion relation at a given energy (Fermi surface) for these operators is necessarily reducible, but the reducibility is not necessarily a consequence of a symmetry of the graph. It is a consequence of the graph's construction as two identical periodic subgraphs coupled by a quantum graph that may not be symmetric. Asymmetric coupling causes a detuning of the complex resonance emanating from the embedded eigenvalue as the graph that supports the bound state is perturbed.

ELI SHLIZERMAN

University of Washington

Dynamics of Caenorhabditis Elegans Worm Neuronal Network

The nervous system of the Caenorhabditis elegans (C. elegans) worm is appealing to study, since it is a tractable fully functional neuronal network (comprised of 302 neurons) for which electro-physical connectivity map (connectome) is fully resolved. While the C. elegans static connectome is complete, understanding the neural circuits that control its sensorimotor responses is challenging because both the neurons and their interactions within the network are dynamic. In my talk I will describe our recent work in which we have established a computational dynamical model for the C. elegans nervous system and able to employ it for analysis of stimulations associated with body movements.

SINJINI SIKDAR

University of Florida

An Integrative Exploratory Analysis of -Omics Data from the ICGC Cancer Genomes Lung Adenocarcinoma Study

It is known that all agents that cause cancer (carcinogens) also cause a change in the DNA sequence. In order to identify such often subtle changes, we attempt to integrate multiple molecular profile data sets released by the International Cancer Genome Consortium (ICGC). The list of data sets includes matched gene and microRNA expression profiles, somatic copy number variation, DNA methylation, and protein expression profiles for lung adenocarcinoma patients receiving treatments. We consider both unsupervised and supervised learning techniques (clustering and penalized regression) to identify interesting molecular markers corresponding to each type of -omics profiles that can differentiate patients. Associations between important markers of two types have been studied. An adaptive ensemble binary regression model has been presented that uses the entirety of available -omics profiles leading to a more accurate clinical prognosis for the patients in the sample. This integrated study provides a more comprehensive picture of lung adenocarcinoma.

GIDEON SIMPSON

Drexel University

Stochastic Processes and Diffusive Molecular Dynamics

Diffusive Molecular Dynamics (DMD) is a novel approach to problems in molecular dynamics that aims to reach the diffusive time scale of milliseconds and beyond. To accomplish this, DMD “averages out” the vibrational time scale of femtoseconds and evolves probability densities at atomistic sites. This requires the approximation of a probability distribution in an extended state space by a synthetic approximate distribution, which can easily be sampled. The mean occupancy at the atomic sites are then evolved according to a system of coupled ODEs, under a so-called Master Equation, but no underlying stochastic process is given in the current formulation. In this work, we propose and examine a stochastic process which gives rise to similar dynamics as DMD. This primitive model also offers a way to connect DMD to a more traditional MD models.

ANDREW SPENCE

Temple University

Modeling Gait Regulation to Understand the Control of, and Constraints Shaping, Locomotion

One of the grand challenges for modern science is to understand how animals move. To move, legged animals typically choose a specific gait (for example walk, trot, or gallop) that is thought to optimize locomotion under various evolutionary constraints (energetic cost, stability, escape from predation). Treating the legs as oscillators, a gait can be thought of as a set of phase relationships between the legs that evolves over time. This talk will present research that seeks to model gait, taking a dynamical systems approach, to gain insight into both the neuromechanical mechanisms that underlie it and the ultimate constraints that have shaped it. Two main contributions will be presented: first, the finding that dogs, when walking on rough terrain, exhibit gait regulation that appears shaped by concern for static stability; second, the finding that both the gait and gait transitions of dogs can be modeled by a symmetric potential that has a body mass dependent phase shift between fore- and hindlimbs. We will highlight areas where we feel this phase- and dynamical systems based approach has brought insight into the experimental work.

WANDA STRYCHALSKI

Case Western Reserve University

Computational Challenges in Simulating Models with Intracellular Flow

The cytoplasm is a complex material consisting of organelles, the cytoskeleton, and liquid cytosol. The cytoplasm has been modeled on the continuum level as an elastic material, viscoelastic material, porous gel, and viscous fluid, depending on the timescale and relevant cellular under consideration. Recent work suggests that cytoplasmic streaming plays an important role in cell motility. The rheological properties of the cytoplasm affect pressure propagation and fluid flow in migrating cells that exhibit cytoplasmic streaming. Some animal cells use blebs, spherical membrane protrusions driven by cytoplasmic flow, for migration. The interpretation of recent experiments found that cytoplasmic elasticity is necessary to limit bleb size. Other experiments and modeling point to the importance of cytoplasmic poroelasticity in blebbing dynamics. Here we discuss a poroelastic immersed boundary method for simulating the relative motion of the cytosol flowing through the cytoskeleton in the cytoplasm. We also discuss the construction of highly accurate approximations to the delta function to address the problem of spurious velocities that arise during simulations of bleb expansion.

XIAOCHUAN TIAN

Columbia University

Trace Theorems for Some Nonlocal Function Spaces

Nonlocal integral-differential equations and nonlocal balance laws have been proposed as effective continuum models in place of PDEs for a number of anomalous and singular processes in physics and material sciences. In this talk, we work on nonlocal function spaces with spatially heterogeneously defined nonlocal interactions, which effectively bridge local(PDEs) and nonlocal models by allowing nonlocality shrinking to zero at certain points. Mathematically, we present an extension of the classical trace theorem on the new nonlocal function spaces such that nonlocal and local coupling is possible through matching the boundary trace. This result is novel in the sense that the boundary trace is attained without imposing regularity of the function in the interior of the domain.

PEI WANG

Icahn School of Medicine at Mount Sinai

A New Method for Joint Network Analysis Reveals Common and Different Co-Expression Patterns Among Genes and Proteins in Breast Cancer

In this paper, we focus on characterizing common and different co-expression patterns among RNAs and proteins in breast cancer tumors. To address this problem, we introduce Joint Random Forest (JRF), a novel non-parametric algorithm to simultaneously estimate multiple co-expression networks by effectively borrowing information across protein and gene expression data. The performance of JRF was evaluated through extensive simulation studies using different network topologies and data distribution functions. Advantages of JRF over other algorithms which estimate class specific networks separately were observed across all simulation settings. JRF also outperformed a competing method based on Gaussian graphic models. We then applied JRF to simultaneously construct gene and protein co-expression networks based on protein and RNAseq data from CPTAC-TCGA breast cancer study. We identified interesting common and differential co-expression patterns among gene and proteins. This information can help to cast light on the potential disease mechanisms of breast cancer.

JONATHAN WEARE

University of Chicago

Understanding Umbrella Sampling Approaches to Rare Event Simulation

I will discuss an ensemble sampling scheme based on a decomposition of the target average of interest into subproblems that are each individually easier to solve and can be solved in parallel. The most basic version of the scheme computes averages with respect to a given density and is a generalization of the Umbrella Sampling method

for the calculation of free energies. We have developed a careful understanding of the accuracy of the scheme that is sufficiently detailed to explain the success of umbrella sampling in practice and to suggest improvements including adaptivity. For equilibrium versions of the scheme we have developed error bounds that reveal that the existing understanding of umbrella sampling is incomplete and leads to a number of erroneous conclusions about the scheme. Our bounds are motivated by new perturbation bounds for Markov Chains that we recently established and that are substantially more detailed than existing perturbation bounds for Markov chains. They demonstrate, for example, that equilibrium umbrella sampling is robust in the sense that in limits in which the straightforward approach to sampling from a density becomes exponentially expensive, the cost to achieve a fixed accuracy with umbrella sampling can increase only polynomially. I will also discuss extensions of the stratification philosophy to the calculation of dynamic averages with respect a given Markov process. The scheme is capable of computing very general dynamic averages and offers a natural way to parallelize in both time and space.

