2015 Georgia Scientific Computing Symposium

Saturday, February 28, 2015

Georgia Institute of Technology

9:30 **Registration, Poster Setup, Coffee**

9:50 **Opening Remarks** – Edmond Chow, Georgia Institute of Technology

Session 1 – Chair: Alessandro Veneziani, Emory University

10:00 Yuliya Babenko, Kennesaw State University
Adaptive Approximation and Interpolation: Error Analysis and Construction of the Partitions

10:50 Juan Gutierrez, University of Georgia
The Case for Science Engineering: Systems Biology of Malaria

11:40 **Poster Blitz** – Chairs: Sung Ha Kang and Edmond Chow, Georgia Institute of Technology

12:00 **Lunch and Posters**

Session 2 – Chair: Alexandra Smirnova, Georgia State University

1:30 Haesun Park, Georgia Institute of Technology
Nonnegative Matrix Factorization for Large-scale Clustering and Topic Discovery

2:20 Lars Ruthotto, Emory University
Numerical Methods for Hyperelastic Image Registration

3:10 **Break and Posters**

Session 3 – Chair: Ming-Jun Lai, University of Georgia

3:50 Martin Short, Georgia Institute of Technology
Mathematics and Computing for Increased Security

4:40 Xiaojing Ye, Georgia State University
Fast Decentralized Gradient Descent Method

5:30 **Adjourn**

6:00 **Dinner** – *Zen on Ten Asian Bistro & Sushi Bar*

Sponsored by the School of Computational Science and Engineering, Georgia Institute of Technology

Abstracts of Invited Presentations

Yuliya Babenko
Department of Mathematics
Kennesaw State University

Adaptive Approximation and Interpolation: Error Analysis and Construction of the Partitions

Approximation by various types of splines is one of the standard procedures in many applications. In all these applications, there is a standard distinction between uniform and adaptive methods. In the uniform case, the domain of interest is decomposed into a partition where elements do not vary much. Adaptive partitions, on the other hand, take into consideration local variations in the function behavior and therefore provide more accurate approximations. However, adaptive methods are highly nonlinear and no polynomial time algorithm exists to provide an optimal approximant for each given function. Therefore, the next natural question would be to construct asymptotically optimal sequences of partitions and approximants on them.

We begin this talk by presenting the exact asymptotics of the optimal error in the weighted L_p-norm, $1 \le p \le \infty$, of linear spline interpolation of an arbitrary bivariate function $f \in C^2([0,1]^2)$. We further discuss the applications to adaptive mesh generation for finite element methods, and explore connections with the problem of approximating the convex bodies by polytopes. In addition, we provide the generalization of this result to asymmetric norm.

We give a brief review of known results and introduce a series of new ones. The proofs of these new results lead to algorithms for the construction of asymptotically optimal sequences of triangulations for linear interpolation. Moreover, we derive similar results for other classes of splines and interpolation schemes, in particular for splines over rectangular partitions and their generalizations. Finally, we shall discuss the harmonic splines, their advantages and disadvantages compared to polynomial splines.

Juan B. Gutierrez
Department of Mathematics
Institute of Bioinformatics
University of Georgia

The Case for Science Engineering: Systems Biology of Malaria

Half the world population is currently at risk of malaria infection, with 200 million clinical cases and 600,000 deaths in 2012. Even though this disease has attracted substantial research resources in the last century, the detailed characterization of the dynamics of malaria is still an open question. Existing mathematical models of malaria infection are rudimentary, and lack the immune data to expand the level of detail to useful predictive levels. The Malaria Host Pathogen Interaction Center (MaHPIC), a research consortium comprised by UGA, Emory, GT, and CDC is producing information about the disease at unprecedented levels of detail. In this talk I will present recent developments by our MaHPIC group in the mathematical modeling of the blood stage of malaria infection using a coupled system of differential equations comprised of two transport PDEs and a set of ODEs. I will also present the challenges in calibrating this type of model with 'omic technologies (transcriptomics, lipidomics, proteomics, metabolomics, and clinical data). Our preliminary model is able to reproduce the clinical presentation of malaria: severe anemia on first infection, and coexistence of host and parasites in subsequent infections. The computational framework necessary to process the information for this project is reusable, and highlights commonalities among different disciplines that could leverage large-scale studies.

Haesun Park
School of Computational Science and Engineering
Georgia Institute of Technology

Nonnegative Matrix Factorization for Large-scale Clustering and Topic Discovery

In recent years, many constrained low rank approximations have been widely utilized in large-scale data analytics where the applications reach far beyond the classical areas of scientific computing. In this talk, we discuss some properties, algorithms, and applications of Nonnegative matrix factorization (NMF) for clustering and topic modeling of document data. A distinguishing feature of the NMF is the requirement of nonnegativity in the low rank factors, which enhances the interpretability and modeling capability for many applications. We offer new methods using the framework of NMF for efficient and effective clustering and topic modeling of large-scale text data. Our substantial experimental results show that rank-2 NMF based hierarchical and flat topic discovery methods called HierNMF2 and FlatNMF2 are far superior to other existing methods such as LDA (Latent Dirichlet Allocation) and k-means in terms of both scalability and solution quality.

