Abstracts

Plenary Speaker

Exploring the Effects of Order of Events in Population Models with Discrete Time

Suzanne Lenhart

University of Tennessee at Knoxville

Careful consideration of the order of events will be discussed for formulating population models with discrete time. Two examples will show how the order of events can affect optimal control results; the control actions include harvesting and augmentation of a population . One of the models is an integrodifference system which is continuous in its spatial variable..

Career Panel Discussion: Finding a Job

Panelists:

- Elise Zipkin (Research Ecologist at U.S. Geological Survey)
- Marco Enriquez (Sr. Applied Mathematician at the MITRE Corporation)
- Barry Thorton (National Security Agency)
- Anthony Kearsley (Research Mathematician at National Institute of Standards & Technology)

Student Paper Presenters

Secondary Intracranial Aneurysm Formation Due to the Effects of a Primary Aneurysm

Bruno Beltran (`bbeltr1@tigers.lsu.edu`)
Louisiana State University [Advisor: Dr. Baojun Song]

Computational fluid dynamics has been employed extensively to model single aneurysm development. We extend these ideas to model how the hemodynamic instabilities caused by a primary aneurysm might impact secondary aneurysm formation. Specifically, we study the risk of developing a secondary aneurysm on the anterior communicating artery given a primary aneurysm at the bifurcation between the posterior communicator artery and the basilar artery. A relative decrease in wall shear stress of 0-4 percent is interpreted as indicating that the removal of an intracranial aneurysm will not delay the formation of further aneurysms nearby, contrary to what was expected.

This work was done in collaboration with Courtney Bruce, Daniel Burkow, and Sarah Erickson.

Transmission Eigenvalues and the Void

Isaac Harris (`iharris@udel.edu`)
University of Delaware [Advisor: Dr. Fioralba Cakoni]

The transmission eigenvalue problem is a new class of eigenvalue problems that have recently appeared in inverse scattering theory for inhomogeneous media. I am working on the inverse electromagnetic scattering problem for anisotropic inhomogeneous media with voids. My main goal is to study the inverse problem of determining the material properties of the medium and the void. This is an important problem since it arises in nondestructive testing of exotic materials. The transmission eigenvalue problem is non self-adjoint and nonlinear which make its mathematical investigation interesting and challenging. Theoretical and Numerical results will be given.

This work was done in collaboration with Jiguang Sun.

Monte Carlo Simulations Probing the Effects of the Disjointing Potential Function on Grain Boundary Premelting

James Hickman (`jh6810@gmail.com`)
George Mason University [Advisor: Dr. Yuri Mishin]

The work being presented studies the emergence of a liquid phase in the Copper-Silver system below the melting temperature at the interface between two grains with different crystallographic orientations. This phenomenon is commonly refereed to as grain boundary (GB) premelting. The current study primarily focuses on probing this liquid layer via the application of Monte Carlo molecular simulations using an interatomic potential obtained from the Embedded Atom Model (EAM). This potential is used to describe the interactions between the various particles. The premelting phenomenon can be understood by the presence of an excess in Gibbs free energy at the GB relative to the bulk. However, a second factor known as the disjointing potential function is also present which is associated with an overlap of density waves in the interfacial region. It is the goal of this work to obtain the functional form of the disjointing potential for this system based on the simulation results described above.

Volume-Constrained Problems of a Linear Nonlocal Convection-Diffusion Equation

Zhan Huang (zxh117@psu.edu)
Pennsylvania State University [Advisor: Dr. Qiang Du]

We propose and study the homogenous Dirichlet and Robin volume-constrained problems associated with a linear nonlocal convection-diffusion equation. As the horizon parameter vanishes, our well-posed formulations converge to boundary-value problems of convectional local convection-diffusion equation. We show that they enjoy features like maximum principle and conservation law, just as their local correspondence do. Monte Carlo simulations and finite difference schemes are applied to show the effects of time, kernel, horizon and different volume constraints. Moreover, we also reveal that, different nonlocal volume-constraint formulations are actually analogous to different finite-difference discretizations of local boundary value problems.