AO YUAN

Georgetown University

U-Statistics for Some Missing Data Models with Conditional Kernel

For incomplete data models, the classical U-statistic estimator of a functional parameter of the underlying distribution cannot be computed directly since the data are not fully observed. To estimate such a functional parameter, we propose a U-statistic using a substitution estimator of the conditional kernel given the observed data. This kernel estimator is obtained by substituting the nonparametric maximum likelihood estimator for the underlying distribution function in the expression of the conditional kernel. We study the asymptotic properties of the proposed U-statistic for several incomplete data models, and in a simulation study, we assess the finite sample performance of the Mann-Whitney U-statistic with conditional kernel in the current status model. The analysis of a real-world data set illustrates the application of the proposed methods in practice.

EMILIO ZAPPA

NYU - CIMS

Computational Methods for the Study of Self-Assembly of Sticky-Spheres Clusters

Sticky-spheres clusters appear in many areas of condensed-matter physics and materials science, e.g. colloids. In this talk I will present some computational methods for the study of self-assembly of particles interacting with short-range potentials. This work involves Monte-Carlo algorithms to sample and compute the volume of differentiable manifolds.

YUPING ZHANG

University of Connecticut

Leveraging Diverse Omics Data to Infer Regulations in Complex Diseases

Recent advances in high-throughput biotechnologies have generated unprecedented types and amounts of data for biomedical research. It is likely that integrating results from diverse experiments may lead to a more unified and global view of complex diseases such as cancer. In this talk, we will address statistical issues in data integration and present a new statistical learning method for integrating diverse omics data. Our method provides an integrated picture of commonalities and differences across tumor types. The performance of our method will be demonstrated through simulations and applications to real cancer data.

YILONG ZHANG

New York University

Concordance Probability in Survival Models

An unmet significant challenge in the treatment of many early-stage cancers is the lack of effective prognostic models to identify patients who are at high risk of disease progression. The only way to identify these patients currently is to await disease recurrence. By then, the best chance to treat the cancer may have been lost. For example, about 90% of resected stage-1 melanoma patients are cured. Accurate and timely identification of high risk cancer patients can save more lives and reduce the number of cured cancer patients who receive costly over-treatment.

Mixture cure models can account for cure fractions in patients population can be more suitable prognostic models than ordinary survival models such as Cox Proportional Hazard models or Proportional Odds models that ignore the existence of cure fractions. We define new prognostic metrics to evaluate the prognostic accuracy for mixture cure models that considering the cure fraction. The asymptotic theory of these estimators is also established. Intensive simulations are provided to show the validity of these estimators in limit sample.

PENGCHENG ZHOU

Carnegie Mellon University

A Hybrid Model for Source Extraction of Microendoscope Calcium Imaging Data

Calcium imaging has been an important tool for recording population neurons. Recent innovations in imaging techniques allow neuroscientists record over hundreds of neurons within broad brain areas. Microendoscope is an one-photon imaging technique that can image large scale neural circuits of deep brain regions on freely behaving animals. This type of data has strong fast-fluctuating background, low signal-to-noise ratio (SNR) and high spatial overlaps. These features pose an important statistical challenge to isolate neurons and extract their activities automatically. Although this imaging technique has been popularized in neuroscience community, the tools for processing its data are very limited. In this work we propose an algorithm to simultaneously identify all neurons' spatial footprints and temporal activities. It is based on Constrained Nonnegative Matrix Factorization (CNMF) method proposed by Liam Paninski group (Pnevmatikakis et. al., Neuron 2016; Yang et. al., Neuron 2016), but specialized for microendoscopic data. The original CNMF method approximates the background with a rank-1 NMF and assumes the background is much weaker than neural signals. However, the background of microendoscopic data has high ranks and is much stronger than neural signals (over 10 times larger). These violations limit the applications of CNMF on this type of data. Here we used a hybrid model to model neural signals with CNMF and model background with Singular Vector Decomposition (SVD). Our SVD approximation can better approximate the background and significantly increase the speed of the model fitting. We also developed special procedures to extract neurons with the least contamination from the background. We tested our method with many datasets and it shows great advantages in performance of source extraction over the most widely used PCA/ICA approach. Our algorithm provides a powerful tool for analyzing microendoscopic data.

FREDERIK ZIEBELL

Heidelberg University

Revealing the Dynamics of Neural Stem Cells in the Adult Hippocampus

In the adult hippocampus, neural stem cells (NSCs) continuously produce new neurons. Although multiple studies identify qualitative NSC features like their age-related decline, a quantitative understanding is still missing. Here, we develop a quantitative model of hippocampal neurogenesis based on newly generated and already published data. We show that the data best fit a model in which NSCs return to quiescence after division and have the ability of becoming activated repeatedly. Moreover, we show that about 40% of the NSC decline can be attributed to direct transformation into astrocytes. Additionally, we demonstrate that aged NSCs remain longer in quiescence and have a higher probability to become re-activated versus being depleted. Finally, our model explains that Dickkopf-1 deletion expands the pool of NSC by increasing their activation and not, as previously speculated, by increasing the rate of symmetric divisions. Altogether, this model provides a framework to interpret changes in NSC dynamics.

JIMMIE ADRIAZOLA AND HARDIK DARI

New Jersey Institute of Technology

Diffusion Limited Aggregation and Saffman-Taylor Instability in Non-Newtonian Hele-Shaw Flow

Diffusion Limited Aggregation and Saffman-Taylor We carry out experimental, theoretical, and computational study of Saffman-Taylor instability in a Hele-Shaw flow involving injection of a less viscous fluid into a more viscous one in a thin gap between two plates. The aim of this project is to study the instability when the more viscous fluid is non-Newtonian, with viscosity that depends on shear rate. To characterize the properties of the emerging patterns, we use several methods to calculate the fractal dimension based on the data collected from experimental trials and extensive simulations of diffusion limited aggregation type. We further quantify the instability development in both the experiments and simulations using Fourier analysis and compare the results to the analytical ones obtained by linear stability analysis.

This work was carried out during the 2015-2016 school year by NJIT undergraduates as part of an applied mathematics Capstone project. Partial support by NSF grant No. 1211713 is acknowledged.