This work is supported in part by DARPA XDATA and NSF/DHS FODAVA programs.

Lars Ruthotto
Department of Mathematics and Computer Science
Emory University

Numerical Methods for Hyperelastic Image Registration

Image registration is an essential task in almost all areas involving imaging techniques. The goal of image registration is to find geometrical correspondences between two or more images. Image registration is commonly phrased as a variational problem that is known to be ill-posed and thus regularization is commonly used to ensure existence of solutions and/or introduce prior knowledge about the application in mind.

This talk presents a nonlinear regularization functional based on the theory of hyperelastic materials, which overcomes limitations of the most commonly used linear elastic model. In particular, the hyperelastic regularization functional guarantees that solutions to the variational problem exist and are one-to-one correspondences between the images, which is a key concern in most applications.

The focus of this talk is on accurate and fast numerical methods for solving hyperelastic image registration problems. Further, the potential of hyperelastic schemes is demonstrated for real-life medical imaging problems and efficient numerical solution of PDEs.

Martin Short
School of Mathematics
Georgia Institute of Technology

Mathematics and Computing for Increased Security

A current trend in research is to turn to advanced mathematics and computing to solve an ever expanding array of social problems. In this talk, I will give a few concrete example of this, with the specific social problem under consideration being criminal behavior. I will discuss how statistical models of property crime, given large training data sets, can be used to predict when and where criminal events will occur, allowing police to decrease crime measurably by devoting resources accordingly. I will also discuss how similar models can be applied to gang violence, and how the resulting mathematics can help resolve unsolved gang crimes within large historical data sets. Finally, I will explore, through the application of game theoretic ideas, how we can try to deal with criminals who strategically alter their behavior to account for the predictions that police might make of future criminal activity.

Xiaojing Ye
Department of Mathematics and Statistics
Georgia State University

Fast Decentralized Gradient Descent Method

We consider the decentralized consensus optimization problem on a connected network where each node privately holds a part of objective function and data. The goal is to find the minimizer for the whole objective function while each node can only communicate with its neighbors during computations. We present a fast decentralized gradient descent method whose convergence does not require diminishing step sizes as in regular decentralized gradient descent methods, and prove that this new method can reach optimal (and unimprovable) convergence rate of $O(1/k^2)$ where k is the communication/iteration number. Numerical experiments also show that it significantly outperforms existing methods. Applications to seismic tomography on large-scale wireless sensor networks will be presented.

Poster Presentations

Deniz Alacam, Georgia State University
Network Bursting in Inhibitory Neuronal Circuits

Alessandro Barone, Emory University
HiMOD and HiPOD Methods for Solving Direct and Inverse Problems in Internal Fluid Dynamics

Vladimir Bondarenko, Georgia State University
Computer Simulation of the Beta1-Adrenergic Regulation of Ionic Dynamics in Mouse Ventricular Myocytes

Marta Canadell, Georgia Institute of Technology
Computation of Normally Hyperbolic Invariant Manifolds

Neranjan Suranga Edirisinghe, Georgia State University
Perfect Infection with Imperfect Virus: Influenza Infection Modeling

Fatma Tokmak Fen, Georgia State University
Nonlinear Second Order Impulsive Boundary Value Problems

Mehmet Onur Fen, Georgia State University
The Input/Output Mechanism of Chaos Generation

Xiuxiu He, Georgia State University
Modeling Cell Migration

Seong Jun Kim, Georgia Institute of Technology
Path Optimization with Limited Sensing Ability

Ming-Jun Lai, University of Georgia
Polygonal Splines and Their Applications

Wuchen Li, Georgia Institute of Technology
A Newton Algorithm in Method of Evolving Junctions for Solving Shortest Path Problem

Hui Liu, Georgia State University
On Generalized Cross Validation for Regularization Parameter Selection in the Model of Plasmodium falciparum *Malaria*

Aftab Patel, Georgia Institute of Technology
New Parallel Preconditioners for Non-symmetric Linear Systems

Talayeh Razzaghi, Clemson University
Multigrid Inspired Support Vector Machines

George Slavov, University of Georgia
Spline Solution of Nonlinear Reaction-Diffusion PDE for a Population Density over Irregular Domains

Joseph Vokt, Georgia Institute of Technology
A Structured Cholesky Factorization for Fock Matrix Construction

Zhengkai Wu, Georgia Institute of Technology
Towards Real-time 3D Simulation of Multi-axis Machining

Boyi Yang, Emory University
Novel In-Human Four Dimensional Wall Shear Stress Calculation of a Coronary Bioresorbable Scaffold using Optical Coherence Tomography Images and Blood Flow Simulations