FACM '17

FRONTIERS IN APPLIED AND COMPUTATIONAL MATHEMATICS

New Jersey Institute of Technology
Newark, New Jersey
June 24 – 25, 2017

Program Guide a l d Abstracts

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

NJIT
New Jersey Institute
of Technology

ORGANIZING COMMITTEE

FRONTIERS IN APPLIED AND COMPUTATIONAL MATHEMATICS
NEW JERSEY INSTITUTE OF TECHNOLOGY
NEWARK, NEW JERSEY
JUNE 24 – 25, 2017

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Michael Booty

Linda Cummings

Casey Diekman

Yixin Fang

Brittany Froese

Shidong Jiang

Ji Meng Loh

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COMMITTEE STAFF

Alison Boldero

Amy Dougher

Fatima Ejallali

Pauline Ford

Michelle Llado-Wrzos

TABLE OF CONTENTS

FRONTIERS IN APPLIED AND COMPUTATIONAL MATHEMATICS

MESSAGE FROM THE ORGANIZING COMMITTEE

Welcome to Frontiers in Applied and Computational Mathematics 2017 (FACM '17). This is the fourteenth 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.

This year the focus is on industrial mathematics and statistics in industry, with the conference themes including applications in materials science, fluid dynamics, electromagnetics, mathematical biology, and modeling and statistical analysis for pharmaceutical applications.

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 the 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 and to 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: Michelle Llado-Wrzos, Fatima Ejallali, Alison Boldero, Amy Dougher and Pauline Ford.

FACM '17 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 fourteenth conference on Frontiers in Applied and Computational Mathematics (FACM). This year, rather than starting with a focus on specific scientific topics, the meeting addresses the question of how industry currently or potentially makes use of innovations in the mathematical sciences. This is, of course, a large and messy question to which we can hope for only limited and preliminary answers in the course of such a brief meeting. Yet we also hope that bringing together those who have an understanding of specific industrial problems with mathematical scientists expert in diverse mathematical methods and techniques will facilitate an exchange of ideas that might both advance science and enhance the effective fulfilment of human needs.

We are pleased this year to hold the majority of FACM events in the recently renovated Central King Building (CKB). These renovations were the largest single investment ($86.3 million) from New Jersey's 2013 Building Our Future Bond Act. We trust that the facilities will provide a comfortable setting for interaction and collaboration.

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 (the site each April of the Essex County Cherry Blossom Festival featuring over five thousand cherry trees), the Newark Museum (situated very close to the way from NJIT to the Robert Treat Hotel where 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. 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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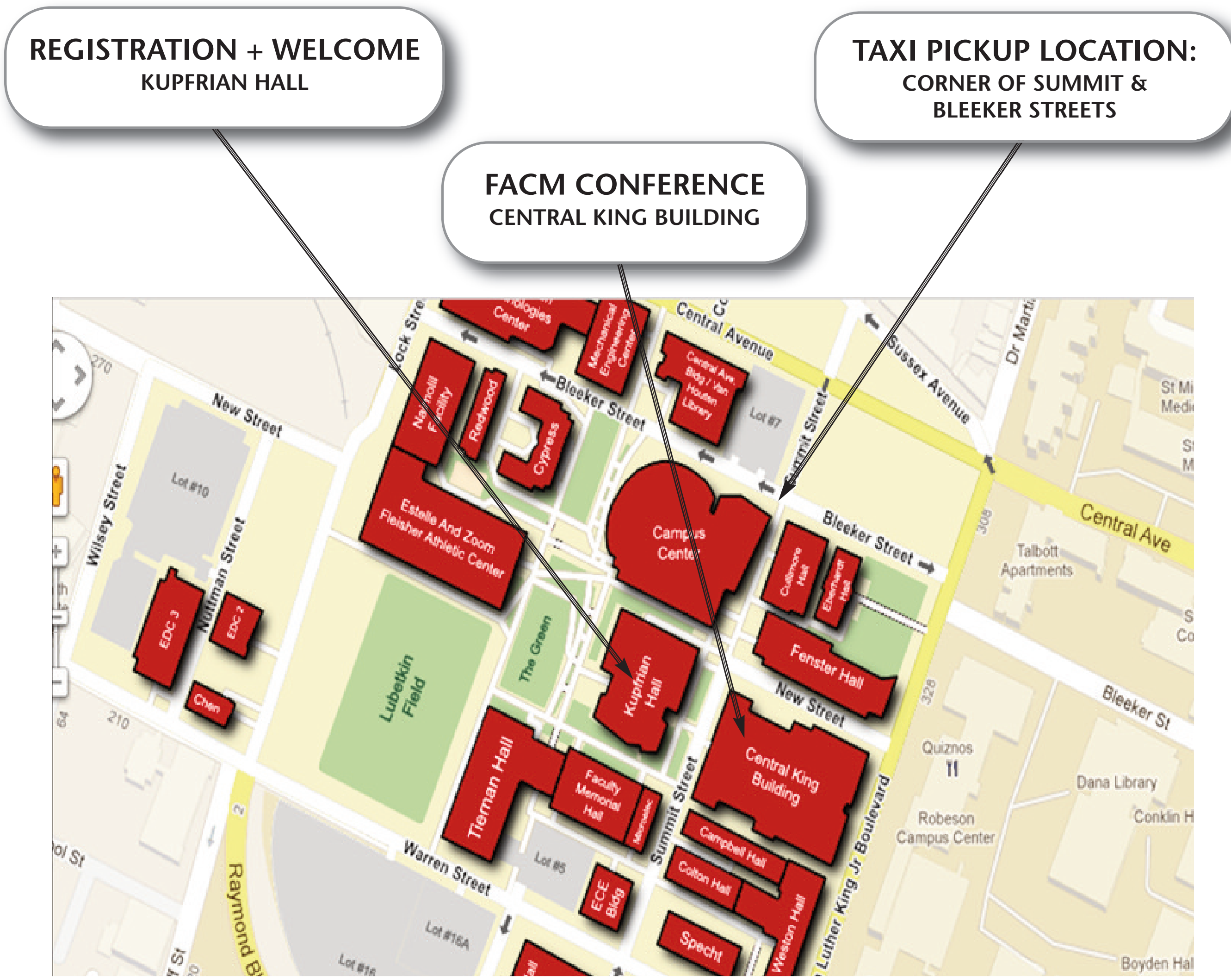
Telephone either one and request pick up at "NJIT campus, corner of Summit and Bleeker Streets." This is near the guard station at Parking Lot 7 by Cullimore Hall. If you plan to pay with a credit card instead of cash, tell them when you call because some drivers only accept cash.



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GUEST ACCESS TO THE NJIT NETWORK

JUNE 24 - 25, 2017

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): **guest649**

Password: **allegro53**

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 26, 2017.

PROGRAM SCHEDULE

SATURDAY, JUNE 24

Time	Event	Location
8:15 – 8:45 a.m.	Registration + Coffee/ Pastries	Kupfrian Hall, Theater Lobby
	Set Up Posters	CKB, Ground Floor Lounge (Lower Level)
8:45 – 9:00 a.m.	**Introductory Remarks**	Jim Wise Theater, Kupfrian Hall
	Jonathan Luke, Chairperson,	
	Department of Mathematical Sciences	
	Welcoming Remarks	
	Atam Dhawan, Vice Provost for Research, NJIT	
9:00 – 10:00 a.m.	**Plenary Lecture I**	
	Cleve Moler, MathWorks	Jim Wise Theater, Kupfrian Hall
	The Evolution of MATLAB	
10:00 – 10:30 a.m.	Coffee Break	CKB, 1st Fl. Lounge
10:30 – 1:00 p.m.	**Minisymposia I, II and III**	
1:00 – 2:15 p.m.	Lunch	CKB, 1st Fl. Lounge
	Poster Session	CKB, Ground Floor Lounge (Lower Level)
2:15 – 3:15 p.m.	**Plenary Lecture II**	CKB, Rm. 303
	Jon Chapman, University of Oxford	
	Mathematical Modelling of Lithium Ion Batteries	
3:15 – 3:45 p.m.	Coffee Break	CKB, 1st Fl. Lounge
3:45 – 6:15 p.m.	**Minisymposia IV, V, and VI**	
6:15 – 9:00 p.m.	**Cocktail Reception**	Eberhardt Hall, University Club
	Banquet	Eberhardt Hall, Rm. 112

PROGRAM SCHEDULE

SUNDAY, JUNE 25

Time	Event	Location
8:30 – 9:00 a.m.	Registration	CKB Study Lounge, Rm. 101
	Coffee/ Pastries	CKB, 1st Fl. Lounge
	Set Up Posters	CKB, Ground Floor Lounge (Lower Level)
9:00 – 10:00 a.m.	**Plenary Lecture III**	CKB, Rm. 303
	Gregory Luther, AOX Northrop Grumman	
	Business-Driven R&D: Leveraging Mathematical and Optical Science	
10:00 – 10:30 a.m.	Coffee Break	CKB, 1st Fl. Lounge
10:30 – 1:00 p.m.	**Minisymposia VII, VIII, and IX**	
1:00 – 2:00 p.m.	Lunch	CKB, 1st Fl. Lounge
	Poster Session	CKB, Ground Floor Lounge (Lower Level)
2:00 – 3:00 p.m.	**Plenary Lecture IV**	CKB, Rm. 303
	Jianying Hu, IBM T. J. Watson Research Center	
	Computational Health Methods for Next Generation Healthcare	
3:00 – 3:15 p.m.	Coffee Break	CKB, 1st Fl. Lounge
3:15 – 5:30 p.m.	**Minisymposia X, XI, and XII**	

PROGRAM EVENTS

SATURDAY MORNING

PLENARY LECTURE I

9:00 – 10:00 a.m.	**Cleve Moler,** MathWorks *The Evolution of MATLAB* Location: Jim Wise Theater, Kupfrian Hall

MINISYMPOSIA I, II, AND III

	Minisymposium I Mathematical Modeling of Membrane Filtration Location: CKB, Rm. 120 Chair: Ian Griffiths (University of Oxford)	**Minisymposium II** Application of Computational Biology Models, Algorithms and Data Science to Establish Proof of Mechanisms and Predict Therapeutic Response in Patient Subpopulations Location: CKB, Rm. 124 Co-Chairs: Ruth Abrams and Karim Azer (Sanofi)	**Minisymposium III** Data Science in Industry Location: CKB, Rm. 126 Chair: Yixin Fang
10:30 – 11:00 a.m.	**Ian Griffiths** University of Oxford *How Do Gradients in Porosity Make a Better Filter?*	(10:30 - 10:55 p.m.) **Avi Ma'ayan** Icahn School of Medicine at Mount Sinai *Mapping the Mammalian Gene Expression Space for Drug and Target Discovery*	**Howard Karloff** Goldman Sachs *Big Data Analytics and Modeling for Financial Institutional Compliance*
11:00 – 11:30 a.m.	**Uwe Beuscher** W.L. Gore & Associates, Inc. *Investigation of the Correlation Between Gas/Liquid Porometry and Particle Filtration Using Simple Network Models*	(10:55 - 11:20 a.m.) **Ruth Abrams** Sanofi *LIFE (Linear in Flux Expression methodology) Enables Modeling and Mechanistic Understanding of Patient Populations with Differential Responses to Therapy*	**Yang (Steve) Liu** KCG Holdings, Inc. *Application of Statistical Analysis on Signal Research*

Continued on next page

SATURDAY MORNING

MINISYMPOSIA I, II, AND III

11:30 – 12:00 a.m.	**Pejman Sanaei** NJIT *Internal Structure and Morphology Profile in Optimizing Filter Membrane Performance*	(11:20 - 11:45 a.m.) **Narges Razavian** NYU School of Medicine *Deep Learning in Healthcare: Biomarker Discovery and Predictive Modeling*	**Yushun Lin** Citi Cards *Statistics in Credit Card Marketing*
12:00-12:30 p.m.	**Sal Giglia** MilliporeSigma *Filtration Modeling for New Membrane Filter Development*	(11:45 - 12:10 p.m.) **Chanchala Kaddi** Sanofi *Quantitative Systems Pharmacology Model of Acid Sphingomyelinase Deficiency and the Enzyme Replacement Therapy Olipudase Alfa is an Innovative Tool for Linking Pathophysiology and Pharmacology*	**Samiran Ghosh** Wayne State University *Use of Historical Information via Bayesian Approach in Non-Inferiority Trial: With Application*
12:30-1:00 p.m.	**Armin Krupp** University of Oxford *Stochastic Modelling of Membrane Filtration*	(12:10 - 12:35 p.m.) **Marylens Hernandez** *LAM Therapeutics* *Expression-based Computational Drug Repurposing for Rare Diseases*	(12:30 - 12:50 p.m.) **Nan Chen** Courant Institute, New York University
		(12:35 - 1:00 p.m.) **Joon Ha** National Institutes of Health *A Mathematical Model Predicts a Delayed Insulin Peak During an Oral Glucose Tolerance Test as a High Risk Factor for Diabetes*	