Advisor: Lou Kondic (NJIT)

Collaborators: Andres Alban, Jake Brusca, Zouhair Draben, Ibin Abdul-Hakeem, Nicholas Hale, Michael Lam (NJIT Lab Assistant), Jacob Moorman, Armando Rosa, Enkhsanaa Sommers, Thomas Tu, and Bryan Valerio (NJIT)

MAHDI BANDEGI AND DAVID SHIROKOFF

New Jersey Institute of Technology

Approximate Global Minimizers of Pairwise Interactions

A wide range of material systems exhibit energy driven pattern formation governed by an underlying non-convex energy functional. Although numerically finding and verifying local minima to these functionals is relatively straight-forward, the computation and verification of global minimizers is much more difficult. Here the verification of global minimizers is often important in understanding the material phase diagram, especially at low temperatures. In this talk I will examine a general class of model functionals: those arising in non-local pairwise interaction problems. I will present a new approach for computing approximate global minimizers based on a convex relaxation of the underlying energy landscape, along with a recovery technique. The approach is sometimes exact, and also provides a numerical recovery guarantee for the approximate minimizer that is often within a few percent of the global minimum. The approach sometimes predicts exact lattice minimizers, and generates a dual decomposition for the energy landscape that leads to the emergence of new preferred low energy length scales.

AMNEET PAL SINGH BHALLA

The University of North Carolina at Chapel Hill

Immersed Boundary Method for Cardiovascular Applications

The immersed boundary method is an approach to solving coupled fluid-structure interaction (FSI) equations on the same computational grid and without employing mesh conforming discretizations. Ever since its introduction in 1970's by Peskin to model blood flow through mammalian heart, explicit version of IB method has become a standard tool to handle FSI in various biological applications involving elastic membranes. In the limit of high stiffness, the explicit IB method suffers from severe timestep size restriction. In this work, we extend the original IB method to model FSI for rigid bodies by solving for distributed Lagrange multipliers along with fluid velocity and pressure, and also present our recent work on developing scalable solvers for implicit discretization of the IB method. These extensions will eventually lead to model cardiovascular components testing devices, such as pulse duplicator devices, that have both rigid and stiff elastic structures in a unified framework. Some cardiovascular applications in this regard will be presented.

Advisor: Boyce E. Griffith (UNC)

RUI CAO

New Jersey Institute of Technology

A Hybrid Numerical Method for Electro-Osmotic Flow with Deformable Interfaces

When a drop or vesicle is suspended in a viscous electrolyte and a direct current (D.C.) electric field is applied, the drop interface or vesicle membrane and the suspending fluid are driven into motion. This occurs due to the attraction and repulsion of ions, which causes a thin diffuse charge double layer to form adjacent to an interface that is called a 'Debye layer'. The electric field exerts a force on the charge inside the Debye layer. This force together with interfacial surface tension or the elastic properties of the membrane govern the deformation and fluid motion.

By taking into account the ion concentration and related governing equations, we construct a model that describes the evolution of the drop interface or vesicle membrane. This combines an asymptotic analysis of the Debye layers with the boundary integral method for determining the fluid velocity and electrostatic potential, and leads to an accurate and efficient numerical method for solving this nonlinear moving boundary problem.

Advisors: Michael Booty and Michael Siegel (NJIT)

NAN CHEN

NYU - CIMS

Filtering Nonlinear Turbulent Dynamical Systems through Conditional Gaussian Statistics

A conditional Gaussian framework for filtering complex turbulent systems is introduced. Despite the conditional Gaussianity, such systems are nevertheless highly nonlinear and are able to capture the non-Gaussian features of nature. The special structure of the filter allows closed analytical formulae for updating the posterior states and is thus computationally efficient. An information-theoretic framework is developed to assess the model error in the filter estimates. Three types of applications in filtering conditional Gaussian turbulent systems with model error are illustrated. First, dyad models are utilized to illustrate that ignoring the energy-conserving nonlinear interactions in designing filters leads to significant model errors in filtering turbulent signals from nature. Then a triad (noisy Lorenz 63) model is adopted to understand the model error due to noise inflation and underdispersion. It is also utilized as a test model to demonstrate the efficiency of a novel algorithm, which exploits the conditional Gaussian structure, to recover the time-dependent probability density functions associated with the unobserved variables. Furthermore, regarding model parameters as augmented state variables, the filtering framework is applied to the study of parameter estimation with detailed mathematical analysis. A new approach with judicious model error in the equations associated with the augmented state variables is proposed, which greatly enhances the efficiency in estimating model parameters. Other examples of this framework include recovering random compressible flows from noisy Lagrangian tracers, filtering the stochastic skeleton model of the Madden-Julian oscillation (MJO) and initialization of the unobserved variables in predicting the MJO/Monsoon indices.

Advisor and Collaborator: Andrew J. Majda (NYU – CIMS)

SUNIL DHAR AND YALIN ZHU

New Jersey Institute of Technology

Multivariate Logistic Type Models Based on Inverse Sampling Scheme

Discrete or count data arises in the biomedical or health care experiments naturally. The outcome variables of interest are the number of rare events. A widely used model for categorical data analysis is the multinomial logistic regression model. Negative multinomial models and extended negative multinomial or generalized inverse sampling scheme are used when at least one distinct rare event categories are observed. The new model based on this generalized inverse sampling scheme for several rare events is developed. The natural log of the ratio of the expected response appears similar to the multinomial logistic model under the inverse sampling scheme. Based on the response events relative to a rare event, the maximum likelihood estimator can be computed by creating score equations and the Hessian matrix of the likelihood. The covariance matrix for the new model is obtained for developing the inference by inverting the Hessian matrix.

CASEY DIEKMAN

New Jersey Institute of Technology

Entrainment Maps: A New Tool for Understanding Properties of Circadian Oscillator Models

Circadian oscillators found across a variety of species are subject to periodic external light-dark forcing. We have developed a new tool called an entrainment map to assess whether, and at what phase, a circadian oscillator entrains to the external forcing. This is a one-dimensional map that can be determined analytically, and numerically, by understanding the underlying phase space structure of the circadian oscillator. Using the map, we are able to determine conditions for existence and stability of phase-locked solutions. In addition, we consider the dependence on various parameters such as the photoperiod and intensity of the external light as well as the mismatch in intrinsic oscillator frequency with the light-dark cycle. We show that the entrainment map yields more accurate predictions for phase locking than methods based on the phase response curve. The map also gives insight into the amount of time required to achieve entrainment as a function of initial conditions, the bifurcation of stable and unstable periodic solutions that leads to loss of entrainment, and the complicated dynamics that occur just beyond the range of entrainment.

Collaborator: Amitabha Bose (NJIT)

SZU-PEI FU

New Jersey Institute of Technology

Coarse-grained Molecular Dynamics Simulations of Lipid Bilayer Membrane

Lipid bilayer membranes have been extensively studied by coarse-grained molecular dynamics (CGMD) simulations, where several lipids are coarse-grained into a particle of size 4~6 nm. Yuan et al. proposed a pair-potential between these coarse-grained lipid particles to capture the mechanical properties of a lipid bilayer membrane (such as gel-fluid-gas phase transitions of lipids and bending rigidity). In this work both explicit and implicit solvent CGMD simulations are performed. The explicit-solvent model uses Lennard-Jones (L-J) potential to account for hydrodynamic interactions (HIs) and His are incorporated via Rotne-Prager-Yamakawa (RPY) tensor in implicit solvent approach. We also consider the effects of cytoskeleton on the lipid membrane dynamics as a model for red blood cell (RBC) dynamics. To demonstrate that the proposed methods can capture observed dynamics of vesicles and RBC, we focus on two sets of studies: 1. Vesicle shape transitions with varying enclosed volume; 2. RBC shape transitions with different enclosed volume.

