Georgia Scientific Computing Symposium

Emory University

February 20, 2016

9:30	Registration, Poster Setup, Coffee
9:50	Opening Remarks
10:00	Michele Benzi, Emory University *Numerical Analysis of Quantum Graphs*
10:50	Alexandra Smirnova, Georgia State University *On Stable Parameter Estimation for Inverse Problems in Epidemiology*
11:40	Poster Blitz
12:00	Lunch and Posters
1:30	Qing Zhang, University of Georgia *Two-Time Scale Markovian Systems: Near-Optimal Controls and Applications*
2:20	Molei Tao, Georgia Institute of Technology *Two Numerical Methods for Multiscale (Stochastic) Differential Equations*
3:10	Group Photo – outside 2nd floor entrance
3:25	Break and Posters
3:50	Phanish Suranarayana, Georgia Institute of Technology *Towards Large and Fast Density Functional Theory Calculations*
4:40	Steven Hamilton, Oak Ridge National Laboratory *Acceleration of Monte Carlo Radiation Transport Eigenvalue Calculations*
5:30	Reception

Titles and Abstracts of Invited Talks

Michele Benzi

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Numerical Analysis of Quantum Graphs

We consider the numerical solution of eigenvalue and boundary-value problems for differential equations posed on graphs or networks. More specifically, the talk is concerned with quantum graphs, which are metric graphs endowed with a self-adjoint differential operator (Hamiltonian) acting on functions defined on the graph's edges with suitable side conditions. We describe and analyze the use of a linear finite element method for discretizing a class of simple Hamiltonians.

The solution of the discrete equations is achieved by means of a (non-overlapping) domain decomposition approach. For model elliptic problems and a wide class of graphs, we show that a combination of Schur complement reduction and diagonally preconditioned conjugate gradients results in optimal complexity. We also discuss time-dependent problems of parabolic type. Numerical results are presented for both simple and complex graph topologies.

This is joint work with Mario Arioli (University of Wuppertal).

Alexandra Smirnova
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On stable parameter estimation for inverse problems in epidemiology

Stable estimation of key epidemiological parameters at the onset of a new infectious disease is paramount in assisting public health authorities to rapidly assess the situation in order to determine whether the pathogen in question is capable of generating sustained local or global outbreaks. In particular, it is important to characterize the contribution of potential animal reservoirs (e.g., poultry) as well as human-to-human transmission to the overall pattern of disease spread. Moreover, a quantification of the rate of viral transmission to humans and the effectiveness of control measures is particularly useful to guide public health responses and provide a comprehensive risk assessment to emerging and re-emerging infectious disease threats. The main challenge of our research is to develop novel methods for the reliable estimation of transmission parameters relating to the dynamics of a pathogen and the contribution of different transmission pathways to the overall force of infection during an epidemic outbreak. This requires fitting model predictions to limited data comprised by aggregated time series of incident cases over some time period. In my talk I will present problem-oriented regularized computational algorithms aimed to improve existing techniques for reliable parameter estimation in ODE-constrained disease transmission models.

This is joint work with G. Chowell, H. Liu, L. deCamp, M. Sheppard.

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Two-Time Scale Markovian Systems: Near-Optimal Controls and Applications

Many real-life systems are of large scale and complex. An effective way of reducing computational complexity is to formulate the underlying problems as a two-time-scale system. Following a singular perturbation approach, one can obtain the associated limiting problem that is simpler to solve. In this talk, I will present various two-time scale systems, their convergence, near-optimal controls and applications. In particular, the talk will focus on asymptotic expansions of the corresponding probability distributions, convergence of occupation measures, asymptotic normality, among others. Applications in LQG control, the Wonham filter, and financial engineering will also be included.

Molei Tao
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Two numerical methods for multiscale (stochastic) differential equations

Motivated by rich applications, we are interested in controlling systems that are characterized by multiple scales, geometric structures, and randomness. This talk will focus on two computational steps in this long term investigation, both concerning long time solutions to differential equations with small parameters. The first half of the talk devotes to stiff equations. We developed integrators that do not resolve fast scales in these systems but still capture their effective contributions. These integrators require no identification of underlying slow variables or processes, and therefore work for a broad spectrum of systems (including stiff ODEs, SDEs and PDEs). They also numerically preserve intrinsic geometric structures (e.g., symplecticity, invariant distribution, and other conservation laws), which leads to improved long time accuracy.