SATURDAY AFTERNOON

PLENARY LECTURE II

2:15 – 3:15 p.m **Jon Chapman**, University of Oxford
Mathematical Modelling of Lithium Ion Batteries
Location: CKB, Rm. 303

MINISYMPOSIA IV, V, AND VI

	Minisymposium IV	Minisymposium V	Minisymposium VI
	Minisymposium IV Continuum Mechanics Problems at the Interface Between Academia and Industry Location: CKB, Rm. 120 Co-Chairs: Demetrios Papageorgiou and Darren Crowdy (Imperial College London)	**Minisymposium V** Optimal Transport with Industrial Applications Location: CKB, Rm. 124 Co-Chairs: Yuan-Nan Young and Brittany Froese	**Minisymposium VI** Mathematical Applications Supporting Research, Development and Cost-Effectiveness in the Pharmaceutical Industry Location: CKB, Rm. 126 Chair: Anna Georgieva Kondic (Merck)
3:45 – 4:15 p.m.	**Peter Buchak** LowReTech LLC *Fabrication of Specialty Optical Fibers*	**Emily Walsh** University of West England, UK *A Moving Mesh Method based on Optimal Transport for Numerical Weather Prediction*	**Nelson Lee Afanador** Merck & Co., Inc *A Descent into the Proximity Matrix of Unsupervised Random Forest*
4:15 – 4:45 p.m.	**Radu Cimpeanu** Imperial College London *Making a Splash: From High Speed Droplet Impact to a Novel Methodology for Water Retention Calculation*	**Emmanuel Maitre** Grenoble Institute of Technology *Constrained Optimal Transportation and Applications*	**Chris Penland** AstraZeneca Pharmaceuticals *A Quantitative Systems Pharmacology Model for Potassium Homeostasis with Applications to Late Stage Drug Development*

Continued on next page

SATURDAY AFTERNOON

MINISYMPOSIA IV, V, AND VI

4:45 – 5:15 p.m.	**Charles Maldarelli** Levich Institute and CCNY *Continuum and Molecular Dynamic Studies of the Hydrodynamics of Colloid Particles at a Fluid Interface*	**Yunan Yang** The University of Texas at Austin *Optimal Transport and the Quadratic Wasserstein Metric for Seismic Inversion*	**Helen Moore** Bristol-Myers Squibb *Optimal Control for Combination Therapy Optimization*
5:15 – 5:45 p.m.	**Ehud Yariv** Technion *Singular-Perturbation Analysis of Phoretic Self-Propulsion*	**Giulio Trigila** New York University *Data Driven Optimal Transport*	**Yuan Xiong** Certara Strategic Consulting *Time-To-Event Analysis to Support Clinical Study Design and Dose Justification in Drug Development*
5:45 – 6:15 p.m.			**David Turner** Merck & Co., Inc *Challenges with Pembrolizumab Exposure-Response Assessments*

SUNDAY MORNING

PLENARY LECTURE III

9:00 – 10:00 a.m	**Gregory Luther,** AOX Northrop Grumman *Business-Driven R&D: Leveraging Mathematical and Optical Science* Location: CKB, Rm. 303

MINISYMPOSIA VII, VIII, AND IX

	Minisymposium VII Low Reynolds Number Technologies: Theory & Applications Location: CKB, Rm. 120 Chair: Darren Crowdy (Imperial College London)	**Minisymposium VIII** Listening to the Heart and Brain: Current Challenges in Multiscale Modeling Location: CKB, Rm. 124 Co-Chairs: Tuan M. Hoang Trong and James Kozloski (IBM)	**Minisymposium IX** Computational Electromagnetics and Photonics Location: CKB, Rm. 126 Co-Chairs: Zydrunas Gimbutas (NIST) and Sharad Kapur (Integrand Software, Inc.)
10:30 - 11:00 a.m.	**Marc Hodes** Tufts University *Transport Phenomena on Superhydrophobic Surfaces*	(10:30 - 10:55 a.m.) **Tuan M. Hoang Trong** IBM Research *Challenges of Modeling Whole-Cell Neurons*	**Carlos Borges** The University of Texas at Austin *Reconstruction of a Compactly Supported Sound Profile In The Presence of Noisy Background Random Medium*
11:00 - 11:30 a.m.	**Alan Lyons** City University of New York *Multi-Functional Superhydrophobic Surfaces: From Singlet Oxygen Generation to Anti-Reflectivity*	(10:55 - 11:20 a.m.) **Kim "Avrama" Blackwell** George Mason University *Computational Approaches to Understanding Habit Learning and Parkinson's Disease*	**Zydrunas Gimbutas** National Institute of Standards and Technology *Modeling Scanning Microwave Impedance Spectroscopy*
11:30 - 12:00 p.m.	**Nicolas Hadjiconstantinou** MIT *On the Limits of Fourier's Law and Kinetic Extensions for Confined Solid-state Materials*	(11:20 - 11:45 a.m.) **Viatcheslav Gurev** IBM *Coupled Biophysical and Regression Models of Cardiac Electrophysiology and Mechanics*	**Sharad Kapur** Integrand Software, Inc. *Large-scale Electromagnetic Simulation for Radio Frequency Integrated Circuit Design*

Continued on next page

SUNDAY MORNING

MINISYMPOSIA VII, VIII, AND IX

12:00 - 12:30 p.m.	**Darren Crowdy** Imperial College London and NJIT *Theoretical Advances in Understanding Superhydrophobic Slip*	(11:45 - 12:10 p.m.) **Adam Ponzi** IBM Research *Striatal Network Modelling in Relation to Huntington's Disease*	**Mike O'Neil** Courant Institute, New York University *Electromagnetics and the Laplace-Beltrami problem*
12:30 - 1:00 p.m.		(12:10 - 12:35 p.m.) **James Kozloski** IBM Research *Modeling Relationships Between Clinical Progression and Circuit Dysfunction in Huntington's Disease*	**Manas Rachh** Yale University *High Order Layer Potential Evaluation in Three Dimensions Using Quadrature by Expansion (QBX)*
		(12:35 - 1:00 p.m.) **Stephen Krieger** Mount Sinai *The Topographical Model of Multiple Sclerosis*	

SUNDAY AFTERNOON

PLENARY LECTURE IV

2:00 – 3:00 p.m.	**Jianying Hu**, IBM T. J. Watson Research Center *Computational Health Methods for Next Generation Healthcare* Location: CKB, Rm. 303

MINISYMPOSIA X, XI, AND XII

	Minisymposium X Stochastic Modeling of Physical Systems Location: CKB, Rm. 120 Chair: Kyongmin Yeo (IBM)	**Minisymposium XI** Pharmaceutical Statistics Location: CKB, Rm. 124 Chair: Dai Feng (Merck) and Yixin Fang	**Minisymposium XII** Computational and Modeling Challenges Location: CKB, Rm. 126 Chair: Michael Booty
3:15 – 3:45 p.m.	**Minseok Choi** POSTECH *Model Reduction for Stochastic Fluid Flows: Time-Dependent Karhunen-Loeve Type Decomposition Methods*	**James Cai** Roche Innovation Center, NY *New Data and New Analytics in Pharmaceutical R&D*	**Aloknath Chakrabarti** Indian Institute of Science, Bangalore *The Role of Wiener-Hopf Technique in Problems of Scattering of Electromagnetic Waves by Multiple Scatterers*
3:45 – 4:15 p.m.	**Youngdeok Hwang** IBM T. J. Watson Research Center *Bayesian Pollution Source Identification via an Inverse Physics Model*	**Jie Cheng** Abbvie Inc. *A Novel Approach to Patient Subgroup Identification and Its Applications to Clinical Trial Data*	(3:45 - 4:05 p.m.) **Sara Pålsson** *KTH Royal Institute of Technology* *Simulation of Surfactant-Covered Droplets in Two-Dimensional Stokes Flow*
4:15 – 4:45 p .m.	**Kyongmin Yeo** IBM Research *Spectral Inverse Model for Advection-Diffusion Problem with a Limited Number of Data*	**Shihua Wen** Novartis Pharmaceuticals Corporation *Benefit-Risk Assessment Using Patient-Level Data*	(4:05 - 4:25 p.m.) **Zecheng Gan** University of Michigan *Boundary Integral and Image-Moment Hybrid Method for Simulations of Solvated Proteins*

Continued on next page

SUNDAY AFTERNOON

MINISYMPOSIA X, XI, AND XII

4:45 – 5:15 p .m.	**Yibo Zhao** Rutgers University *Efficient Gaussian Process Modeling Using Experimental Design-Based Subagging*	**Dai Feng** Merck & Co., Inc. *Building Quantitative Structure–Activity Relationship Models Using Bayesian Additive Regression Trees*	(4:25 - 4:45 p.m.) **Gokberk Kabacaoglu** UT at Austin - ICES *Deformability-Based Cell-Separation Through Deterministic Lateral Displacement*
5:15 – 5:30 p.m.	(5:15 - 5:35 p.m.) **Joe Klobusicky** Rensselaer Polytechnic Institute *Two One Dimensional Models from Grain Boundary Coarsening*		(4:45 - 5:05 p.m.) **George (Georgios) Karamanis** Tufts University *Extended Graetz-Nusselt Problem for Liquid Flow in Cassie State Over Isothermal Parallel Ridges*
			(5:05 - 5:25 p.m.) **Qi Tang** Rensselaer Polytechnic Institute *A Stable FSI Algorithm for Rigid Bodies and Incompressible Flows*

PLENARY SPEAKERS

JON CHAPMAN

University of Oxford

Mathematical Modelling of Lithium Ion Batteries

A framework is presented for modelling the physical and chemical dynamics of a lithium-ion battery using the method of multiple scales to derive a macroscopic model from a detailed electrode microstructure. The result is a porous electrode model similar in flavour to the standard model of Newman, but in which the macroscopic parameters such as permeability are directly related to the microscopic electrode structure. The model includes both electrokinetic transport phenomena and mechanical deformation due to electrode swelling, and is thus able to predict local mechanical stresses. These in turn may lead to cracking with a resulting degradation of battery performance

JIANYING HU

IBM T. J. Watson Research Center

Computational Health Methods for Next Generation Healthcare

Next generation healthcare will be driven by prevention and treatment strategies that take individual variability into consideration. Much of this variability is captured in the large amount of data of different types that has become available: clinical encounters, lab results, diagnostics, medications, genomics, and increasingly, physiological, lifestyle, social behavioral and environmental data. The challenge is how to leverage modern methodologies from machine learning, data mining, visual analytics and decision science, to extract insights from all this data collected over large populations, in order to apply them at patient level to improve outcomes for health and wellness. The overarching goal of Computational Health Research is to enable this journey from complex and diverse health data to useful insights for individuals. At the Center for Computational Health at IBM Research we have been systematically developing advanced data science methodologies for healthcare, ranging from intelligent data preparation and pattern extraction, to complex models for insights generation, to behavioral analysis for personalized interventions. These methodologies have been applied to a wide range of use cases in personalized care delivery and care management, care pathway analytics and practiced based evidence, risk prediction and disease progression modeling, real world evidence for drug discovery, and patient and user engagement. I will discuss these methodologies, use cases, lessons learned and important future directions.

GREGORY LUTHER

AOX Northrop Grumman

Business-Driven R&D: Leveraging Mathematical and Optical Science

We describe several case studies where mathematical and optical sciences are leveraged to achieve business-driven objectives using current frameworks for business R&D.

CLEVE MOLER

MathWorks

The Evolution of MATLAB

We show how MATLAB has evolved over more than 30 years from a simple matrix calculator to a powerful technical computing environment. We demonstrate several examples of MATLAB applications. We conclude with a discussion of current developments, including parallel computation on multicore, multicomputer, and cloud systems.

RUTH ABRAMS

Sanofi

LIFE (Linear in Flux Expression methodology) Enables Modeling and Mechanistic Understanding of Patient Populations with Differential Responses to Therapy

Quantitative Systems Pharmacology (QSP) models mathematically represent the relevant biology of a disease, and how it is impacted by the mechanism of action of a treatment of interest. These models are often calibrated to simulate the response of an average patient to this treatment. In order to adapt the model to represent patient subgroups with different levels of responsiveness to treatment, it is necessary to identify QSP model parameters corresponding to sources of variability in patient biology. Once these parameters are selected, one can create distributions for these parameters which generate variability in model outputs that encompasses the diversity seen in clinical response. There are empirical methods of doing this, which tailor parameters to fit patient baseline and endpoint values. We have developed the Linear In Flux Expressions (LIFE) method based on the principles of control theory to mechanistically represent dependencies between parameters so that core parameters controlling variability in the disease can be more easily identified, and variability induced in these parameters can be propagated through connected parameters in the model to maintain the same baseline biology. LIFE allows us to determine boundaries on parameter distributions guided not only by literature on each individual parameter value, but by the constraint that variability in the core parameter must induce a physiologically reasonable level of variability for all connected parameters in the model as well.