Advisors: Yuan-Nan Young and Shidong Jiang (NJIT)

SHUYUE MIKI HAN

New Jersey Institute of Technology

A New Defibrillation Mechanism: Termination of Reentrant Waves by Propagating Action Potentials Induced by Nearby Heterogeneities

Introduction. Recently, there has been a major effort to develop new, low-energy defibrillation methods. These methods would be less damaging and less traumatic for the patient, and would save battery energy. However, these methods have not been entirely successful, due in part to an incomplete understanding of all the mechanisms present that may help or hinder the process of terminating the rotating waves present during fibrillation. Here we describe a new mechanism whereby a far-field electric field pulse terminates waves that are rotating in the vicinity of a blood vessel, plaque deposit or other heterogeneity in the gap junction conductivity.

Method and Results. We ran a series of two-dimensional computer simulations based the Barkley model of the excitable electrical dynamics of the heart. The parameters used (a = 0.6, b = 0.075), put the simulations in the regime of stably rotating spiral waves, between the sub-excitation and meandering spiral wave regimes. A rotating spiral wave was initiated in the vicinity of a non-conducting obstacle representing the heterogeneity. Conditions mimicking the application of an electric field pulse caused a semicircular action potential wave to be launched from the heterogeneity. The interaction of this wave with the rotating wave resulted in termination of all wave activity.

Conclusion: These simulations demonstrate a new mechanism by which a low-energy electric field pulse can interact with structures within cardiac tissue to terminate the reentrant waves associated with fibrillation. The mechanism studied here only requires the spiral wave to be nearby, but not necessarily, pinned to an obstacle, and thus extends the effectiveness of the electric field pulses used in low-energy defibrillation. Consideration of this mechanism alongside those already discovered could result in the development of improved, low-energy defibrillation protocols.

Advisor and Collaborator: Niels Otani (RIT)

Collaborators: Valentin Krinski and Stefan Luther (Max Planck Institute for Dynamics and Self-Organization)

GAL HASPEL

New Jersey Institute of Technology, Department of Biological Sciences

A Model of the C. Elegans Locomotion Network Demonstrates Multiple Solutions for the Distribution of Oscillators that Produce Coherent Undulatory Motor Output

Neuronal oscillators underlie rhythmic behavior, and particularly locomotion, in all animals in which the neural mechanism has been determined. Caenorhabditis elegans is the only animal for which an organism-level connectome exists; yet it is unknown how its nervous system generates locomotor behavior. The original electron micrographic dataset is incomplete, but we recently described an extrapolated and complete neuromuscular network that spans the full length of an animal and includes all motoneurons, muscles, and chemical and electrical synapses. The output of the network is the activity pattern of the muscle cells, which can be directly interpreted as body curvature.

We developed an ordinary differential equations model of the locomotion circuit and populated the model with two kinds of nodes: passive (for non-oscillatory motoneurons and muscle cells) and oscillating (for autonomously oscillating motoneurons). In the most extreme cases, the motoneurons were either all passive or all oscillating. We systematically assayed all 128 combinations of the seven motoneuron classes being oscillatory. For each distribution of oscillators we optimized synaptic parameters for the network simulation to try to produce a propagating dorsoventral alternation of muscular activity in forward or backward directions. Several distributions have produced undulatory-like motor programs in both forward and backward directions.

Collaborators: Haroon Anwar, Jordan Storms, Antonio Jurko, Casey Diekman, and Gal Haspel

(Department of Mathematical Sciences and Department of Biological Sciences, New Jersey Institute of Technology)

DAVID HORNTROP

New Jersey Institute of Technology, Department of Biological Sciences

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

Much recent research on modeling and optimization of servicing costs for Non-Renewing Free Replacement Warranties (NR-FRW) assumes that a consumer's usage profile is constant and known. Such an assumption is unrealistic for moderately high value consumer durables. In such cases, it would be pragmatic to assume that the manufacturer/seller is uncertain about any customer's usage rate of the product; the usage rate is modeled by a probability distribution of the usage for target customers. This research seeks to model and minimize the expected costs of pragmatic servicing strategies for NR-FRW warranties, using a Copula based approach to capture the adverse impact of increasing product usage rate on its time-to-failure. Since exact analytical solutions to these models are typically not obtainable, numerical methods using MATLAB and the Simulated Annealing algorithm for globally optimal cost minimization are used for computational solution. These methods and results are compared with those obtained from a well-known benchmark numerical example and then new results are derived.

Collaborator: Sonia Bandha (D&B)

JIANJUN HUANG

Worcester Polytechnic Institute

Studying the Flagellum Motility Near a Wall by Using Regularized Singularities

Method of regularized singularities with images for modeling flagellar motility is presented. The technique is used to study the concentration phenomenon of microorganisms near a surface.

Advisor: Sarah Olson (WPI)

EMEL KHAN

New Jersey Institute of Technology

Investigating Frequency Preferences of Chemical Systems in Response to Periodic Forcing

Oscillatory chemical reactions where the reactants concentration changes periodically, such as the Belousov-Zhabotinsky (BZ) reaction, are prototypical examples of nonlinear oscillators. How these systems interact with oscillatory inputs is not well understood. In this study, we investigate the frequency preference responses models of chemical reactions to periodic inputs. We use three canonical models: the Brusselator, the Oregonator and Lengyel Epstein models. We explore three different regimes of the unforced models: sustained oscillations (a stable limit cycle), damped oscillations (a stable focus), and non-oscillatory behavior (a stable node). Sustained oscillations can be either in small or large amplitude regimes(SAO and LAO, respectively).We vary the strength (A) and frequency (f) of the forcing signal and characterize concentration of the responses using concentration profile(curves of concentration amplitude versus the input frequency f) and Arnold Tongues to identify the entrainment properties in the A-f parameter space. Our results pave the way for the analysis of more complex biochemical systems such as the cyanobacterial circadian clock.

Advisors and Collaborators: Horacio G. Rotstein and Casey O. Diekman (NJIT)

LENKA KOVALCINOVA

New Jersey Institute of Technology

Scaling Properties of Force Networks for Compressed Particulate Systems

We consider, computationally and experimentally, the scaling properties of force networks in the systems of circular particles exposed to compression in two spatial dimensions. The simulations consider polydisperse and monodisperse particles, both frictional and frictionless, and in experiments we use monodisperse and bi-disperse frictional particles. While for some of the considered systems we observe consistent scaling exponents describing the behavior of the force networks, we find that this behavior is not universal. In particular, we find that frictionless systems, independently of whether they partially crystallize under compression or not, show scaling properties that are significantly different compared to the frictional disordered ones. The findings of non-universality are confirmed by explicitly computing fractal dimension for the considered systems. The results of the physical experiments are consistent with the results obtained in simulations of frictional disordered systems.

Advisor and Collaborator: Lou Kondic (NJIT)

Collaborator: Arnaud Goullet (NJIT)

MICHAEL LAM

New Jersey Institute of Technology

Breakup of Partially Wetting Thin Nematic Liquid Crystal Film

We consider very thin (less than a micrometer) nematic liquid crystal (NLC) on a horizontal substrate, focusing on the breakup up of partially wetting films. Particular attention is paid to the interplay between the bulk elasticity and the anchoring (boundary) conditions at the substrate and free surface. Numerical simulations of a perturbed at film show that, depending on the initial average thickness of the film, satellite droplets form and persist on time scales much longer than dewetting. Formulating the model in terms of a structural disjoining pressure (elastic response and van der Waals interaction), simulations further suggest that satellite droplets form when the initial average thickness corresponds to a positive structural disjoining pressure.