Exterior-Point Method for Support Vector Machines

Byong Kwon (bkwon1@masonlive.gmu.edu)
George Mason University [Advisor: Dr. Igor Griva]

This talk presents an exterior-point method (EPM) for training support vector machines. The EPM is an algorithm based on the nonlinear rescaling and augmented Lagrangian methods, which can be used to solve constrained, nonlinear optimization problems.

This work was done in collaboration with Veronica Bloom, and Anna-Rose Wolff.

Comparison of Tests of Homogeneity of Binomial Proportions

Peter Linton (pet3@umbc.edu)
University of Maryland Baltimore County [Advisor: Dr. Anindya Roy]

In this talk I present a review of tests of homogeneity of binomial proportions in the statistics literature. For sparse data, most test procedures may fail to perform well. A review of nine classical and recent testing procedures will be presented along with an empirical comparison of powers and size.

This work was done in collaboration with Martin Klein.

Numerical Methods for Conservation Laws using Chebfun

Matthew Moye (mmoye@udel.edu)
University of Delaware [Advisor: Dr. Tobin Driscoll]

This project aims to extend the Chebfun package in Matlab to solve for scalar hyperbolic conservation laws. An algorithm proposed by Fijavž et. al is based on the principle that the area under the solution curve changes in time according to the flux at the boundaries, even after shocks develop. The initial data is parameterized so that it can be evolved by the method of characteristics. Given a convex/concave flux and a piecewise smooth initial condition, spectrally accurate quadrature and rootfinding are used to apply the equal area principle in order to locate shocks and compute a physically meaningful solution at any given time.

This work was done in collaboration with Tonatiuh Sanchez-Vizuet.

Shape Optimization of Superhydrophobic Surfaces using Energy Landscape Considerations

Kellen Petersen (kellen@cims.nyu.edu)
New York University [Advisor: Dr. Weiqing Ren]

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

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

This work was done in collaboration with Benedikt Wirth.

A Symbolic Algorithm to Compute Lax Pairs in Matrix Form for Nonlinear Evolution Equations

Jacob Rezac (rezac@math.udel.edu)
University of Delaware [Advisor: Dr. Willy Hereman]

Integrable nonlinear partial differential equations (PDEs) can often be expressed in terms of a compatibility condition called a Lax pair. While Lax pairs are important, for example, in finding solutions of these PDEs with the inverse scattering transform, straightforward methods for their calculation are rare. We will present a direct algorithmic method for the construction of a class of Lax pairs in matrix form for completely integrable nonlinear PDEs. The technique is based on scaling symmetry properties which reduce the problem to one of solving nonlinear algebraic equations. As such, it can be implemented in any computer algebra system. Prototype Mathematica software will be demonstrated for nonlinear integrable evolution equations, including the Korteweg-de Vries, sine-Gordon, and nonlinear Schrodinger equations.

A Mathematical Model for Cholera Dynamics with Movement of Population

Nourridine Siewe (siewe.nourridine@bison.howard.edu)
Howard University [Advisor: Dr. Abdul-Aziz Yakubu]

A mathematical model for the dynamics of cholera is presented. A chronological account of previous cholera models is presented, from which we eventually derive one that, while conforming to literature, summarizes the most celebrated recent models.We take into account the hyper-infectious and lower infectious natures of the Vibrio cholerae, as well as the two known states of human infection by cholera. Preliminary analysis is done and a patchy model is formulated, assuming non-homogeneity of human populations in space.

This work was done in collaboration with M.I. Teboh-Ewungkem, and G.A. Ngwa.

Optimization Techniques with Applications to Infectious Diseases

Alexandra Signoriello (alsignoriello@ursinus.edu)
Ursinus College [Advisor: Dr. Mohammed Yahdi]

Optimization techniques are critical when studying infectious diseases because of the randomness and uncertainty in biological systems. Data fitting and computational optimization techniques are applied to two infectious disease models; Influenza (Flu) and Vancomycin-Resistant Enterococci (VRE). The applications result in a better understanding of the roles of the parameters and the network in the system, which will ultimately lead to better prevention techniques.