The second half considers systems perturbed by small noise. The goal is to quantify what noises can do and utilize them. Noise-induced transitions are characterized by optimizing probabilities given by Freidlin-Wentzell large deviation theory. In gradient systems, transitions between metastable states were known to cross saddle points. We investigate nongradient systems, and show transitions may instead cross unstable periodic orbits. Numerical tools for identifying periodic orbits and for computing transition paths are proposed. If time permits, I will also describe how these results help design control strategies.

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Towards large and fast Density Functional Theory Calculations

Electronic structure calculations based on Density Functional Theory (DFT) have been remarkably successful in describing material properties and behavior. However, the large computational cost associated with these simulations has severely restricted the size of systems that can be routinely studied. In this talk, previous and current efforts of the speaker to develop efficient real-space formulations and massively parallel implementations for DFT will be discussed. These include linear scaling methods applicable to both insulating and metallic systems.

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Acceleration of Monte Carlo Radiation Transport Eigenvalue Calculations

Accurate solution of radiation transport eigenvalue problems plays an important role in the design and analysis of nuclear reactors as well as the safe storage and operation of many nuclear systems. Monte Carlo methods offer the most accurate solutions due to their ability to treat the entire phase space of energy, angle, and space without discretization. The standard approach to solving Monte Carlo eigenvalue calculations is a stochastic version of power iteration, which is subject to slow convergence even for deterministic solvers. This situation is compounded with the statistical errors inherent to Monte Carlo calculations, with inadequate sampling and iteration-to-iteration correlations resulting in further convergence difficulties, including the inability to diagnose convergence. In this talk, we will describe several methods that have been used to accelerate the convergence of Monte Carlo eigenvalue calculations. We will then discuss recent work using deterministic radiation transport solvers to accelerate the convergence of Monte Carlo solvers, circumventing difficulties with existing approaches. Early results indicate that the new approach is capable of improving the rate of convergence as well as the robustness of existing solvers for several challenging test problems.

Posters

Each poster presenter will have one minute during the poster blitz to briefly describe an overview of their poster. This is a rapid fire event! Poster presenters should line up on the left side of the room, in the order given below. When one person finishes, the next person steps up.

1. Asfaw, Tesfaye
   Georgia State University
   Markov Models for the Kinetics of Human Cardiac Sodium Channel

2. Bhattarai, Rosahn
   Georgia State University
   Using Predator Carrying Capacity for a Pathogenic Vector-Dynamic Differential Model

3. de Camp, Linda
   Georgia State University
   Inverse Problems and Ebola Virus Disease Using an an Age of Infection Model

4. Díaz de Alba, Patricia
   University of Cagliari and Emory University
   Numerical method for data inversion in Geophysics

5. French, Shateil
   Georgia State University
   Memory Consolida/on of Binary Inputs

6. Garvey, Clarissa
   Emory University
   Singular Value Decomposition Approximation using Kronecker Products

7. Herring, James
   Emory University
   Phase Recovery from the Bispectrum in Astronomical Imaging

8. Lanterman, Jay
   University of Georgia
   A Polygonal Spline Method for General 2nd-Order Elliptic PDEs and Applications

9. Lefieux, Adrien
   Emory University
   Cardiovascular Mathematics: from theory to practice

10. Lupo Pasini, Massimiliano
    Emory University
    Monte Carlo Accelerated Iterative Methods for Sparse Linear Systems

11. Mullins, Paula
    Georgia State University
    A model for the β_1*-adrenergic regulation of mouse ventricular myocyte contraction*

12. Rozier, Kelvin
    Georgia State University
    Biochemical aspects of the β_1*- and* β_2*-adrenergic signaling systems in mouse ventricular myocytes through computational modeling*

13. Sheppard, Michael
    Georgia State University
    Stable Identification of System Parameters in Infectious Disease Modeling

14. Sirb, Benjamin
    Georgia State University
    Decentralized Delayed Gradient Descent

15. Walsh, J. D.
    Georgia Institute of Technology
    Computing Optimal Coupling Systems by Blending Continuous and Discrete Models

16. Wang, Chunmei
    Georgia Institute of Technology
    Weak Galerkin Finite Element Methods

17. Wolfson-Pou, Jordi
    Georgia Institute of Technology
    Reducing Communication in Distributed Asynchronous Iterative Methods

18. Wu, Samy
    Emory University
    jlnv - A Flexible julia *Package for Parallel PDE Parameter Estimation*

19. Yashtini, Maryam
    Georgia Institute of Technology
    Fast Algorithms for Nonconvex Optimization with Application to Image Inpainting