Advisor and Collaborator: Linda Cummings (NJIT)

Collaborators: T.-S. Lin and Lou Kondic (NJIT)

PILHWA LEE

University of Michigan

Physical Mechanisms of Cancer in the Transition to Metastasis

Whether a tumor is metastatic is one of the most significant factors that influence the prognosis for a cancer patient. The transition from a non-metastatic tumor to a metastatic one is accompanied by a number of genetic and proteomic changes within the tumor cells. These protein-level changes conspire to produce behavioral changes in the cells: cells that had been relatively stationary begin to move, often as a group. Here we ask the question of what cell-level biophysical changes are sufficient to initiate evasion away from an otherwise static tumor. We use a mathematical model developed to describe the biophysics of epithelial tissue to explore this problem. The model is first validated against in vitro wound healing experiments with cancer cell lines. Then we consider the behavior of a group of mutated cells within a sea of healthy tissue. We find that moderate increases in cell-ECM adhesion accompanied by a decrease in cell-cell adhesion and/or Rho family of small GTPase activation can cause a group of cells to break free from a tumor and spontaneously migrate. This result may explain why some metastatic cells have been observed to up-regulate integrin, down-regulate cadherin and activate Rho family signaling.

Collaborator: Charles Wolgemuth (University of Arizona)

YOONSANG LEE

NYU – CIMS

Preventing Catastrophic Filter Divergence Using Adaptive Additive Inflation for Baroclinic Turbulence

Ensemble based filtering or data assimilation methods have proved to be indispensable tools in atmosphere and ocean science as they allow computationally cheap, low dimensional ensemble state approximation for extremely high dimensional turbulent dynamical systems. For sparse, accurate and infrequent observations, which are typical in data assimilation of geophysical systems, ensemble filtering methods can suffer from catastrophic filter divergence which frequently drives the filter predictions to machine infinity. A two-layer quasi-geostrophic equation which is a classical idealized model for geophysical turbulence is used to demonstrate catastrophic filter divergence. The mathematical theory of adaptive covariance inflation by Tong et al. and covariance localization are investigated to stabilize the ensemble methods and prevent catastrophic filter divergence. Two forecast models, a coarse-grained ocean code, which ignores the small-scale parameterization, and stochastic superparameterization (SP), which is a seamless multi-scale method developed for large-scale models without scale-gap between the resolved and unresolved scales, are applied to generate large-scale forecasts with a coarse spatial resolution 48x48 compared to the full resolution 256x256. The methods are tested in various dynamical regimes in ocean with jets and vorticities, and catastrophic filter divergence is documented for the standard filter without inflation. Using the two forecast models, various kinds of covariance inflation with or without localization are compared. It shows that proper adaptive additive inflation can effectively stabilize the ensemble methods without catastrophic filter divergence in all regimes. Furthermore, stochastic SP achieves accurate filtering skill with localization while the ocean code performs poorly even with localization.

Advisor and Collaborator: Andrew Majda (NYU - CIMS)

Collaborator: Di Qi

RANDOLPH LEISER

New Jersey Institute of Technology

Network Response to Periodic Inputs

Human pancreatic beta cells are located within the pancreas and are responsible for producing the hormone insulin. They are found in clusters of endocrine cells known as the Islets of Langerhans. Despite being a heterogeneous population, all beta cells within an islet as well as all islets synchronize in phase. The goal of this project was to investigate what role this heterogeneity, or differences, between the cells' properties plays in their function when the cells are electrically coupled with a gap junction. Different cells will respond differently to unique inputs, and this response can be better or worse depending on the scenario (e.g. insulin production activity). We have looked at a minimal network of electrically coupled cells and examined how differences in their parameter values affect the attributes of the network response to periodic input. The simplicity of the model allowed us to directly see the effects of parameter variation by examining the analytic solution. However, when multiple copies of a model are involved, the analysis becomes more complex. To understand the underlying dynamic mechanisms, we used dynamical systems tools (phase-plane analysis), noting how parameter changes move the nullclines and how these movements interact to produce the observed behavior.

Advisor: Horacio G. Rotstein (NJIT)

FRANCISCO MARTINEZ

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Breather Solutions for a Model Type FPU Using Birkhoff Normal Forms and Applications in Biomolecules

We present results on spatially localized oscillations in some inhomogeneous nonlinear lattices of Fermi-Pasta-Ulam (FPU) type derived from phenomenological nonlinear elastic network models used in the study of protein vibrations. The main feature of the FPU lattices we study is that the number of interacting neighbors varies from site to site, and we see numerically that this spatial inhomogeneity leads to spatially localized normal modes in the linearized problem. This property is seen in 1-D models, as well as a 3-D models obtained from protein data. The spectral analysis of these examples suggests some non-resonance assumptions that can be used to show the existence of invariant subspaces of spatially localized solutions in Birkhoff normal forms. We also study some periodic orbits on these subspaces and show some results of integration.

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VICTOR MATVEEV

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A Novel Approximation Method for Single-Channel Ca2+ Nanodomains

Localized calcium (Ca2+) signals control some of the most fundamental physiological processes, including synaptic transmission as well as its activity-dependent plasticity. Computational and mathematical modeling played a crucial role in the understanding of spatio-temporal Ca2+ dynamics that drives these processes, and showed that Ca2+ concentration around a single Ca2+ channel reaches a quazi-equilibrium distribution (known as the Ca2+ "nanodomain") within about 10 microseconds after the opening of the channel, and collapses as rapidly after the closing of the channel. Such localization of Ca2+ in time and space is achieved by its rapid diffusion as well as its binding to its multiple interaction partners collectively called Ca2+ buffers and Ca2+ sensors. One of the successes of mathematical modeling was the development of several analytic approximations describing the equilibrium concentration of Ca2+ as a function of distance from the open Ca2+ channel, such as the Rapid Buffering Approximation (RBA) and the Linear Approximation (LA). Each of these approximations has a particular applicability parameter regime created by the interplay between the properties of Ca2+ buffers, in particular their mobility and Ca2+ binding rates, and the strength of the Ca2+ current. Here we present a novel approximation method which does not require a particular range of the relevant Ca2+ and buffer parameters, and is based on matching the low-distance and large-distance asymptotic behavior of the concentration function. Even at low orders, the resulting approximation is as accurate as previously developed asymptotic approximations for a wide range of modeling parameters, but its validity extends beyond the parameter range of applicability of RBA and LA. The usefulness of the resulting approximation is two-fold: first, together with the previously developed approximations, the novel method provides a deeper intuition into the dependence of Ca2+ nanodomain properties on the relevant buffering parameters, and second, it constitutes an efficient numerical tool in the modeling of the Ca2+ signals underlying presynaptic and postsynaptic phenomena.