Using Bioinformatic Approaches to Predict Gene Expression from Promoter Structure in Acute Myeloid Leukemia

Natalie Stanley (stanleyn@dickinson.edu)
Dickinson College [Advisor: Dr. Jeffrey Forrester, and Dr. Michael Roberts]

The HL-60 cell line can be used as an experimental model for acute myeloid leukemia, an important hematological cancer. These cells can be induced to behave normally in culture. As the cancerous cell changes into one that is macrophage-like, its gene expression patterns are altered. To analyze these changes, we performed a cluster analysis of microarray data and grouped the genes based on their temporal expression patterns throughout this transition. The control of gene expression is orchestrated by a class of proteins called transcription factors, whose binding sites are present in the promoters of the cellular genes. Often, transcription factor binding sites, or motifs, are over-represented in DNA sequences, and can be determined computationally. After using an algorithm to obtain statistically significant motifs from each expression cluster, we utilized a Nave Bayes Model to predict gene expression patterns, based on the presence or absence of the individual motifs. This talk will give an overview of the Nave Bayes Model in the context of gene expression in acute myeloid leukemia. In addition, it will explore how to optimize the models parameters to allow for the most accurate recapitulation of the expression clusters.

Mean-field Model of Systemic Risk

Chao Tian (tian_c@math.psu.edu)
Pennsylvania State University - University Park [Advisor: Dr. Qiang Du]

Systemic risk is the risk that in an interconnected system of agents that can fail individually, a large number of agents fails simultaneously or nearly so, leading to the overall failure of the system. In this talk we present a system of bistable mean-field model of systemic risk motivated by the phenomena of dynamical phase transitions and metastability for ferromagnetic Curie-Weiss models with continuous spin. Similar models have been proposed in chemical kinetics, statistical physics, and large economic systems.

Analysis and Comparison of Different Approximations to Nonlocal Diffusion and Linear Peridynamic Equations

Xiaochuan Tian (xzt101@psu.edu)
Penn State University [Advisor: Dr. Qiang Du]

We consider the numerical solution of nonlocal constrained value problems associated with linear nonlocal diffusion and nonlocal peridynamic models. Two classes of discretization methods are presented which include standard finite element methods and quadrature based finite difference methods. We discuss the applicability of these approaches to nonlocal problems having various singular kernels and study some basic numerical analysis issues concerning these discrete schemes. We illustrate the similarities and differences of the resulting nonlocal stiffness matrices and establish properties such as discrete maximum principles. We pay particular attention to the issue of convergence in both the nonlocal setting and the local limit. The latter reveals that while some methods tend to converge to the intended solutions, other methods lead to the possibility of convergence to unintended local limits. Our results thus offer important guidance to practical applications of nonlocal models.

Stochastic and Agent Based Models of the Effect of Preventive Measures on a Nosocomial Infection

Jayant Velagala (javelagala@ursinus.edu)
Ursinus College [Advisor: Dr. Mohammed Yahdi]

Nosocomial infections claim about 100; 000 lives per year. About one-third of infections contracted in intensive care units (ICU) are caused by Vancomycin-Resistant Enterococci (VRE). Stochastic and Discrete-time Markov chains approaches are used to understand the VRE dynamics and the impact of preventive measures both at the compartmentally structured model of ICU patients as well as at the agent based model. The models take in consideration the uncertainty of the parameter values and transitions. In particular, critical health condition of a patient is linked to the most effective level of chlorhexidine baths to significantly reduce VRE infections and mortality rate.

Quality Control of Sensor Data and Data Provenance Tracking

Yujia Zhou (zhouy@dickinson.edu)
Dickinson College [Advisor: Dr. Emery Boose, Dr. Barbara Lerner, and Dr. Leon Osterweil]

In this research, we developed R programs to detect and fix quality control problems of data from the meteorological station at Harvard Forest. In order to provide a Data Derivation Graphs (DDG) that can record the full provenance of data, we built a process simulating scientists initial processing of the raw data and the reprocessing after some of the quality control techniques are updated. We implemented this process in both Kepler and Little-JIL to compare the data provenance graphs they produce from identical processes. We found that while Kepler is easier to use for scientists with no programming background, Little-JIL has a much stronger visualization tool for drawing comprehensive DDGs and stores more information in them.

Student Poster Presenters

A New Twist on Computing the Matrix Exponential

Bruno Beltran (bbeltr1@tigers.lsu.edu)
Louisiana State University [Advisor: Dr. Frank Neubrander]

Traditionally, methods involving "scaling and squaring" and low order Pade approximants have been employed to calculate e^{tA}. New results prompt the exploration of the use of higher order Pade approximants without scaling and squaring, which we find to have comparable accuracy and computational cost to the methods built into Matlab, and a much lower cost than those built into Mathematica. We extend our results to develop an efficient numerical method for the inversion of the Laplace transform.