We demonstrate the usefulness of this method on a model of cholesterol metabolism, where the LIFE method allows us to identify mechanisms differentiating low vs. high statin responders. A new cholesterol treatment, anti-PCSK9 therapy, is given in combination with statins, and leverages mechanistic synergies with statins which may upregulate PCSK9 expression. With the LIFE method we can use insight gained into the mechanisms controlling statin responsiveness to predict how well anti-PCSK9 therapy, alone or in combination with statins, will work on these patient subgroups.

(Authors: Ruth Abrams, Sean McQuade, Jeff Barrett, Benedetto Piccoli, Karim Azer)

NELSON LEE AFANADOR

Merck & Co., Inc

A Descent into the Proximity Matrix of Unsupervised Random Forest

Unsupervised methods, such as principal component analysis, have gained popularity and widespread acceptance in the data analysis community. Unsupervised random forest (URF) is an additional method capable of discovering underlying patterns in the data. However, the number of applications of URF has been limited. One possible cause for this is the belief that random forest can only be used in a supervised analysis setting. In this talk we will discuss the use of URF as an unsupervised learning method, and explore its properties in light of competing dimensionality reduction methods. Several examples will be presented.

UWE BEUSCHER

W.L. Gore & Associates, Inc.

Investigation of the Correlation Between Gas/Liquid Porometry and Particle Filtration Using Simple Network Models

In order to better understand the performance of microporous membranes for particle filtration, it is important to determine and measure the appropriate membrane structural properties that influence filtration. One such property is the pore size distribution and a common technique for measuring pore sizes or porous structures is gas/liquid capillary porometry. In this method, the pore size is determined by measuring the capillary pressure distribution of the sample, which is correlated to a pore size distribution using a very simple model structure of parallel capillaries. A numerical study using a simple network model for the porous material, however, has shown that the morphological structure strongly influences the porometry results. Model structures with different morphology and pore size information lead to varying porometry results at similar filtration behavior and vice versa. An attempt is made to correlate numerical porometry and filtration performance as is often done in experimental studies. Finally, the limitations of porometry in predicting filtration behavior are illustrated.

KIM "AVRAMA" BLACKWELL

George Mason University

Computational Approaches to Understanding Habit Learning and Parkinson's Disease

Parkinson's Disease, normal habit learning, and addiction are related by the role of a critical molecule called Dopamine. The association of reward (which triggers dopamine in the brain) with prior actions or context produces learning whose repetition leads to habits. In contrast, the absence of dopamine produces motor deficits. On the cellular level, dopamine initiates a cascade of intracellular events that modifies cell properties, which in turn modify circuit dynamics and behavior. Computer modeling, constrained by experiments, is an approach to investigate the interactions between dopamine and other molecules, and the effect of dopamine on cell and circuit properties. I describe development of software to facilitate development of these large scale models of signaling molecules. I will explain simulations demonstrating the role of dopamine in synaptic plasticity. I also will present a model of electrical activity and calcium dynamics, which evaluates how different spatio-temporal patterns of stimulation interact with dopamine to control synaptic plasticity.

CARLOS BORGES

The University of Texas at Austin

Reconstruction of a Compactly Supported Sound Profile In The Presence of Noisy Background Random Medium

We address the problem of reconstructing an unknown compact sound profile embedded in a random noisy background medium given the full aperture far field measurements of the scattered field for multiple angles of incidence at multiple frequencies. The fast Poincar\'{e}-Steklov solver of Gillman et.al is used to simulate the forward scattering problem and its Frech\'{e}t derivative. The recursive linearization algorithm of Chen is used for doing continuation in the frequency to obtain increasingly accurate reconstructions of the object and at each frequency we apply the Gauss-Newton method to recover a band-limited approximation of the sound-profile. Using this stable and accurate framework, we make a comprehensive study of methods for recovering the sound profile embedded in a random noisy background medium in different situations.

PETER BUCHAK

LowReTech LLC

Fabrication of Specialty Optical Fibers

Microstructured, multicore, and other specialty optical fibers are increasingly finding applications in the communications, medical, and petroleum industries, among others. However, a major bottleneck in their development is the difficulty of fabricating them. Optical fibers are made by heating glass preforms and drawing them into fiber. Because surface tension causes the cross section to deform, the geometry of the fiber depends in a nontrivial way on the preform geometry and on the parameters used to draw it. Currently, fabricators rely on trial and error to design preforms and select draw parameters. As a consequence, fabricating specialty fibers is time-consuming and expensive.

In this talk, we give an update on our theoretical and experimental work on the fluid dynamics of fiber drawing. Mathematical models that exploit the geometry of fiber drawing eliminate the need to simulate the full flow numerically. This allows fabricators to rapidly calculate the influence of preform design and draw parameters on the geometry of specialty fibers, making it practical to determine in advance how to produce a desired fiber.

JAMES CAI

Roche Innovation Center, New York

New Data and New Analytics in Pharmaceutical R&D

Data analysis has long been an integral part of the pharmaceutical R&D. One prominent example is the statistical analysis in clinical trials. Despite this, the interdisciplinary science of drug discovery and translational research is still largely an experimental and observational practice, conducted in biology and chemistry labs. In recent years, the emergence of various forms of Big Data, derived from new technologies such as next-generation sequencing of the human genome and wearable sensors, digitization of traditionally analog information such as pathology images and patient medical records, combined with the widespread use of the internet and social media, has made it possible and necessary to apply more advanced data analytics. In this talk I will discuss the growing role of Data Science as a new function in pharmaceutical R&D, and the application of advanced analytics, e.g., machine learning in drug research. I will highlight areas where new insights were gained through quantitative analysis, with examples of how they impacted the progress of our drug projects. I will also discuss the challenges that remain and may require more applied research.

ALOKNATH CHAKRABARTI

Indian Institute of Science, Bangalore

The Role of Wiener-Hopf Technique in Problems of Scattering of Electromagnetic Waves by Multiple Scatterers

The Wiener- Hopf technique and its recent developments are found to be highly advantageous and effective, both analytically as well as computationally, in handling a class of problems of scattering of Electromagnetic and Acoustic Waves, by Multiple Scatterers, present in a medium of known properties. As examples of multiple scatterers, two and three semi-infinite planes, with varieties of arrangements in the medium and with general type of boundary conditions on their surfaces are examined in detail. The resulting two-dimensional boundary value problems under consideration are shown to be amenable to the Wiener-Hopf technique, leading finally to the solution of a system of Fredholm integral equations of the second kind which are best solved numerically.

NAN CHEN

Courant Institute, New York University

A Simple Dynamical Model for El Nino with Wind Bursts and the Mechanisms of the 2014-2016 Delayed Super El Nino

In this talk, we present a simple modeling framework for the El Nino. A simple parametrization of wind bursts is coupled to the atmosphere and ocean model that is otherwise deterministic, linear and stable. The wind bursts parameterization involves a state-dependent (multiplicative) noise that describe both the westerly and easterly winds. The coupled system succeeds in simulating all kinds of El Nino events as well as their statistical features in the eastern Pacific. This modeling framework is also applied to understand the delayed 2014-2016 super El Nino, which is a new type of El Nino and has great social impacts. It is revealed by the model that both westerly and easterly wind bursts are crucial in the formulation of the delayed El Nino. The theoretical findings here suggest that the delayed super El Ni\~no events are not necessarily unusual and could reoccur in the future.

Advisor: Andrew J. Majda

Collaborators: Andrew J. Majda, Sulian Thual, and Samuel N. Stechmann

JIE CHENG

Abbvie Inc.

A Novel Approach to Patient Subgroup Identification and Its Applications to Clinical Trial Data

Precision medicine is an important direction for future drug development. Central to precision medicine is the ability to effectively identify patient subgroups that are likely to benefit from a certain treatment. However, due to multiple testing, subgroup analysis is well known for its tendency to produce spurious results if not done with extreme care. In this talk, we will present a random permutation based patient subgroup identification procedure and demonstrate its effectiveness using randomized clinical trial datasets.

MINSEOK CHOI

POSTECH

Model Reduction for Stochastic Fluid Flows: Time-Dependent Karhunen-Loeve Type Decomposition Methods

We present a hybrid methodology for stochastic PDEs based on the dynamically orthogonal (DO) and bi-orthogonal (BO) expansions that provide a low dimensional representation for square integrable random processes. The solution to SPDEs follows the characteristics of KL expansion on-the-fly at any given time. We prove the equivalence of the two approaches and provide a unified hybrid framework of those methods by utilizing an invertible and linear transformation between them. Numerical examples are presented to illustrate the proposed methods.

RADU CIMPEANU

Imperial College London

Making a Splash: From High Speed Droplet Impact to a Novel Methodology for Water Retention Calculation

A new methodology for the calculation of water collection efficiency on aircraft surfaces is discussed. The approach incorporates the detailed fluid dynamical processes often ignored in this setting, such as the drop interaction with the surrounding air flow, drop deformation, rupture and coalescence, as well as the motion of the ejected microdrops in the computational domain. Direct numerical simulations using the volume-of-fluid technique are performed using modelling assumptions which enable us to take advantage of the disparity of lengthscales in the system. The analysis shows a high degree of flexibility and can be used efficiently when considering changes in geometry (aircraft design), flow conditions and cloud characteristics. The interaction with our industrial partners will also be a point of focus, in particular in the context of developing a framework that incorporates the above analysis in an industrial work pipeline with no additional computational cost, thus making direct use of several hundreds of thousands of hours of CPU time on local supercomputing facilities. The methodology is finally applied to representative test geometries in collaboration with our partners.

DARREN CROWDY

Imperial College London and NJIT

Theoretical Advances in Understanding Superhydrophobic Slip

This talk will survey a number of recent theoretical advances in understanding the slip properties of flows over unidirectional superhydrophobic surfaces. The role of meniscus curvature, non-uniform pressure gradients and non-Newtonian fluid effects will be discussed.

DAI FENG

Merck & Co., Inc

Building Quantitative Structure–Activity Relationship Models Using Bayesian Additive Regression Trees

Quantitative structure–activity relationship (QSAR) is a very commonly used technique for predicting biological activity of a molecule using information contained in the molecular descriptors. The large number of compounds and descriptors and sparseness of descriptors pose important challenges to traditional statistical methods and machine learning (ML) algorithms (such as random forest (RF)) used in this field.

Recently, Bayesian Additive Regression Trees (BART), a flexible Bayesian non-linear regression approach, has been demonstrated to be competitive with widely used ML approaches. Instead of only focusing on accurate point estimation, BART is formulated entirely in a hierarchical Bayesian modeling framework, allowing one to also quantify uncertainties and hence to provide both point and interval estimation for a variety of quantities of interest.

We studied BART as a model builder for QSAR and demonstrated that the approach tends to have predictive performance comparable to RF. More importantly, we investigated BART's natural capability to handle truncated (or qualified) data and generate interval estimates for molecular activities as well as descriptor importance, which could not be easily acquired through other approaches. We will present the encouraging results obtained.

ZECHENG GAN

University of Michigan

Boundary Integral and Image-Moment Hybrid Method for Simulations of Solvated Proteins

We present our recent work on a numerical Boundary Integral Equation (BIE) method, and a semi-analytical Image-Moment hybrid method for efficient and accurate simulations of electrostatic fields in systems consisting multiple proteins in solvent. The BIE is coupled with treecode for fast kernel summation, and is applicable to arbitrary shaped dielectric interface; while the hybrid method combines analytical image charge solution of dielectric spheres with the Method of Moments, and is accelerated by the fast multipole method (FMM). Numerical results from both methods are presented, showing that the induced charge on the dielectric interfaces can significantly change the interaction energy of solvated proteins.

Advisor: Robert Krasny

Collaborators: Shidong Jiang and Weihua Geng

SAMIRAN GHOSH

Wayne State University

Use of Historical Information via Bayesian Approach in Non-Inferiority Trial: With Application

Clinical trials are acceptable gold standard for determining whether an intervention works for particular disease. However it requires substantial resources to be successful in making that determination. These resources can be quantified not only as a monetary cost, but also from an ethical view point as it requires exposing subjects to an unverified treatment regime from which benefits are yet to be determined. Hence reducing sample size if possible without undermining the integrity of the trial is always desirable. Historical trials often provide substantial information for legacy disease areas in many cases. Noninferiority trials are unique because they are dependent upon historical information in order to make meaningful interpretation of their results. Bayesian paradigm provides a natural framework in incorporating this historical information as a prior, which could reduce sample size burden substantially. In this talk we will review some of these Bayesian approaches from Noninferiority point of view with some application in depression trial.