ALI MEHDIZADEHRAHIMI AND AMIR MOLAVI

Northeastern University

Nonlocal Theory and Multiscale Nonlinear Boundary Condition for Continuum Models of Biomolecular Electrostatics

Electrostatic interactions between biomolecules and the surrounding aqueous media play an important role in biological processes. Implicit-solvent models consider the problem as a continuum media made of two regions with different dielectric constants. These standard continuum models are faster than atomistic molecular-dynamics simulations, however, they are unable to grasp some important physics of the problem such as, 1) the effects of the first layers of the solvent (the hydration shell) which do not behave like a bulk material, 2) asymmetrical response of the standard Poisson-Boltzmann model to the sign change of the applied field, and, 3) nonlocal behavior of dielectric function of water molecules in small length scales. In this research, we improved the traditional continuum models, by defining a nonlinear boundary condition, to address the effects of the hydration shell. We also utilized the nonlocal dielectric theory accompanying with BEMPP boundary element solver to calculate the electrostatic potentials more precisely.

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ENSELA MEMA

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Flexoelectric Effects in a Freedericksz Transition Cell

The Freedericksz transition is an important phenomenon that occurs in a nematic liquid crystal (NLC) layer confined between two parallel bounding plates, across which an external field is applied. It is observed that at low field strengths the NLC molecules align parallel to the bounding plates throughout the layer. As the field strength is increased a transition occurs to a nontrivial molecular configuration in which the molecules align partially with the applied field in the interior of the layer while aligning parallel to the plates at the boundaries. At yet higher field strengths the molecules align parallel to the electric field everywhere. We investigate these transitions mathematically, particularly focusing on the influence of the flexoelectric effect, which previous studies neglected but which may significantly affect the transitions.

Advisor: Linda J. Cummings (NJIT)

NAGA ADITYA MUSUNURI

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Fluid Dynamics of Hydrophilous Pollination

The aim of this work is to understand the physics underlying the mechanisms of two-dimensional aquatic pollen dispersal, known as hydrophily, that have evolved in several genera of aquatic plants, including Halodule, Halophila, Lepilaena, and Ruppia. We selected Ruppia maritima, which is native to salt and brackish waters circumglobally for this study. We observed two mechanisms by which the pollen released from male inflorescences of Ruppia is adsorbed on a water surface: 1) inflorescences rise above the water surface and after they mature their pollen mass falls onto the surface as clumps and disperses as it comes in contact with the surface; 2) inflorescences remain below the surface and produce air bubbles which carry pollen mass to the surface where it disperses. In both cases dispersed pollen masses combined with others under the action of lateral capillary forces to form pollen rafts. The formation of porous pollen rafts increases the probability of pollination since the attractive capillary force on a pollen raft toward a stigma is much larger than on a single pollen grain. The presence of a trace amount of surfactant can disrupt the pollination process as the pollen is not captured or transported on the water surface.

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PEJMAN SANAEI

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Investigating the Performance of Pleated Membrane Filters

Pleated membrane filters are widely used in many applications, and offer significantly better surface area to volume ratios than equal area unpleated membrane filters. However, their filtration characteristics are markedly inferior to those of equivalent unpleated membrane filters in dead-end filtration. While several hypotheses have been advanced for this poor performance, one possibility is that the flow field induced by the pleating leads to spatially nonuniform fouling of the filter, which in turn affects performance. We investigate this hypothesis by developing a simplified model for the flow and fouling within a pleated membrane filter. Our model accounts for the pleated membrane geometry (which affects the flow), for porous support layers surrounding the membrane, and for two membrane fouling mechanisms: (i) adsorption of very small particles within membrane pores; and (ii) blocking of entire pores by large particles. We use asymptotic techniques based on the small pleat aspect ratio to solve the model, and we compare solutions to those for the closest-equivalent unpleated filter.

Advisor: Linda Cummings (NJIT)

MICHAEL SENTER

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A Model of Muscle Response to Neuronal Spike Activity

An important component of locomotion is sensing the environment and reacting appropriately to it. The nervous system actuates and controls this movement. A model was developed to investigate how spike-train signals from a motor neuron results in dynamic force generation in muscle. With the help of this model, relationships between spike-train frequency, intracellular calcium dynamics in muscle, and force generation were investigated. This model can be coupled with a model of locomotion. A potential application of this model can be made to the control of muscles attached to an inverted pendulum, such as has been used in modeling insect walking.

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Collaborator: Katie Newhall (UNC-CH)

IVANA SERIC

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Direct Computations of Marangoni-Induced Flows Using a Volume of Fluid Method

The volume of fluid (VOF) interface tracking methods have been used for simulating a wide range of interfacial flows. An improved accuracy of the surface tension force computation has enabled the VOF method to become widely used for simulating flows driven by the surface tension force. We present a new method for including variable surface tension in a VOF based Navier-Stokes solver. The tangential gradient of the surface tension is implemented using an extension of the classical continuum surface force model that has been previously used for constant surface tension simulations. Our method can be used for computing the surface gradients of surface tension that is temperature or concentration dependent.

Advisors: Shahriar Afkhami and Lou Kondic (NJIT)

BALJEET SINGH

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Reflection of Thermoelastic Waves at a Non-Free Thermally Insulated Surface

Sinha and Sinha (J. Phys. Earth, 22, 237–244, 1974) studied a problem on reflection of thermoelastic waves at a stress free thermally insulated solid half-space in context of Lord and Shulman theory of generalized thermoelastcity. He showed the existence of three plane waves (two longitudinal and a shear) in a homogeneous, linear and isotropic thermoelastic medium. He also obtained reflection coefficients of reflected waves theoretically and numerically for incident plane waves. However, the boundary surface may be non-free with various constraints in actual engineering problems. In the present paper, a problem on reflection of thermoelastic waves at a non-free surface is considered. The non-free surface is modeled as a surface with distributed elastic constraint or support. Each mass point at the surface is subjected to the normal and tangential translation constraint. The reflection coefficients of various reflected waves are obtained for new boundary conditions at non-free surface. For a particular numerical example, the reflection coefficients are also computed and shown graphically against the angle of incidence for different boundary parameters.

JEFFREY SLEPOI

Montclair State University

Numerical Detection of Wave-Breaking in the Short Pulse Equation

The Short-Pulse Equation (SPE) is a model for ultra-short optical pulses. Pulse solution of the SPE provides analytical tools to determine existence of the break and its timing. Numerical analysis of the pattern of Fourier coefficients over time allows to accurately determine the break. Same technique can be used for other initial conditions (IC) which don't have an analytical solution. Modified Gaussian IC has a wide analytical parameter gap between well-posedness and wave-breaking. Established numerical method is used to significantly diminish the gap to almost a border line.

Advisor: Dr. A. David Trubatch (MSU)

YIBELTAL TEREFE

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Global Stability for Continuous and Discrete SIS-Diffusion Epidemiological Models

The classical SIS system is extended into a reaction-diffusion equation to model the spatial spread of a disease. It is shown that the disease-free equilibrium (DFE) is globally asymptotically stable (GAS) when the basic reproduction number R0 is less than or equal to 1; it is unstable when R0>1. In the latter case, there appears an endemic equilibrium (EE) which is GAS. On the other hand, we construct nonstandard finite difference schemes which theoretically and computationally replicate these stability properties of the equilibria.

