Twenty-Sixth Annual University of Alabama System Applied Mathematics Meeting

Saturday, November 2, 2013

University of Alabama

All sessions will be held in Gordon Palmer Hall on the campus of the University of Alabama.

9:30-10:00	Refreshments	Room 301
10:05	Welcoming remarks	Room 208
10:10	Dr. Leila Setayeshgar (UAH) Large Deviations and Importance Sampling for a Feed-forward Network	Room 208
10:50	Dr. Wei Zhu (UA) Simulation on Liquid Crystal Elastomers Using Spectral Methods with a New Preconditioner	Room 208
11:30	Lunch	Area restaurants
1:10	Dr. Shannon Starr (UAB) Quantum spin systems	Room 208
1:50	Yunzhu He (UAH) Wavelet estimator in nonparametric regression model and simulation study	Room 208
2:10	Ajay Mahato (UAB) The Inverse Volatility Problem for American Options	Room 208
2:30	Wufeng Tian (UA) A fast ADI algorithm for geometric flow equations in biomolecular surface generation	Room 208
2:50	Refreshments	Room 301
3:15	Faculty discussion	Room 302
3:15	Student discussion	Room 346

Abstracts

Large Deviations and Importance Sampling for a Feed-forward Network, Leila Setayeshgar (UAH)

Queuing networks arise in many application areas including, but not limited to, communications, telecommunications, and ethernet design and their analysis leads to a better understanding of such systems. In this talk, we begin by considering a d-dimensional feed-forward network with a priority service policy. We show that the family of scaled state processes satisfies the sample path large deviations principle, where we employ the weak convergence approach. We then restrict our attention to the two-dimensional network, and explicitly identify the exponential decay rate of the probability a rare event, namely, the total population overflow associated to the network. Finally, we use importance sampling – an efficient rare event simulation technique – to estimate the probability of interest. (This is joint work with Prof. Hui Wang)

Simulation on Liquid Crystal Elastomers Using Spectral Methods with a New Preconditioner, Wei Zhu (UA)

Liquid crystal elastomers (LCEs) are soft complex materials of enormous technological importance because of their remarkable responsiveness to excitations. In our previous work, we proposed a non-local continuum model to study the dynamical behaviors of LCEs. The preliminary simulation demonstrated that the model can successfully capture the shape changing phenomena observed in real experiments and other features of LCEs. However, due to the complexity of governing equations, the simulation is very time-consuming. In this talk, we introduce a novel preconditioner for solving the velocity equation using Chebyshev spectral collocation method and present new simulations to show its efficiency.

Quantum spin systems, Shannon Starr (UAB)

Quantum spin systems are mathematical models to try to explain magnetic systems. The main difficulty is the quantum nature of the models. For some special models one can try to overcome this problem by using diagrammatic methods a-la Feynman and Kac. This leads to random systems instead of quantum ones. I will describe how this works and what partial results it has led to, so far.

The Inverse Volatility Problem for American Options, Ajay Mahato (UAB)

The inverse problem of determining equity volatility from a knowledge of American option prices for a range of exercise prices and maturities is solved by minimization of a convex functional. We illustrate the method using examples drawn from recent market data.

***Wavelet estimator in nonparametric regression model and simulation study*, Yunzhu He (UAH)**

Wavelet analysis has been proved to be a powerful tool for the nonparametric estimation. In this talk, we consider the nonparametric regression model with long range dependent noise and short range dependent noise by using wavelet methods. The main purpose is to do comparative simulation study to different wavelet methods. In addition, a new two-dimensional function estimator is proposed.

***A fast ADI algorithm for geometric flow equations in biomolecular surface generation*, Wufeng Tian (UA)**

In this paper, a new alternating direction implicit (ADI) method is introduced to solve potential driven geometric flow partial differential equations (PDEs) for biomolec- ular surface generation. For such PDEs, an extra factor is usually added to stabilize the explicit time integration. However, two existing ADI schemes are also based on the scaled form, which involves nonlinear cross derivative terms that have to be evaluated explicitly. This affects the stability and accuracy of these ADI schemes. To overcome these difficulties, we propose a new ADI algorithm based on the unscaled form so that cross derivatives are not involved. Central finite differences are employed to discretize the nonhomogenous diffusion process of the geometric flow. The proposed ADI algo- rithm is validated through benchmark examples with analytical solutions, reference solutions, or literature results. Moreover, quantitative indicators of a biomolecular surface, including surface area, surface-enclosed volume, and solvation free energy, are analyzed for various proteins. The proposed ADI method is found to be uncondition- ally stable and more accurate than the existing ADI schemes in all tests. This enables the use of a large time increment in the steady state simulation so that the proposed ADI algorithm is very efficient for biomolecular surface generation.