SAL GIGLIA

MilliporeSigma

Filtration Modeling for New Membrane Filter Development

Since the development more than 80 years ago of the early models of fouling through membrane filters, simulations of filtration behavior have continued to be mostly based on a simple macroscopic approach. Although phenomenologically useful, this approach is constrained by a number of simplifying assumptions that have limited its utility for aiding development of new filters. In recent years, however, advances in 3D-electron microscopy, introduction of highly sophisticated modeling software, and availability of increasingly powerful computers have enabled a leap forward in filtration simulation and visualization. In this talk, case studies will be presented where these new modeling tools (using a microscopic approach) have assisted in guiding development of new filtration technologies and have provided insights and key understandings into mechanisms of filter fouling.

ZYDRUNAS GIMBUTAS

National Institute of Standards and Technology

Modeling Scanning Microwave Impedance Spectroscopy

In this talk, we will discuss our recent work in building numerical tools for modeling Scanning Microwave Impedance Spectroscopy (sMIM). We propose to use a complex-valued capacitance solver for impedance extraction of simple targets embedded in thin film layered media.

(This is joint work with Andrew Dienstfrey.)

IAN GRIFFITHS

University of Oxford

How Do Gradients in Porosity Make a Better Filter?

When you change the air filter in your car or vacuum you will notice that one side is dirty while the other side is clean. This clogging of a filter on the top surface while the rest of the medium remains relatively clean is generic, and leads to filter failure before reaching its full potential. A porosity-graded filter, whose porosity decreases with depth, resolves this problem by allowing contaminants to penetrate more deeply and evenly into the medium before being trapped. However, the optimal porosity gradient that maximizes the trapped contaminant is unknown.

In this talk we use homogenization theory to derive a macroscopic model for the fluid flow and particle trapping within a porosity-graded depth filter. We use the resulting model to show how particle trapping is more evenly spread through the filter for a decreasing porosity compared with a uniform porosity. By quantifying the removal rate, we show how a given operating regime can be fine-tuned to improve filter efficiency. We discuss the implications of this work for industry, and a collaboration that we now have with vacuum cleaner company Dyson as a result as we strive to find the best filter for a given task.

VIATCHESLAV GUREV

IBM

Coupled Biophysical and Regression Models of Cardiac Electrophysiology and Mechanics

Computational multi-scale models of the heart are promising tool for diagnostics of cardiovascular diseases with the potential to predict development of pathologies such as myocardial infarction and heart failure. We are developing computational methods that combine biophysical and statistical models to address the complexities of the cardiovascular system. The main idea of such methods is to use results of mechanistic simulations of cardiac electrophysiology and mechanics for subsequent application of algorithms from statistics and machine learning. In some cases, the application of simulation does not add much predictive value over statistical and machine learning approaches alone. For example, the cardiotoxic effect of drugs can be classified without explicit computation of the electrical responses of the heart cells; machine learning on in vitro assay data alone will suffice for existing data sets. In other applications in cardiac mechanics, we see important benefits from combining mechanistic models with statistical modeling and machine learning. Recently, our group built a pipeline to construct 3D models of cardiac mechanics from databases of cardiac MRI and trained regression models on simulation results. Our coupled approach allows us to simulate the coupling of cardiac mechanics and blood circulation in real time, to perform optimization in a very large parametric space and to define new quantitative indexes of cardiac function.

JOON HA

National Institutes of Health

A Mathematical Model Predicts a Delayed Insulin Peak During an Oral Glucose Tolerance Test as a High Risk Factor for Diabetes

Identifying an early sign of metabolic dis-function of a risk factor for diabetes is necessary to prevent and delay onset of the disease. We have updated our mathematical model for beta-cell mass and function (Ha et al. Endo 2016) to study a risk factor for diabetes during an oral glucose tolerance test (OGTT). Model simulations confirmed the result of an unpublished cohort data set (ENDO Annual Meeting 2017), showing that a delayed time to glucose peak during an OGTT is a high risk factor. Furthermore, the model predicts that a delayed time to insulin peak precedes that to glucose peak. Longitudinal simulations show that both beta-cell dysfunction and insulin resistance contribute to the delay in time to insulin peak. In addition, the model predicts that the delay in time to insulin peak is more prominent in those with impaired glucose tolerance (IGT) than those with impaired fasting glucose (IFG).

NICOLAS HADJICONSTANTINOU

Mechanical Engineering, MIT

On the Limits of Fourier's Law and Kinetic Extensions for Confined Solid-state Materials

We use a Hilbert procedure to obtain asymptotic solutions to the Boltzmann equation modeling phonon transport in crystalline materials in the limit of a small but finite mean-free path (or Knudsen number, Kn, defined as the ratio of the mean free path to the characteristic system lengthscale). This procedure yields the continuum equations and boundary conditions governing phonon-mediated heat transfer over a range of lengthscales, starting from the traditional heat conduction equation (Kn→0) and transitioning to a regime where the latter fails (Kn>0.1). We show that deviations from the traditional heat conduction equation originate at the system boundaries, while the Fourier constitutive relation remains robust in the bulk at least up to second order in the Knudsen number. This can be explained by noting that Fourier's law does not hold within a few mean free paths from a boundary due to the inhomogeneity introduced by the latter. Using a boundary layer-outer solution matching approach, effective boundary conditions accounting for this effect are derived up to second order in the Knudsen number.

We also show that the asymptotic solution procedure can be used to solve the Kapitza resistance problem associated with an interface between two materials (within the Boltzmann equation approximation). The well-known temperature jump at the interface is shown to be a result of the incompatibility between the distribution functions in the two materials, requiring a two-sided boundary layer matching procedure.

All results are validated via comparisons with low-variance deviational Monte Carlo simulations for a variety of material models. The physical origin of deviational Monte Carlo simulations will be briefly discussed as well as implications for multiscale simulation.

MARYLENS HERNANDEZ

LAM Therapeutics

Expression-based Computational Drug Repurposing for Rare Diseases

Drug repurposing offers a way to identify potential treatments for diseases that currently have no cure by "repurposing" known drugs. Doing this computationally further reduces the cost and increases efficiency of the drug development process. In the present study, we use a computational approach based on gene expression to accelerate the discovery of new treatments for rare diseases. Our method relies on the premise that if a drug's gene expression perturbation is opposite to a disease gene expression phenotype, then that drug could be a potential treatment for that disease. Towards this goal, we first built a gene expression database for around 400 different rare diseases, with 1500 high quality gene expression signatures. Then, we defined the gene expression (perturbation) profile for our drugs-of-interest. Finally, we implemented and integrated three different metrics to compute the similarity between drug expression profiles and disease-gene expression signatures, and assigned a p-value to each drug-disease pair. A drug-disease pair would only be considered as a high confidence prediction when the match was statistically significant and most of the expression signatures for the particular disease were significantly associated with the drug. This methodology was able to capture and replicate positive control diseases that we had already validated in preclinical models, and allowed us to predict with confidence new indications for our drugs.

TUAN HOANG TRONG

IBM Research

Challenges of Modeling Whole-Cell Neurons

The neuron type is attributable not only in their morphology, but also in their wide range of synaptic inputs on different dendritic locations. This enables neurons from different region of the brain to handle differently the inputs they receive via thousands of synapse structures. However, how the complete dendritic morphology contributes to the function of a single neuron is still largely unknown. Modeling the detailed of spines on neurons can increase the complexity of the model to a few orders of magnitude in terms of number of compartment to be solved. Furthermore, the functional role of neurons, in terms of plasticity, neuronal energy metabolism, and propagating the signal to the spike initiation site to coordinate the communication in the brain, is also mediated by different intracellular signaling systems, in that calcium plays an important role. In this work, we present out effort to develop a graph-based simulation system to tackle such challenging problem.

MARC HODES

Tufts University

Transport Phenomena on Superhydrophobic Surfaces

In nature, liquids may be suspended upon micro- or nano-scale hydrophobic (water-repelling) protrusions, as in the case of, e.g., the lotus leaf and the Namib Desert beetle, both of which exhibit so-called superhydrophobic (SH) surfaces. Biomimetic structures with the same properties may be achieved using modern micro- and nano-fabrication techniques. In this talk I will discuss how momentum, heat and mass are transferred between SH surfaces and liquids suspended over a lubricating gas phase upon them in the unwetted (Cassie) state. Specifically, I will show how one can compute the key engineering parameters, i.e., Poisueille number and Nusselt number, for flows in diabatic microchannels using various analytical and numerical techniques. Attention will then turn towards applications that SH surfaces enable such as enhanced heat removal from electronics and drag reduction on underwater objects such as ships or swimming robots. Finally, I will discus outstanding needs relevant to achieving more realistic models of transport phenomena on SH surfaces, e.g., capturing high Knudsen number effects in the gas-phase which lubricates the liquid phase.

YOUNGDEOK HWANG

IBM T. J. Watson Research Center

Bayesian Pollution Source Identification via an Inverse Physics Model

Behavior of air pollution is governed by the complex dynamics, in which air quality of a site is affected by the pollutants transported from neighboring locations via phys- ical processes. To estimate the source of observed pollution, it is crucial to take the atmospheric condition account. Traditional approach to build empirical models uses observations, but is not able to incorporate the physical knowledge. This drawback becomes particularly severe for the situations where a near-real time source estimation is needed. In this paper, we propose a Bayesian method to estimate the pollution sources, by exploiting both the physical knowledge and observed data. The proposed method uses a flexible approach to utilize the large scale data from the numerical weather prediction model while incorporating the physical knowledge into the model.

GOKBERK KABACAOGLU

The University of Texas at Austin - IC

Deformability-Based Cell-Separation Through Deterministic Lateral Displacement

Fast and reliable separation of biological cells is an essential for various applications in micro- and nano-fluidics. Microscale separation devices are of great interest since they operate with smaller sample sizes in shorter times than the traditional methods do. Huang et al. [1] presented deterministic lateral displacement (DLD) as a size-based microfluidic particle separation technique and used it to separate rigid particles. Here we systematically analyze the separation of deformable capsules from their dense suspensions through DLD in two dimensions. In particular, we study vesicles which are capsules filled with a Newtonian fluid. Vesicle flows are good proxies for flows of biological cells such as red blood cells. We use our in-house algorithms for the simulation of vesicles suspended in a Stokesian fluid [2]. Our method is based on an integral equation formulation of the Stokes equations coupled to the continuum models of vesicles.

A DLD device consists of rows of posts in a flow channel and the posts are shifted vertically by a fixed amount in the flow direction. Flowing particles either move along the length of the channel or are pushed laterally by the posts. The separation of rigid spherical particles from dilute suspensions through DLD depends only on the particle size and is well understood. The effectiveness of separation by DLD is less understood for deformable particles and for dense particle suspensions. In this talk, I will first present the DLD theory for rigid particles and our method for the simulation of vesicle flows. Then I will show how different a single biological cell behaves in a DLD device than a spherical rigid particle does. Finally, I will discuss how particle-particle interactions in dense suspensions affect the particle separation.

[1] L. R. Huang, E. C. Cox, R. H. Austin and J. C. Sturm, Science, 2004, 304, 987–990.
[2] B. Quaife and G. Biros, Journal of Computational Physics, 2014, 274, 245-267.

Advisor: George Biros

CHANCHALA KADDI

Sanofi

Quantitative Systems Pharmacology Model of Acid Sphingomyelinase Deficiency and the Enzyme Replacement Therapy Olipudase Alfa is an Innovative Tool for Linking Pathophysiology and Pharmacology

Olipudase alfa (rhASM) is an investigational enzyme replacement therapy in development for the treatment of nonneurological manifestations of acid sphingomyelinase deficiency (ASMD), traditionally known as Niemann-Pick disease types A and B. ASMD is clinically heterogeneous, affecting multiple organ systems, with clinical manifestations including hepatosplenomegaly, infiltrative pulmonary disease, and hyperlipidemia [1].

A phase 1b trial of olipudase alfa treated five adults with chronic visceral ASMD (Niemann-Pick type B), and demonstrated improvements in clinical markers including spleen and liver volume, infiltrative lung disease, and stored sphingomyelin [2, 3]. Phase 2/3 adult and phase 1/2 pediatric trials are ongoing.

We present a quantitative systems pharmacology (QSP) model to support the development of olipudase alfa. The model utilizes a mechanistic, multi-scale approach to link the enzymatic activity deficiency driving ASMD with consequent lipid accumulation, cellular abnormalities, and organ-level clinical manifestations.