Advisor: Jean Lubuma (University of Pretoria)

ROSA MARIA VARGAS-MAGAÑA

Universidad Nacional Autónoma de México (UNAM)

A Whitham-Boussinesq Long-Wave Model for Variable Topography

We study the propagation of water waves in a channel of variable depth using the long-wave asymptotic regime. We use the Hamiltonian formulation of the problem in which the non-local Dirichlet-Neumann operator appears explicitly in the Hamiltonian, and propose a Hamiltonian model for bidirectional wave propagation in shallow water that involves pseudo-differential operators that simplify the variable-depth Dirichlet-Neumann operator. The model generalizes the Boussinesq system, as it includes the exact dispersion relation in the case of constant depth.

A numerical approach based on Galerkin Fourier discretization is developed to evaluate the nonlocal term, and numerical results are shown to demonstrate that the spectrum of the corresponding linear operator is physically relevant for a set of bottom profiles. Finally, time-evolving simulations are conducted to test the overall performance of the long-wave model. Numerical integration also suggests that the constant depth nonlocal Boussinesq model can capture qualitative features of the evolution obtained with higher order approximations of the Dirichlet-Neumann operator.

Advisor and Collaborator: Panayotis Panayotaros (IIMAS - UNAM)

SHAOBO WANG

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A High Order Integral Equation Method for Solving the Heat Equation with Complex Geometries in Three Dimensions

We show that a high order integral equation method can be constructed for solving the heat equation with complex geometries in three dimensions. Specially the heat kernel can be approximated by an efficient separated sum-of-exponentials. Surface integral with singularity can be solved with spectral order of accuracy. We can achieve 9-10 digits accuracies for solving the heat equation in three dimensions. The algorithms can be parallelized in a straightforward manner. Several numerical examples are presented to illustrate the accuracy and stability of these approximations.

Advisor and Collaborator: Shidong Jiang (NJIT)

Collaborator: Jing Wang

SHUOLUN WANG

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Modeling Soft Dielectric Viscoelastomers with Application to Electromechanical Instabilities

Soft dielectric materials undergo large deformations in response to an electric field, which has garnered significant attention as a smart active material. Applications of these materials are varied, and include actuators that convert an applied electric field into mechanical motion, and energy harvesting devices that convert mechanical input into electrical energy and medical devices. However, it has been experimentally shown that these materials suffer from electro-mechanical instabilities that are still not well known. They include pull-in, creasing, and cavitation, all of which are caused by coupling between large deformation and electric field. Depending on the application, such instabilities may be desired, or may lead to catastrophic failure. Our work aims to elucidate the onset of these electro-mechanical instabilities in the presence of inelastic effects by 1) developing finite element formulations for electro-mechanically coupled behavior, 2) modeling VHB4910, a soft dielectric material widely used in industry, and 3) numerical simulations of pull-in, creasing, and cavitation with the purpose of understanding when they occur.

Advisor and Collaborator: Shawn Chester (NJIT)

Collaborator: Bosnjak, Nikola Srdjan (Group Member)

ARJUN YADAW

Icahn School of Medicine at Mount Sinai

A Comprehensive, Multi-Scale Dynamical Model of Cannabinoid (CB1) Receptor Regulated Neurite Outgrowth

The outgrowth of neurites is a complex whole cell level process by which a neuron starts to acquire the morphological and functional capability for information transmission over a long distance. Such a change in cellular state depends on the coordinated functioning of multiple sub-cellular processes at different levels. A major question is how these subcellular processes act in a coordinated manner to produce this whole cell response.

To identify the sub cellular processes associated with neurite outgrowth, Neuro 2A cells were stimulated with the CB1 cannabinoid receptor agonist with HU210 for multiple time points (2h,4h,6h and 8h), followed by RNA-seq to identify HU2010 triggered differentially expressed genes. The up regulated genes were subjected to Gene Ontology enrichment analysis to predict up regulated sub cellular processes that they belong to. Among the inferred subcellular processes are vesicular transport, microtubule organization and elongation and membrane lipid metabolism.

Based on these inferences, we built a dynamical multicompartment ODE model that integrates models of membrane production at the cell body, membrane delivery to the axonal tip via microtubule based vesicular transport and axonal microtubule growth. We predicted that such a large-scale model should simulate neurite-outgrowth and CB1 receptor stimulation of the processes. We find that we are able to simulate neurite outgrowth using the subcellular processes identified from the mRNA-Seq experiments and incorporating changes in the levels of proteins encoded by upregulated genes leads to significant increases in the rate of neurite outgrowth. Details of the simulations will be presented.

Advisor and Collaborator: Professor Ravi Iyengar (Icahn School of Medicine at Mount Sinai)

Collaborators: Jens Hansen, Mustafa Siddiq, Vera Rabinovich, Laura Thompson, and Julia Bond (Icahn School of Medicine at Mount Sinai)

YIMING YU

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Biased Monte Carlo Simulations to Compute Phase Slip Probabilities in a Mode-Locked Laser Model

We consider the probability that a mode-locked laser with active feedback will experience a phase slip when subjected to small-amplitude random perturbations such as amplified spontaneous emission noise generated by the gain medium. To quantify the likelihood of this rare event, we reduce the infinite-dimensional model to a finite-dimensional system of stochastic ordinary differential equations (SODE) and study optimal paths computed using the geometric minimum action method, including using these paths in biased Monte Carlo simulations.

Advisor: Richard O. Moore (NJIT)

YING ZHANG

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CAPM Model as Factor Model with Drawdown Measure

The CAPM model has been used for decades for portfolio optimization, and different risk measures yield different Beta of a portfolio. Conditional Drawdown-at-Risk (CDaR) is defined as average of specified percentage of the largest drawdowns over an investment horizon. The portfolio beta under this risk measure is well developed. However, less has been done on the CAPM factor model with CDaR. We investigate the CAPM model with one factor with CDaR. From this perspective, we fit the market data to this linear model and calculate the error. When minimizing the error, we get the same portfolio beta with this factor model as in the optimization problem. And more results will come from the multi-factor model with CDaR and replication of the market index.

Advisor: Michael Zabarankin (Stevens Institute of Technology)

YALIN ZHU

New Jersey Institute of Technology

Multiple Hypotheses Testing for Discrete Data

In applications such as studying drugs adverse events (AE) in clinical trials and identification of genes differentially expressed in microarray experiments, the experiments are usually conducted using control and study groups to detect the significant signals. In these kinds of experiments, the data consists of frequency counts. In the analysis of such data, researchers often face multiple hypotheses testing based on discrete test statistics. Incorporating this discrete property of specific data results in development of more powerful multiple testing procedures than traditional ones.

We propose several stepwise procedures controlling FWER, which allow to use the CDF of p-values to determine the testing threshold. We show that the proposed procedures strongly control the FWER and are more powerful than the existing ones for discrete data. Through some simulation studies and real data example, the proposed procedures are shown to outperform the existing procedures in terms of the FWER control and power. By using similar ideas, we modify the critical thresholds of Benjamini-Hochberg (BH) procedure, Benjamini-Yekutieli (BY) procedure and step down Romano-Shaikh (RS) procedure to develop more powerful FDR controlling procedures for discrete data. We also present simulation studies to compare the proposed procedure with BH procedure.