This work was done in collaboration with Avery St. Dizier, and Tyler Wales.

Categorizing Objects in Lipid Microscope Images from the Ocular Surface

Dylan Chapp (dchapp@udel.edu)
University of Delaware [Advisor: Dr. Richard Braun]

The lipid layer of the tear film is the outermost layer of the tear film. By examining images obtained by high-resolution microscopy of the lipid layer, the overall health of the tear film can be characterized. In particular there are several types of local-level features indicative of clinical conditions. These features are easy for a human observer to detect, but the number of images produced per patient necessitates an automatic classification scheme. We develop such a scheme in Matlab to classify images by means of clustering algorithms and local-level statistical information.

This work was done in collaboration with Tianyu Qiu, and P.E. King-Smith.

Modeling the Wnt Pathway in the Human Colonic Crypt

Brooks Emerick (emerick@math.udel.edu)
University of Delaware [Advisor: Dr. Gilberto Schleiniger]

A series of chemical reactions within a single cell known as the Wnt pathway, plays an important role in colonic crypt development, cell proliferation, and oncogenesis. In this model, we analyze the behavior of several key players of the Wnt pathway and expand an ODE system into a PDE system along the major crypt axis. This allows us to track the evolution of protein concentration gradients along this axis, which can help us define a specific cell type at each level of the crypt or determine the crypt's condition.

This work was done in collaboration with Bruce Boman.

Prisoner Reform Programs and Their Impact on Recidivism

Kimberly Gutstein (khg7.kg@gmail.com)
Humboldt State University [Advisor: Dr. Luis Melara]

The California prison system has a high percentage of people who return to prison within a three year period after release. A mathematical model is formulated to study the eeffectiveness of Reentry Court programs first time offending parolees designed to reduce the prison return rates when implemented alone or in conjugation with an in prison educational program. Parolees who participated in both in/out of prison programs are referred to as an ideal class in the model. Stability analysis and numerical simulations were carried out to study the impact of the programs. The results show that the reentry program reduces the recidivism rate more than the Basic Educational program within the prison system, but only when social influence of criminals is low outside of prison. However, for populations with high rates of social influences, incarceration rates should be large in order to get the same impact of the reentry program.

This work was done in collaboration with Brenda Martinez, Itelhomme Fene, and Wilson Alvarez.

Modeling Shale Gas Production Using the Cobb-Douglas Production Function

Frank Liao (fliao@student.hagerstowncc.edu)
Hagerstown Community College [Advisor: Dr. Yuying Xie]

The Cobb-Douglas Production Function has been widely used in economics to demonstrate the relationship between input factors and the output, which usually represents the maximum production level. In this research, we attempt to utilize the Cobb-Douglas Production function to analyze the shale gas production and employment data, and validate predictions regarding the booming shale gas drilling, including the potential production level in the near future and the employment generated from shale gas industry.

Perturbation Methods and Green Oxidation Catalysts

Diego Torrejon (dtorrejo@masonlive.gmu.edu)
George Mason University [Advisor: Dr. Maria Emelianenko]

Oxidation, a process in which oxygen is added to break pollutants or organic wastes, is important in many industries. However, this process often uses chemicals that can result in the production of hazardous substances, so it is imperative to be able to control the process to make it environmentally safe.

In this poster, we study the problem of suicidal inactivation of enzymes and man-made oxidation catalysts. Based on experimental data obtained from our colleagues at Carnegie Mellon University, we formulate a system of differential equations that models chemical reactions and analyze its numerical and analytical properties. The main goal is to be able to estimate the rates of the reactions based on limited experimental observations. The nonlinear 3-dimensional ODE system under investigation does not allow for an exact solution. However, noticing its similarity with Michaelis-Menten system, we have been able to develop quasi-state approximation of the model that together with perturbation techniques has allowed us to derive an approximate solution matching experimental observations to a high degree of accuracy. It is expected that these novel techniques will yield even more far-reaching results when applied to more realistic systems taking into account complex interactions between the catalysts.