The QSP model was developed by integrating knowledge from ASMD natural history, preclinical, and clinical data, and takes as input patient-specific PK profiles and indicators of disease severity. The model successfully reproduces both transient and long-term patient-specific responses to olipudase alfa. At the molecular level, it describes plasma ceramide and plasma lyso-sphingomyelin profiles; at the organ level, it describes spleen volume and pulmonary function.

Overall, the QSP model enables quantitative representation of systemic treatment responses to olipudase alfa. Due to the clinical heterogeneity of ASMD, this provides insight into treatment effects on different aspects of the overall disease burden, as a function of patient variability. The QSP model provides a platform for addressing clinical questions of interest such as alternative dosing regimens, patient stratification, and pediatric extrapolation.

[1] McGovern et al. (2013) Genet Med 15(8): 618-623

[2] Wasserstein et al. (2015) Mol Genet Metab 116(1-2): 88-97

[3] Thurberg et al. (2016) Am J Surg Pathol, 40(9): 1232-1242

SHARAD KAPUR

Integrand Software, Inc.

Large-scale Electromagnetic Simulation for Radio Frequency Integrated Circuit Design

We describe an electromagnetic simulator for modeling radio frequency (RF) components and circuits. It is a fast, integral-equation based, full-wave field solver that takes advantage of the layout ``regularity'' in typical design. We describe some novel features of the formulation and advances in numeric techniques that allow the simulator to be accurate and fast enough to be used extensively in industry. The solver is two orders of magnitude faster than the finite-element based solvers that were previously widely used. Several designs, fabricated on a variety of process technologies will be presented with comparisons to measurement.

GEORGE (GEORGIOS) KARAMANIS

Tufts University, Department of Mechanical Engineering

Extended Graetz-Nusselt Problem for Liquid Flow in Cassie State Over Isothermal Parallel Ridges

We consider convective heat transfer for laminar flow of liquid between parallel plates that are textured with isothermal ridges oriented parallel to the flow. Two different geometries are analyzed: both plates textured with symmetrically aligned ridges and one plate textured and the other one smooth and adiabatic. The liquid is assumed to be in the Cassie state on the textured surfaces to which a mixed boundary condition of no-slip on the ridges and no-shear along flat menisci applies. The thermal energy equation is subjected to a mixed isothermal-ridge and adiabatic-meniscus boundary condition on the textured surfaces. We solve for the developing three-dimensional temperature profile resulting from a step change of the ridge temperature assuming a hydrodynamically-developed flow with finite axial conduction, i.e., we consider the Extended Graetz-Nusselt problem. Effects of viscous dissipation and volumetric heat generation are also considered. Using the method of separation of variables, the homogeneous part of the thermal problem is essentially reduced to a two-dimensional eigenvalue problem in the transverse coordinates. Expressions are found for the local and fully-developed Nusselt number in terms of the eigenvalues, eigenfunctions, Brinkman number and the volumetric heat generation. Estimates are also provided for the location that viscous dissipation effects become important.

Advisor: Marc Hodes

Collaborators: Marc Hodes (Tufts University, Department of Mechanical Engineering), Toby Kirk (Imperial College London, Department of Mathematics), Demetrios T. Papageorgiou (Imperial College London Department of Mathematics)

HOWARD KARLOFF

Goldman Sachs

Big Data Analytics and Modeling for Financial Institutional Compliance

It is critical for a financial institution to comply with government regulations. The cost of non-compliance can result in criminal indictment, multi-billion-dollar fines and loss of licenses. Our department is responsible for the implementation of controls to detect and monitor insider trading, market manipulation, money laundering, bribery, terrorist financing, and other policy violations.

This talk will focus on how Goldman Sachs' compliance department leverages large quantities of data and modeling methodology to address specific risks. In particular, we will discuss our recent "surveillance" to detect spoofing.

JOE KLOBUSICKY

Rensselaer Polytechnic Institute

Two One Dimensional Models from Grain Boundary Coarsening

We study two simplified models which arose from the study of two dimensional, isotropic coarsening of networks. From the Von Neumann-Mullins n-6 rule, individuals grains in a network change areas at a constant rate that is completely dependent on grain topologies. When a grain vanishes, topologies are reassigned. Multiple mean field models have been developed which attempt to describe the coupled behavior between area evolutions for classes of grains. In this talk, we will focus on two minimal particle system models, and their associated kinetic limits, which capture the nontrivial behavior of grain coarsening. We hypothesize on the relation between methods used in these models, and proofs of convergence for general grain coarsening particle systems.

Advisor: Peter Kramer

Collaborators: Govind Menon and Bob Pego

JAMES KOZLOSKI

IBM Research

Modeling Relationships Between Clinical Progression and Circuit Dysfunction in Huntington's Disease

The progression of Huntington's disease (HD) is marked by clinical changes in cognitive, affective, and motor function among mutant gene carriers, as well as changes in gross morphological measures in patient brain imaging. Animal disease models reveal widespread cellular, synaptic, microcircuit and brain circuit changes due to the mutant Huntington protein (mHTT). Each of these changes emerges at multiple scales, often simultaneously, and their measures therefore overlay the primary risk of mHTT, which accumulates locally, with compensation for this risk, which emerges globally in the brain's circuitry resulting in clinical phenotypes. We have constructed computational neuroscience models of neuronal and circuit electrophysiology across scales, validated against preclinical HD animal model data. We show how cellular, synaptic, microcircuit, and brain circuit functional regulatory units can be discovered using these simulations and then manipulated to effect and predict disease progression, and various outcomes from therapeutic inputs to the models at each scale.

STEPHEN KRIEGER

Mount Sinai

The Topographical Model of Multiple Sclerosis

Relapses and progression contribute to multiple sclerosis (MS) disease course, but neither the relationship between them nor the spectrum of clinical heterogeneity has been fully characterized. The topographical model of MS is a dynamic model of MS disease course that incorporates localization and other drivers of disability to propose a clinical manifestation framework that visualizes MS in a clinically individualized way. The topographical model encapsulates five factors (localization of relapses and causative lesions; relapse frequency, severity, and recovery; and progression rate), visualized utilizing dynamic 3D renderings. The central hypothesis is that progression clinically recapitulates prior relapse symptoms and unmasks previously silent lesions, incrementally revealing underlying lesion topography. Utilization of this model could allow for earlier and more clinically precise identification of progressive MS. The model can be validated, and predictive implications can be empirically tested, through identification and weighting of precise clinical and imaging metrics.

ARMIN KRUPP

University of Oxford

Stochastic Modelling of Membrane Filtration

Porous membranes are used for their particle retention capabilities in a wide range of industrial filtration processes. The underlying mechanisms for particle retention are complex and often change during the filtration process, making it hard to predict the change in permeability of the membrane during the process. Recently, stochastic network models have been shown to predict the change in permeability based on retention mechanisms, but remain computationally intensive.

We show that the averaged behaviour of such a stochastic network model can efficiently be computed using a simple partial differential equation. Moreover, we also show that the geometric structure of the underlying membrane and particle-size distribution can be represented in our model, making it suitable for modelling particle retention in interconnected membranes as well.

YUSHUN LIN

Citi Cards

Statistics in Credit Card Marketing

Credit card marketing programs such as acquisition, balance transfer, retention, creative test, etc. require statistical techniques. This presentation will describe how to apply experimental design, modeling, and optimization for decision making and will focus on modeling. The main modeling related topics include data, feature creation and selection, modeling methods, performance assessments and tracking, model validation and governance, and interpretation of modeling results. Applying machine learning on big data platform is a fast-growing trend in card industry to solve business problems. Software commonly used for both traditional statistical modeling and machine learning will be briefly introduced as well.

YANG (STEVE) LIU

KCG Holdings, Inc.

Application of Statistical Analysis on Signal Research

This presentation will review a few tools in statistical analysis and machine learning and their applications to signal research on US equity market. Examples will be presented in the areas of regression and regularization, model reduction, classification, non-parametric parameter optimization and cluster analysis. Topics such as data cleaning, cross validation, overfitting and production feedback will also be briefly discussed. All examples are derived from real research projects after removing sensitive proprietary IP and after certain simplification.

ALAN LYONS

City University of New York

Multi-Functional Superhydrophobic Surfaces: From Singlet Oxygen Generation to Anti-Reflectivity

By incorporating sufficient roughness into a low surface energy material, superhydrophobicity can be achieved such that droplets of water assume a nearly spherical shape. Additional functionality can be achieved by further modifying the surface structure and/or chemistry. In this presentation, I will discuss two different approaches to increasing the functionality of superhydrophobic surfaces for specific applications. In one approach photo-catalytic particles are partially embedded into the surface enabling the generation of reactive oxygen species that can oxidize conjugated aromatics and efficiently kill microbes. In a second approach, the superhydrophobic surface is made to be optically transparent because the surface features are smaller than the wavelength of visible light. The low refractive index of the fluoropolymer, combined with the hierarchical topography, impart anti-reflective properties. Anti-soiling behavior is observed in the presence of condensed water droplets (i.e. simulated dew). The solid-liquid-vapor triple contact line is highly mobile on the superhydrophobic surface, thus as the liquid water droplet evaporates, it shrinks laterally, sweeping imbibed dust particles into discreet piles that reduce overall scattering.

AVI MA'AYAN

Icahn School of Medicine at Mount Sinai

Mapping the Mammalian Gene Expression Space for Drug and Target Discovery

By processing hundred of thousands gene expression profiles collected from human and mouse cells and tissues, we can impute knowledge about genes and proteins, and prioritize targets and novel small molecules for therapeutic and adverse event associations. We are also developing several software tools and databases that organize and integrate knowledge from many omics resources to enable the discovery of links between genes, pathways, cells, small molecules and phenotypes.

EMMANUEL MAITRE

Grenoble Institute of Technology

Constrained Optimal Transportation and Applications

We consider the dynamic optimal transportation problem between two densities subject to constraints. Those constraints could be either obstacles that densities are not allowed to cross, or rigidity constraints of the optimal plan. Existence of minimizers is proven and an extension of the genuine Benamou-Brenier algorithm is proposed. Applications are satellite images interpolation for weather forcasting and crowd motion in buildings, for which we show some numerical computations.

CHARLES MALDARELLI

Levich Institute and Department of Chemical Engineering, City College of New York

Continuum and Molecular Dynamic Studies of the Hydrodynamics of Colloid Particles at a Fluid Interface

Colloidal-sized particles (10 nm – 10 μm in size) adsorb onto a fluid interface (i.e. a gas/liquid or a liquid/liquid interface) from the continuous phases surrounding the surface and become trapped due to a reduction in their interfacial energy, forming a two dimensional monolayer. Colloid monolayers adsorbed onto the dispersed phase of emulsions and foams are traditionally used in stabilizing dispersions from coalescence. Emerging technologies focus on the self-organization of colloid monolayers formed on the fluid interface of liquid films on solid substrates. Control over later forces (e.g. capillary attraction and electrostatic repulsion) allows the formation of 2D crystalline monolayer phases on substrates as templates for materials fabrication, and textured surface topologies for super-hydrophobic surfaces.

The organization of colloids in a monolayer is a balance between the surface forces and the viscous resistance to particle motion along the surface. This presentation focuses on the surface hydrodynamics. A continuum analytical theory is presented for the drag force on a colloid at a vapor/liquid interface as a function of its immersion depth into the liquid phase, and the theory is extended by numerical calculation to colloids on the fluid interface of a thin film. A hydrodynamic theory is also developed for the viscous resistance due to the mutual approach of two colloids, and Brownian dynamics simulations are presented to understand the role of thermal fluctuations and hydrodynamic interactions in the capillary attraction of colloid pairs. Molecular dynamics calculations are detailed for the drag force on nano-sized colloids translating at a vapor/liquid interface, and a significant reduction in drag is obtained as the nanoparticle translates within the finite-width interfacial zone of the surface.

Experiments are presented to demonstrate how the calculated drag force can be used to accurately model the capillary attraction of two colloids. Experiments measuring the Brownian diffusion coefficient of a colloid at an interface are detailed, and used with the drag force calculation to obtain the colloid immersion depth and three phase contact angle.

HELEN MOORE

Bristol-Myers Squibb

Optimal Control for Combination Therapy Optimization

Combination therapy is increasingly important, but it can be challenging to determine the best regimens to use when there are many drugs and dose levels to choose from. Instead of running experiments with all possible combinations of dose levels, we can use mathematical modeling and optimal control to predict the best regimens. These data- and model-based predictions can then be incorporated into preclinical and clinical testing. I will give an overview of the technique and present examples of how much of a difference optimal control regimens can make.