Advisor: Wenge Guo (NJIT)

ZHENTING ZOU

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Theoretical Basis for Attenuation of Ultrasound

Ultrasound has been used for non-destructive testing of cement based material since the 1940. This method is not only used to find out the bulk material properties but also to detect the microstructure and change in mechanical properties. Velocity and attenuation are commonly measured parameters of the non-destructive ultrasound test. For instance, the ultrasonic pulse velocity method is one of the most common NDT method for material characterization. However, its isolated use for predicting material strength is limited because there is no unique strength-velocity relationship. Pulse velocity itself is not sufficient to obtain a clear picture of intensity of damage as it is insensitive to micro cracks. On the other hand, attenuation of ultrasonic signal can be effectively used for damage studies as it is sensitive to micro cracks. High frequency ultrasound should be used in order to obtain quantitative information of the microstructure of the concrete. However, with higher the frequency, there is higher the attenuation and lower penetration depth. Attenuation refers to as the loss of sound energy when the ultrasonic beam passes through the material. Attenuation has two components, absorption and scattering. Scattering is the reflection of the wave in directions than its original direction of propagation. Absorption is the transfer of energy from ultrasound to the propagating medium, where it is transformed into a different form of energy, mostly heat. Energy can't crate or disappear, hence shock waves would be a possible explanation for this energy transfer. Ultrasound is a compress wave and the speed of sound depends on the material. When ultrasound travel from cement into air, the wave speed is suddenly slowed. But continuous application of ultrasound would continue sending sound waves to air compressing the air. This waves becomes steeper in front and less steep in back, until a shock wave is formed. Typically, a shock wave can be described using three conservation equations. By combine these conservation equations with the equation of the state, equations to describe the relation between the pressure, density, flow speed and temperature in front and behind the shock could be found. Based on these equations a mathematic model was developed to describe the shock wave propagate in an idealized 1-D model to explain the energy transfer from the sound energy to heat absorbed by the material.

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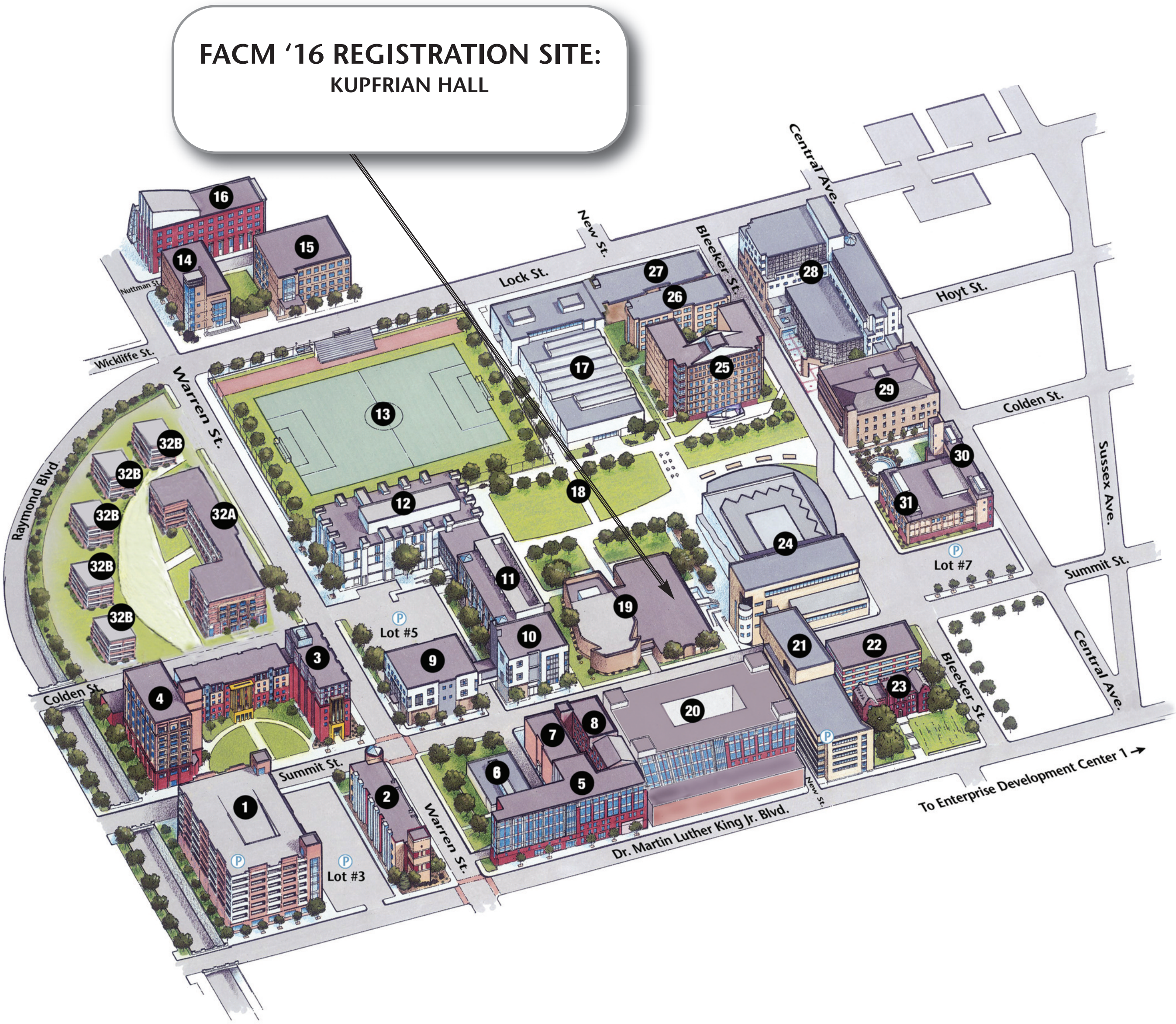
NOTES

NJIT CAMPUS MAP



1 CAMPBELL HALL/STUDENT SERVICES
2 YORK CENTER FOR ENVIRONMENTAL ENGINEERING AND SCIENCE
3 LAUREL RESIDENCE HALL
4 OAK RESIDENCE HALL
5 COLLEGE OF ARCHITECTURE AND DESIGN
6 SPECHT BUILDING
7 COLTON HALL
8 CAMPBELL HALL
9 ECE BUILDING
10 MICROELECTRONICS CENTER
11 FACULTY MEMORIAL HALL
12 TIERNAN HALL
13 LUBETKIN FIELD AT J. MALCOLM SIMON STADIUM
14 CHEN BUILDING
15 ENTERPRISE DEVELOPMENT CENTER 2
16 ENTERPRISE DEVELOPMENT CENTER 3
17 ESTELLE AND ZOOM FLEISHER ATHLETIC CENTER
18 THE GREEN:
19 KUPFRIAN HALL
20 CENTRAL KING BUILDING:
21 FENSTER HALL
22 CULLIMORE HALL:
23 EBERHARDT HALL/ALUMNI CENTER:
24 CAMPUS CENTER
25 CYPRESS RESIDENCE HALL:
26 REDWOOD RESIDENCE HALLS
27 NAIMOLI FAMILY ATHLETIC AND RECREATIONAL FACILITY
28 GUTTENBERG INFORMATION TECHNOLOGIES CENTER
29 MECHANICAL ENGINEERING CENTER
30 CENTRAL AVENUE BUILDING
31 VAN HOUTEN LIBRARY
32A ALBERT DORMAN HONORS COLLEGE
32B GREEK HOUSES

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