MIKE O'NEIL

Courant Institute, New York University

Electromagnetics and the Laplace-Beltrami problem

In the static limit, electric currents along a perfect conductor can be separated into their divergence free, curl free, and harmonic components using the Hodge decomposition. For arbitrarily defined fields, this requires solving the Laplace-Beltrami problem along the surface. Such a separation is useful for electromagnetic computations at all frequencies, and often yields correspondingly well-conditioned integral equation methods. This talk will give an overview of modern integral equation representations for Maxwell's equation and novel integral equations for the Laplace-Beltrami problem.

SARA PÅLSSON

KTH Royal Institute of Technology

Simulation of Surfactant-Covered Droplets in Two-Dimensional Stokes Flow

The interest in fluid mechanics on the micro scale is growing, fueled by e.g. the development in miniaturized biological equipment. On these scales, surface forces dominate volume forces and the flow can be described with the linear Stokes equations. Surface active agents (surfactants) have a large effect on the dynamics of the flow in the presence of drops, as they significantly alter the surface tension.

We simulate the deformation of droplets in two dimensions using a boundary integral formulation, using a specialized method for numerical integration at target points close to the interfaces . This allows us to solve Stokes equations to high accuracy, also for drops in close proximity to each other.

The surfaces of the drops are covered with surfactants. The convection-diffusion equation describing the surfactant concentration is solved with a spectral method. To match the low spatial errors of our methods, we use a cost-efficient adaptive time-stepping method which maintains accuracy both in drop deformation and surfactant evolution

We present our method of simulating deforming surfactant-covered droplets. We show good agreement with analytic results both for clean and surfactant-covered bubbles. In the latter case, we show these analytic results hold in steady state also for drops. Finally, we simulate multiple closely interacting drops in different flow fields.

Advisor: Anna-Karin Tornberg

Collaborator: Michael Siegel

CHRIS PENLAND

AstraZeneca Pharmaceuticals

A Quantitative Systems Pharmacology Model for Potassium Homeostasis with Applications to Late Stage Drug Development

A quantitative systems pharmacology model for potassium homeostasis with applications to late stage drug development Hyperkalemia is a dangerous medical condition defined by an abnormally high level of potassium in the circulation which alters the electrophysiological potential across cell membranes in excitable tissues and increases the risk of life threatening arrhythmias. Zirconium cyclosilicate (ZS) is an orally administered drug that selectively binds potassium in the gastrointestinal tract. We developed a quantitative systems pharmacology (QSP) model that describes the dietary absorption, distribution and excretion of potassium and joined it with models for the potassium binding, transport and elimination by ZS. The model was then used to guide dose selection for planned clinical trials and characterize clinical sensitivity to key manufacturing criteria, both of which are key late stage challenges in which QSP models have rarely been found useful.

MANAS RACHH

Yale University

High Order Layer Potential Evaluation in Three Dimensions Using Quadrature by Expansion (QBX)

The practical application of integral equation methods requires the evaluation of singular or weakly singular integrals on complex geometries. Quadrature by expansion is a recent method developed by Barnett, Epstein, Greengard, Klockner and O'Neil which stems from the observation that a layer potential induces a field which is locally smooth when restricted to either the interior or the exterior of the boundary. In this talk, we present a linear CPU time fast multipole accelerated QBX algorithm for evaluating layer potentials with high order accuracy in three dimensions. Our method is based on an optimized version of the fast multipole method (FMM) which uses diagonal forms for the translation operators. We illustrate the performance of the algorithm with several numerical examples.

NARGES RAZAVIAN

NYU School of Medicine

Deep Learning in Healthcare: Biomarker Discovery and Predictive Modeling

Recent advances in machine learning, and in particular deep learning, has enabled new approaches to biomarker discovery and prediction tasks. In this talk, I will discuss a number of recent applications of deep learning methods in healthcare, from medical imaging biomarker discovery and diagnosis models, to models of time series of lab measurements, to predictive models based on electronic health records. I will further discuss how using non-linearities and back-propagation, coupled with stochastic gradient descent have opened door to many new families of computational and mathematical models, and as an example, will introduce our work on learning multivariate kernels from irregularly measured lab value time series. I will conclude this talk by presenting a number of opportunities for bringing medical and artificial intelligence researchers closer together.

PEJMAN SANAEI

NJIT

Internal Structure and Morphology Profile in Optimizing Filter Membrane Performance

Membrane filters are used extensively in microfiltration applications. The type of membrane used can vary widely depending on the particular application, but broadly speaking the requirements are to achieve fine control of separation, with low power consumption. The solution to this challenge might seem obvious: select the membrane with the largest pore size and void fraction consistent with the separation requirements. However, membrane fouling (an inevitable consequence of successful filtration) is a complicated process, which depends on many parameters other than membrane pore size and void fraction; and which itself greatly affects the filtration process and membrane functionality. In this work we formulate mathematical models that can (i) account for the membrane internal morphology (internal structure, pore size and shape, etc.); (ii) describe fouling of membranes with specific morphology; and (iii) make some predictions as to what type of membrane morphology might offer optimum filtration performance.

QI TANG

Rensselaer Polytechnic Institute

A Stable FSI Algorithm for Rigid Bodies and Incompressible Flows

A stable partitioned algorithm is developed for fluid-structure interaction (FSI) problems involving viscous incompressible flow and rigid bodies. The algorithm remains stable, without sub-iterations, even for zero-mass rigid-bodies when added-mass and viscous added-damping effects are large. A fully second-order accurate implementation of the scheme is developed based on a fractional-step method for the incompressible Navier-Stokes equations and overlapping grids to handle the moving geometry. A number of difficult benchmark problems will be presented to verify the proposed algorithm. In particular, a FSI simulation based on the flow through a bileaflet mechanical heart valve will be presented.

Advisor: J.W. Banks

Collaborators: J.W. Banks, W.D. Henshaw, and D.W. Schwendeman

GIULIO TRIGILA

New York University

Data Driven Optimal Transport

A new data driven algorithm for the solution of the barycenter problem in optimal transport is presented. The algorithm is particularly well suited for the explanation of variability and removal of confounding factors from data set defined in high dimensional spaces. Applications of the algorithm are shown on synthetic and real data sets.

DAVID TURNER

Merck & Co., Inc

Challenges with Pembrolizumab Exposure-Response Assessments

Keytruda (pembrolizumab) remains at the forefront in a rapid expansion of cancer immunotherapy, with several landmark U.S. approvals across various lines of therapy in non-small cell lung cancer (NSCLC), melanoma, classical Hodgkin lymphoma, and head and neck cancer. Pharmacokinetic (PK) dependencies in overall survival (OS) were evaluated in 1453 subjects with melanoma or NSCLC across three pivotal studies of pembrolizumab with either 200 mg or 2 to 10 mg/kg administered every 3 weeks. Kaplan-Meier (K-M) plots of OS, stratified by dose, exposure, and baseline clearance (CL0) were assessed per indication and study. A Cox Proportional Hazards (CPH) Model was implemented to identify imbalances in prognostic factors in high/low NSCLC CL0 subgroups. OS was dose-independent from 2 to 10 mg/kg for melanoma (P = 0.480) and NSCLC (P = 0.171), confirming that 2 mg/kg resides at or near the efficacy plateau in these protocols; however, a strong CL0-OS association was identified for both cancer types. Decreased OS in subjects with higher pembrolizumab CL0 paralleled simultaneous disease severity markers associated with end-stage cancer anorexia-cachexia syndrome and potentially reflects catabolic activity as a marker of disease severity rather than a direct PK-related impact of pembrolizumab on efficacy.

AMAN ULLAH

George Mason University

Using Multiscale Modeling to Understand How Genetic Mutation Lead to Arrhythmia

Point mutations in the Ca2+ cycling proteins, calsequestrin 2 (CASQ2), have been found to underlie the arrhythmic cause of sudden cardiac death (SCD) known as catecholaminergic polymorphic ventricular tachycardia (CPVT-2). Understanding the subcellular mechanisms of CPVT is experimentally challenging because the arrhythmias are rare and the development of SCD are even rarer. For example, an episode of SCD may not occur in an affected individual for many decades if at all. To gain insight into the nature of this rare but potentially lethal class of arrhythmias we developed a multiscale model of cardiac electrical excitation and Ca2+ dynamics in heart cells and tissue with features that would include stochastic gating of channels and subcellular Ca2+ signaling. Models of the genetic mutant forms CASQ2 based on experimental data are incorporated into our models and enables us to explore how the mutations give rise to arrhythmia under conditions of beta adrenergic stimulation. Increased sensitivity to SR lumenal Ca2+ of RyR2, located in the junctional sarcoplasmic reticulum (jSR), leads to reductions in SR calcium content in CPVT-2 as a required by pump-leak balance of Ca2+ in the SR. Furthermore, increased SR Ca2+ content via enhanced SERCA Ca2+ pumping after treatment with catecholamines is attenuated due to the increased SR Ca2+ leak and does not lead to arrhythmia. Instead, in CPVT-2 additional changes (specifically the increased SR volume and decreased SR Ca2+ buffer) are sufficient to destabilize Ca2+ signaling. Therefore the increased SR lumenal Ca2+ sensitivity, increased SR volume and decreased buffering all are important elements in the model to produce cellular Ca2+ signaling alternans at high stimulation rates with simultaneous catecholamine treatment. The cellular Ca2+ instability underlies the multicellular development of extra-systoles.

EMILY WALSH

University of West England, UK

A Moving Mesh Method based on Optimal Transport for Numerical Weather Prediction

I will talk about a moving mesh method based upon ideas from optimal transport theory which is suited to solving PDE problems arising in many applications, but the main focus here will be meteorology. This method can be used to better resolve evolving small scale features in the flow, such as emerging weather fronts. I will also present results that show the meshes produced using this method naturally align to the solution structure, thus resolving the flow more efficiently and accurately.

SHIHUA WEN

Novartis Pharmaceuticals Corporation

Benefit-Risk Assessment Using Patient-Level Data

Structured benefit-risk (BR) assessment has recently been employed by FDA and EMA during the regulatory review process. Value tree, effect tables, and other quantitative BR assessment methodologies have appeared more frequently in regulatory submission packages. However, most of the BR analyses are based on evaluation of aggregated data (e.g., study level summary data). In this presentation, we propose a way to quantify the uncertainty of benefit-risk measure by utilizing patient-level data.

YUAN XIONG

Certara Strategic Consulting

Time-To-Event Analysis to Support Clinical Study Design and Dose Justification in Drug Development

Time-to-event analysis, sometimes referred to interchangeably with survival analysis, has drawn more and more attention from pharmacometricians for its natural link to underlying biological and physiological processes and its elegant theoretical basis in mathematics and statistics. This talk will begin with a brief review of the basic ideas behind time-to-event analysis and its association with traditional pharmacokinetic/pharmacodynamic modeling concepts. Next, real-life examples will be provided on how time-to-event analysis has been used in drug development, either independently or in conjunction with other approaches, to evaluate a drug candidate's efficacy profile, to identify influential covariates, to justify dose selection, and to inform clinical study design.

YUNAN YANG

The University of Texas at Austin

Optimal Transport and the Quadratic Wasserstein Metric for Seismic Inversion

Conventional FWI using the least-squares norm (L2) as a misfit function is known to suffer from cycle skipping. We proposed the quadratic Wasserstein metric (W2) as a new misfit function for FWI. It has been proved to have many ideal properties with regards to convexity and insensitivity to noise. Unlike the L2 norm, W2 measures not only amplitude differences, but also global phase shifts, which helps to avoid cycle skipping issues. We propose two ways of using the W2 metric in FWI: trace-by-trace comparison and global comparison. Numerical results on synthetic models and field data demonstrate the promising future of this new misfit function.

EHUD YARIV

Technion

Singular-Perturbation Analysis of Phoretic Self-Propulsion

Phoretic self-propulsion of micron-size particles is a vibrant research area which has attracted significant attention in the physics, chemistry, and engineering communities. The underlying mechanism is a catalytic reaction at the particle boundary, converting chemical energy into mechanical motion in a viscous liquid solution. When the chemical reaction is nonuniform, this may result in particle motion. In my talk I will describe singular-perturbation analyses of several problems in the field, including: (i) the large-Peclet-number limit; (ii) slender particles; (iii) near-contact particle-wall interactions; (iv) advection-induced propulsion; and (v) regularization of the two-dimensional problem.

KYONGMIN YEO

IBM Research

Spectral Inverse Model for Advection-Diffusion Problem with a Limited Number of Data

We present a spectral inverse model to infer a smooth source function from a limited number of observations in the context of air pollution, where the source-receptor relation is given by an advection-diffusion equation. A smooth source surface is approximated by a set of Gaussian kernels on a pre-defined rectangular mesh system and the generalized polynomial chaos (gPC) expansion is used to represent the model uncertainty due to the fixed mesh system. It is shown that the convolution of gPC basis and the Gaussian kernel provides hierarchical basis functions for a spectral source estimation. The spectral inverse model is formulated as a stochastic optimization problem. We propose a mixed L_1 and L_2 regularization based on the hierarchical nature of the basis polynomials. It is shown that the spectral inverse model is capable of providing a good estimate of the source function even when the ratio of the number of parameters (m) to the number of data (n) is large, m/n > 50.

YIBO ZHAO

Rutgers University

Efficient Gaussian Process Modeling Using Experimental Design-Based Subagging

We address two important issues in Gaussian process (GP) modeling. One is how to reduce the computational complexity in GP modeling and the other is how to simultaneous perform variable selection and estimation for the mean function of GP models. Estimation is computationally intensive for GP models because it heavily involves manipulations of an n-by-n correlation matrix, where n is the sample size. Conventional penalized likelihood approaches are widely used for variable selection. However the computational cost of the penalized likelihood estimation (PMLE) or the corresponding one-step sparse estimation (OSE) can be prohibitively high as the sample size becomes large, especially for GP models. To address both issues, this article proposes an efficient subsample aggregating (subagging) approach with an experimental design-based subsampling scheme. The proposed method is computationally cheaper, yet it can be shown that the resulting subagging estimators achieve the same efficiency as the original PMLE and OSE asymptotically. The finite-sample performance is examined through simulation studies. Application of the proposed methodology to a data center thermal study reveals some interesting information, including identifying an efficient cooling mechanism.

SHUCHI AGRAWAL

Maharaja Agrasen College, University of Delhi

A Model For Microwave Heating of a Ceramic Slab

A reduced mathematical model for the microwave heating of a thin ceramic slab in a TE_{N03} cavity is studied. The study is motivated by an experiment designed by Morris Brodwin (1993) with the goal of uniformly heating a ceramic sample. Here the mode number N varies as a function of time. The more realistic source is replaced by dirac delta functions and non linear radiative losses are neglected. Steady-state solutions of the reduced model are given by exact, closed-form expressions.

Collaborator: Richard Moore

VALERIA BARRA

NJIT

Gravity-driven instabilities of thin viscoelastic films on an inverted plane

The theoretical and numerical study concerned the gravity-driven evolution of the interface of a thin viscoelastic film laying on an inverted plane. The governing equation is obtained as a long-wave approximation of the Navier-Stokes equations, including the gravitational body force, and the Jeffreys model for viscoelastic stresses. The Linear Stability Analysis is performed to compare theoretical predictions of the early stage of the dynamics, with the numerical results obtained. The competing effects of the physical parameters involved on the length and time scales of the instabilities are analyzed, in the linear and nonlinear regimes.

This work was carried out during the 2016-2017 school year by NJIT undergraduate students as part of an applied mathematics Capstone project. Partial support by NSF grant No. 1521717 is acknowledged.

Advisor: Shahriar Afkhami

Collaborators: Elizabeth Daudelin, Diego Rios, Urvya Iyer, Sonali Kamath, and Karl Marcus Schultz

RUI CAO

NJIT

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.

Advisor: Michael Booty

ABHISHEK CHOUDHARY

Rensselaer Polytechnic Institute

Axonal Transport in Cells: Modeling of Motor-Cargo Dynamics

Intracellular transport along the axon by molecular motors is a crucial component for long distance transfer of cargo inside neurons. We mathematically model the movement of a motor-cargo complex along a parallel arrangement of microtubules. The first passage time for a diffusing motor to reattach to a microtubule is computed, and key quantities of interest are derived for a macroscopic viewpoint of effective transport process over multiple motor attachment and detachment events.

Advisor: Dr. Peter R Kramer

LINDA CUMMINGS

NJIT

Modeling flow and fouling in membrane filters: Insights into filter design

We present first-principles models describing flow of particle-laden ``feed solution" through a membrane filter. Particles are removed from the feed via a combination of sieving (large particles) and particle adsorption within pores, leading to fouling of the filter. Such fouling increases the membrane resistance, which in turn impacts the flow. In this presentation we will describe some of our recent and ongoing work modeling membrane filtration and fouling. Particular emphasis is paid to how membrane filter design (in particular, permeability gradients across the membrane, and the internal branching structure of pores) can significantly affect filtration efficiency, as measured by (i) total throughput over a filter lifetime, and (ii) proportion of particles removed from the feed.

Collaborator: Pejman Sanaei

ANDREW DESTEFAN

NJIT

Numerical Methods for Finding Optimal Sampling Paths for Autonomous Vehicles

Autonomous surface vehicles and autonomous underwater vehicles (collectively referred to as AVs) are self-propelled waterborne drones which are commonly used to study various oceanographic properties. In this research, we are particularly interested in using AVs to better understand uncertain surface currents in oceanic domains. This requires determining an optimal sampling path, along which the AV can acquire the most information regarding the ocean currents. We accomplish this by means of the level set method, which is an algorithm capable of solving optimal control problems such as the minimum time-to-travel between two points in a given domain. Kalman filtering techniques are used in conjunction with the level set method for data assimilation purposes.

Advisor: Richard Moore

CASEY DIEKMAN

NJIT

Modeling Circadian Rhythms of Cardiac Arrhythmias

The cardiomyocyte circadian (~24-hour) clock influences multiple intracellular processes, including transcription and contractile function, and has recently been linked to ventricular arrhythmias in mice (Jerayaj et al. (2012) Nature 483:96-100). Circadian rhythms have also been observed in transient outward potassium current (Ito) – a current that dominates mice action potential (AP) repolarization. We used mathematical modeling to study the dynamical mechanisms underlying secondary oscillations during the repolarization phase of the AP. These oscillations, called early afterdepolarizations (EADs), have significance because they are associated with heart failure and arrhythmias. It can be shown that EADs arise from a Hopf bifurcation and that this can occur for certain ranges of the Ito conductance (Zhao et al. (2012) Cardiovascular Research 95:308-316). We investigated how variation of calcium and IKs potassium conductances affects the range over which EADs occur. This allows us to predict the role circadian regulation of currents other than Ito could play in cardiac activity. Finally, we compare our results on daily rhythms in EADs to existing data on the times of day that humans are most likely to suffer sudden cardiac death.

SHIDONG JIANG

NJIT

Unsteady Stokes Flow in Complex Moving Geometries

We present a high-order scheme for unsteady Stokes flow in complex moving geometries. The scheme is built upon an accurate evaluation of the unsteady Stokes layer potentials in complex moving geometries. Several numerical examples are provide to demonstrate the performance of the scheme.

Collaborator: Leslie Greengard

LENKA KOVALCINOVA

NJIT

On Connection Between Topology and Memory Loss in Sheared Granular Materials

We present combined results of discrete element simulations and topological data analysis that allows us to characterize the geometrical properties of force networks. Our numerical setup consists of the system of cylindrical particles placed inside rectangular box with periodic boundary conditions along the horizontal direction. System dynamics is driven by constant shearing speed of the top and bottom walls (in the opposite directions) and pressure applied on the top wall in a dense flow regime. Our study reveals the origin of memory loss in granular systems through local rapid changes in force networks. Surprisingly, our results suggest that the memory loss is driven mainly by pressure even in the case of fixed inertial number. We conclude that the interplay between physical properties of the granular system and force network geometry is a key to understand the dynamics of the sheared systems.

Advisor: Lou Kondic

RANDOLPH LEISER

NJIT

Frequency Response Alternating Map: A Mutually Forced Approach to Resonant Networks

An impedance profile represents the interaction between a neuron and periodic forcing. The interplay of frequency preference and amplitude response give us insight into the preferred forcing for optimal output. However, this idea becomes much more complex when applied to a network. Although resonance has been observed in several neuron types, the resonant properties of neuronal networks and the functionality of the impedance profile are still not well understood. The interactions of multiple frequency preferences can open op behaviors that individual cell would not be capable of alone. The frequency preference of a network is unable to be determined given the intrinsic frequency preference of its cells. We aim to develop a tool that allows us to predict and analyze the resonant properties of a coupled network from the resonant properties of the participating neurons. We test these ideas in a minimal network model of two electrically coupled neurons, measuring the network response in terms of impedances of the two coupled cells.

Advisor: Horacio G. Rotstein

PAN LIU

Carnegie Mellon University

Bilevel training scheme and fractional order TGV regularizers in image processing

A new fractional order seminorm, TGV^r , r ∈ R, r ≥ 1, is proposed in the one-dimensional setting, as a generalization of the standard TGV^k -seminorms, k ∈ N. The fractional TGV^r -seminorms are shown to be intermediate between the standard TGV^k -seminorms of integer order. A bilevel learning scheme is proposed, where under a box constraint a simultaneous optimization with respect to the parameter α and the order r is performed. A numerical implementation of the learning scheme is provided, as well as an example where the optimal reconstruction is achieved for non-integer values of the order of derivation r.

Advisor: Irene Fonseca

Collaborator: Elisa Davoli

MATTHEW MOYE

NJIT

Data Assimilation and Electrophysiological Modeling of Mammalian Circadian Clock Neurons

Recently there has been interest in the application of data assimilation tools to the improvement of neuronal models. Often, the only data one has access to is the measured voltage from a current-clamp experiment with a prescribed injected current. Our work aims to improve understanding of how well one can recover characteristics of excitability such as voltage profile and bifurcation diagrams. Parameter estimation results will be shown from an Unscented Kalman Filter (UKF). We will test the performance on constant currents to replicate the scenario of spontaneous firing in circadian cells. The ability of these various stimulus protocols to enable state and parameter estimation will be assessed using simulated data from the Morris-Lecar model and a biophysical model of mammalian circadian clock neurons in the suprachiasmatic nucleus.

Advisor: Casey Diekman

MOHIT NAKRANI

NJIT

Breakup of Liquid Filaments

In this study, we focus on the breakup of finite size liquid filaments on substrates, using direct numerical simulations. We illustrate the effects of three parameters: Ohnesorge number, the ratio of the viscous forces to inertial and surface tension surfaces, the liquid filament aspect ratio, and a measure of the fluid slip on the substrate, i. e. slip length. Through these parameters, we are able to determine whether a liquid filament breaks up into one or multiple droplets or collapse into a single droplet on the substrate. We compare our results with the results for free standing liquid filaments. We show that the presence of the substrate promotes breakup of the filament. We also discuss the effect of the degree of slip on the break up.

This work was carried out during the 2016-2017 school year by NJIT undergraduate students as part of an applied mathematics Capstone project. Partial support by NSF grant No. 1521717 is acknowledged.

Advisor: Shahriar Afkhami

Collaborators: Andrew Dziedzic, Binah Ezra, Lou Kondic, and Musa Syed

ADAM PONZI

IBM T.J. Watson Research Center

Modeling Striatal Network Dynamics in Disease

Dysregulated striatal information processing is thought to play a crucial role in the pathology of multiple diseases such as Huntingtons, Parkinsons, depression and addiction. Previous striatal network modelling [Ponzi, A and Wickens J (2010). Sequentially switching cell assemblies in random inhibitory networks of spiking neurons in the striatum. Journal of Neuroscience, 30(17), 5894-5911. Ponzi, A and Wickens J, Optimal balance of the striatal medium spiny neuron network. PLoS Comput Biol 9, no. 4 (2013): e1002954] suggested that the normal medium spiny neuron network may be poised close to a critical state between stable and unstable dynamical regimes. To investigate how disease pathologies can affect this balance we made a more detailed computational model of the striatal network comprising more biologically detailed spiny projection neurons with multiple ion channels and fast spiking interneurons.

We first confirm that this more detailed network model also shows a non-trivial critical state in the striatally appropriate parameter regime. Next we explore how a variety of modifications to the individual cell ion channels, to the network structure and synaptic properties and to the excitatory driving, move the network dynamics away from this optimal critical state. We compare these pathological states with experimental observations from disease states to provide insight into the physiological modifications underlying the aberrant network phenotypes and to isolate targets for pharmacological intervention as part of a quantitative network systems pharmacology.

Collaborator: James Kozloski

ZACHARY VAN RIJN, CHANCHALA KADDI, AND KARIM AZER

Translational Informatics, Sanofi U.S.

Multiple-Interface Solver Toolkit (MIST): Efficient and Modular Quantitative Systems Pharmacology Modeling Framework

Multiple-Interface Solver Toolkit (MIST) is a cross-platform software framework for converting established quantitative systems pharmacology (QSP) models into hardware-optimized, compiled software libraries for simulation within high-level languages such as MATLAB © (The MathWorks, Inc., Natick, MA), PHP, Python, and R.

The model, solver, and other necessary components are compiled and packaged together in the form of a software library which provides a consistent front-end interface to the model in the modeler's preferred language. This front-end is not a graphical user interface (GUI) but a function via which the modeler may pass data or receive the final simulation output. During a simulation, all computation is performed by the self-contained library and within pre-allocated memory belonging to that language's interpreter. This avoids redundant data transfer, further reducing overhead which is critical to the efficiency of running successive simulations.

The MIST framework is also capable of supporting massively-parallel distributed simulations using both central- and graphics-processing unit (CPU and GPU) hardware on Windows and Unix-like platforms without requiring the modeler to modify their code, even between initial development and production simulations. Written in C, the MIST framework is portable in that MIST libraries can be compiled to target any architecture (such as x86 or ARM) or platform with a supporting C compiler.

MIST currently uses solvers from the SUNDIALS suite (Hindmarsh et al., Lawrence Livermore National Laboratory) as a back-end, though alternative numerical integration libraries such as Odeint (Ahnert, Mulansky, 2011) or others written in C, C++, and/or Fortran may be used. The Intel ® Math Kernel Library may be utilized for optimized BLAS/LAPACK routines if available. By using a compiled language, additional optimizations, static code analysis, and further hardware-specific profiling and tuning can be performed.

MIST has been tested on three QSP models in the rare disease and immunology therapeutic areas. These models range in scale from 52 to 145 state variables, and are all multi-scale models comprised of PK, molecular, cellular, and organ sub-models. Simulation time has been reduced by a factor of between 40 and 60 compared to the identical hand-optimized MATLAB implementations

While the MIST framework is written in C, modelers are not required to know the language, even to port a model to the MIST framework. In addition, we are currently developing tools to automatically port existing models from MATLAB, R, and other languages into the MIST framework. In the future, we hope to expand MIST to directly perform model order reduction, sensitivity analysis, or optimization, thus providing these hardware-optimized features through any supported front-end interface.

By using the MIST framework, modelers are now able to harness the performance of native Fortran or C models from within their preferred languages, as well as transition seamlessly from development to production environments using the same codebase.

PEJMAN SANAEI

NJIT

Curvature and Stress Driven Tissue Growth in a Tissue Engineering Scaffold Pore

Cell proliferation within a porous tissue engineering scaffold depends sensitively on the choice of pore geometry and flow rates: regions of high pore curvature encourage cell proliferation while a critical flow rate is required to promote growth. When the flow rate is too slow the nutrient supply is limited; too fast and the cells become damaged due to the high shear. As a result, determining appropriate tissue engineering construct scaffold geometries and operating regimes poses a significant challenge that cannot be addressed by experimentation alone. We present a mathematical theory for the fluid flow within a pore of a tissue engineering scaffold, which is coupled to the growth of cells seeded on the on the pore walls. In addition, we exploit the slenderness of a pore that is typical in such a scenario, to derive a reduced model that enables a comprehensive analysis of the system to be performed. Furthermore, we also demonstrate how the simplified system may be used to suggest improvements to the design of a tissue engineering scaffold and the appropriate operating regime.

Advisors: Linda J. Cummings

Collaborators: Ian M. Griffiths and Sarah L. Waters

SOMAYYEH SHEIKHOLESLAMI

The University of Southern Mississippi

Solution of PDEs for first-order photobleaching kinetics using Krylov subspace spectral methods

We show how to solve the first order photobleaching kinetics partial differential equations with prebleach steady state initial conditions using a time-domain method known as a Krylov Subspace Spectral method (KSS method). KSS are explicit methods for solving time-dependent variable-coefficient partial differential equations(PDEs). KSS methods are advantageous compared to other methods because of its high resolution and its superior scalability. We will apply Gaussian Quadrature rules in the spectral domain developed by Golub and Meurant to solve PDEs. We present a simple rough analytical solution, as well as a computational solution that is first-order accurate. We then use this solution to examine short and long time behaviors.

Advisors: James Lambers

Collaborators: James Lambers

DAVID SHIROKOFF

NJIT

Unconditional Stability for Multistep Imex Scheme

Unconditional stability is a desirable property of a time stepping scheme, as it allows the choice of time step solely based on accuracy considerations. Of particular interest are problems for which both the implicit and explicit parts of the ImEx splitting are stiff. Such splittings can arise, for example, in variable-coefficient problems, or the incompressible Navier-Stokes equations. To characterize the new ImEx schemes, we introduce an unconditional stability region, which plays a role analogous to that of the stability region in conventional multistep methods. Moreover, we will show how the new diagrams explain the fundamental stability restrictions of the well-known semi-implicit backward differentiation formulas (SBDF). We further show that the new ImEx coefficients can overcome the limitations of SBDF, and highlight their utility with several examples arising from partial differential equations: such as variable diffusion, advection diffusion and, time permitting a time dependent Stokes equation.

YIXUAN SUN

NJIT

Investigating the Performance of Pleated Membrane Filters

Pleated membrane filters are used in a wide variety of applications to remove particles and undesired impurities from a fluid. In a typical pleated filter cartridge, a membrane filter is sandwiched between two, much more porous, support layers. The resulting three-layer structure is pleated and packed into an annular cylindrical cartridge with mesh walls. The pleated construction allows a large filtration surface area to be confined to a small volume, allowing for rapid filtration. However, filtration performance, as measured by flux processed for a given pressure drop, is inferior when compared to the equivalent area flat (non-pleated) membrane in dead-end filtration. The precise reasons for this difference in performance have so far proved elusive, and likely involve several factors. In order to understand which of the factors play a key role for the performance difference, we investigated the pleated filter via simple first-principles modeling, first to understand the effect of pleating and the role played by the supporting layer; and subsequently, to understand how the details of the membrane's internal structure (the pore shape) affects filtration performance.

Advisor: Linda J. Cummings

Collaborators: Pejman Sanaei, Linda J. Cummings, and Lou Kondic

TADANAGA TAKAHASHI

NJIT

Analyzing Force Networks in Granular Systems using Persistent Homology

Our goal is to use persistent homology to analyze the results from an experiment which aimed to study the force propagation in a 2D granular system under impact. In the experiment, photoelastic particles were exposed to impact causing the photoelastic response proportional to the amount of exerted force. The particles display an elaborate chain-like pattern that spreads as the intruder, the falling object, penetrates the system. We use persistent homology as a means of characterizing the behavior of the force chains in terms of their topological features. We cross validate the information from the persistence diagrams and the physical measurements from the experiment. We have found that the total persistence is highly correlated with the acceleration of the intruder for multiple experiment settings, suggesting that topologically based measures could be used to quantify the material response.

This work was carried out during the 2016-2017 school year by NJIT undergraduate students as part of an applied mathematics Capstone project. Partial support by NSF grant No. 1521717 and by DARPA grant HR0011-16-2-0033 is acknowledged.

Advisor: Lou Kondic

Collaborator: Joseph Ballardo

ANGELO TARANTO AND LENKA KOVALCINOVA

NJIT

Force Chains in Granular Materials

In this project, classical granular measures, percolation theory, and persistent homology are applied to simulated three dimensional particulate systems. The simulations involve compressing the particles to the packing fraction of 0.75. To reduce the effect of noise, we average our results over 20 different realizations of the same nominal simulations. We seek to understand the effect of particle friction and system size on the percolation, topology, and on a set of classical measures for particulate systems. To investigate the effects of both friction and the system size, we consider three different system sizes and three different friction levels. Our particular focus is on analysis of force networks that develop in compressed particulate systems. The results include the comparison of the uncovered force network properties obtained using the techniques considered. Regarding the influence of system size, we find that the results are qualitatively similar, suggesting that the system size does not influence the main features of the force networks. Regarding friction, we find that it plays an important role in determining the properties of force networks, and correspondingly the mesoscopic properties of compressed particulate systems.

This work was carried out during the 2016-2017 school year by NJIT undergraduate students as part of an applied mathematics Capstone project. Partial support by NSF grant No. 1521717 and by DARPA grant HR0011-16-2-0033 is acknowledged.

Advisor: Lou Kondic

Collaborators: Jake Brusca, Sidney Carr, Chao Cheng (Lab Assistant), Robert Cuber, Andrew Firriolo, Christian Granier, Rahul Halder, Beatriz McNabb, Alina Mohit-Tabatabai, Josef Mohrenweiser, and William Ruys

ZICONG ZHOU

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Mesh/Grid Generation thru Deformation Method

The proposed deformation method for Grid Generation is done by solving a so-call div-curl-ODE system and looking for a diffeomorphism that deforms from a uniform mesh to a expected mesh with positive prescribed Jacobian determinant.

Advisor: Liao, Guojun

Collaborators: Liao, Guojun; Chen, Xi; Zhou, Zicong

YALIN ZHU

NJIT

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 can be obtained for developing the inference by inverting the Hessian matrix. Model diagnostic can be checked by computing likelihood, model deviance and Pearson residual.

Advisors: Sunil Dhar and Wenge Guo

Collaborator: Sunil Dhar

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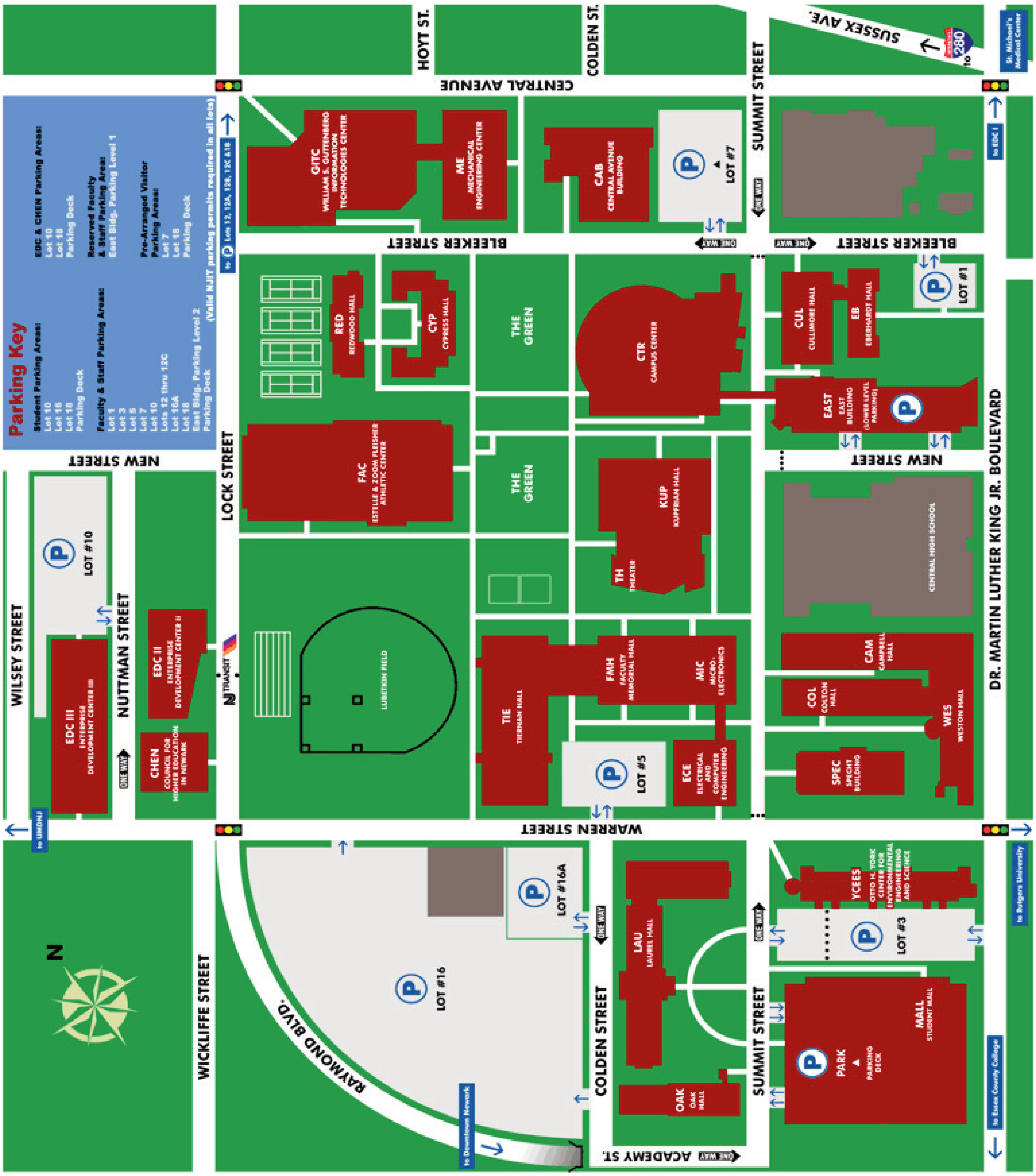
NJIT CAMPUS MAP



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