# Final Program and Abstracts

## SIAM Conference on Computational Science and Engineering

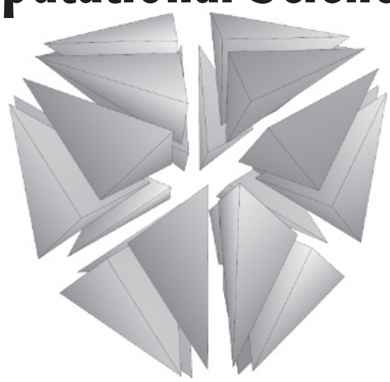

Figure courtesy Thomas A. Brunner and Tzanio V. Kolev, SISC, Vol.33, 5-6

**February 25-March 1, 2013**
**The Westin Boston Waterfront**
**Boston, Massachusetts, USA**

Sponsored by the SIAM Activity Group on
Computational Science and Engineering (CSE)

The SIAM Activity Group on CS&E fosters collaboration and interaction among applied mathematicians, computer scientists, domain scientists and engineers in those areas of research related to the theory, development, and use of computational technologies for the solution of important problems in science and engineering. The activity group promotes computational science and engineering as an academic discipline and promotes simulation as a mode of scientific discovery on the same level as theory and experiment.

The activity group organizes this conference and maintains a wiki, a membership directory, and an electronic mailing list.

2013 is designated as the year of Math of Planet Earth.
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Friday, March 1

# MS245

## Simulation and Modeling Applied to Diffusion Magnetic Resonance Imaging - Part II of II

*9:30 AM-11:00 AM*

*Room:Commonwealth Ballroom C - Concourse Level*

**For Part 1 see MS206**

Diffusion magnetic resonance imaging (DMRI) gives a measure of the average distance travelled by water molecules in a certain medium and can give useful information on cellular structure and structural change when the medium is biological tissue. In this mini-symposium we explore various aspects of the modeling and simulation of DMRI signals and showcase new results on simulation, including Monte-Carlo and PDE approaches, as well as modeling, including analytical and reduced models, going all the way to the determination of tissue microstructure from the DMRI signals.

Organizer: Jing-Rebecca Li
*INRIA, France*

Organizer: Denis Grebenkov
*Ecole Polytechnique, France*

**9:30-9:55 Monte-Carlo Simulation of Diffusion in Fractal Domains**
*Denis Grebenkov*, Ecole Polytechnique, France; Hang Tuan Nguyen, CEA, France

**10:00-10:25 Hermite Functions in Modeling Diffusion MRI Data: From Applications to Fundamentals**
*Evren Ozarslan*, Brigham & Women's Hospital, USA; Cheng Guan Koay, University of Wisconsin, Madison, USA; Peter J. Basser, National Institutes of Health, USA

**10:30-10:55 Diffusion Dynamics in Porous Media**
*Yi-Qiao Song* and Giovanna Carneiro, Massachusetts General Hospital and Harvard Medical School, USA; Larry Schwartz and Michael Prange, Schlumberger-Doll Research, USA

Friday, March 1

# MS246

## The Effect of Noise and Uncertainty on the Analysis of Large Networks

*9:30 AM-11:30 AM*

*Room:Commonwealth Ballroom B - Concourse Level*

Considerable work has been done on developing algorithms and techniques for analyzing the large- scale networks that are used to model interactions in application areas ranging from social networks to bioinformatics to software engineering. Less has been done to understand the impact of the fact that the ways in which these networks are created can make them vulnerable to noise and other perturbations: exact edge weights may depend on imprecise experimental data, the same network might be described using different orderings on the nodes, etc. In this minisymposium speakers will explore sources of noise and uncertainty, how existing algorithms handle noise, and techniques for handling real world networks.

Organizer: Tzu-Yi Chen
*Pomona College, USA*

Organizer: Sanjukta Bhowmick
*University of Nebraska, Omaha, USA*

**9:30-9:55 Quantification of Uncertainty in Network Summary Statistics**
*Eric D. Kolaczyk*, Boston University, USA

**10:00-10:25 On the Resilience of Graph Clusterings**
*Evan Fields* and Tzu-Yi Chen, Pomona College, USA

**10:30-10:55 Evaluating Noise in Complex Networks**
*Sanjukta Bhowmick*, Sriram Srinivasan, and Vladimir Ufimtsev, University of Nebraska, Omaha, USA

**11:00-11:25 Impact of Graph Perturbations on Structural and Dynamical Properties**
Abhijin Adiga, Henning Mortveit, Chris Kuhlman, and *Anil Vullikanti*, Virginia Tech, USA

Friday, March 1

# MS247

## Theoretical and Computational Advances in Time Dependent PDEs - Part III of IV

*9:30 AM-11:30 AM*

*Room:Otis - Lobby Level*

**For Part 2 see MS226**
**For Part 4 see MS266**

Many problems arising in mathematics, physics, biology and engineering can be formulated as the solution of time dependent partial differential equations (PDEs). Both the mathematical analyses and numerical simulations are important tools to understand these PDEs. This minisymposium aims to study recent developments and corresponding works in this area, including both linear and nonlinear equations, both local in time and global in time properties. Different time stepping schemes and spatial discretizations will be covered.

Organizer: Cheng Wang
*University of Massachusetts, Dartmouth, USA*

**9:30-9:55 Numerical Stability of Vortex Soliton under Optical Lattice and Harmonic Potential**
*Qian-Yong Chen*, University of Massachusetts, Amherst, USA

**10:00-10:25 Analysis of Formal Order of Accuracy of WENO Finite Difference Scheme**
*Wai-Sun Don*, San Diego State University, USA

**10:30-10:55 Unconditionally Stable Numerical Scheme for Two Phase Models in Karst Aquifers**
*Xiaoming Wang*, Florida State University, USA

**11:00-11:25 Adaptive Multigrid, Discontinuous Galerkin Methods for Cahn-Hilliard Type Equations**
*Steven M. Wise*, University of Tennessee, USA

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Diffusion-weighted MRI has became an important source of information about the dynamics in and the structure of natural or artificial materials (e.g., rocks, cements, human organs). In spite of intensive research, the relation between the microstructure and the signal formed by diffusing nuclei remains poorly understood, mainly due to lack of efficient algorithms and models for multi-scale porous media. To overcome this limitation, we developed a fast random walk (FRW) algorithm with gradient encoding which exploits the multi-scale character of the medium. In this talk, we present an application of this algorithm to a Menger sponge which is formed by multiple channels of broadly distributed sizes and often used as a model for soils and materials. Using this model, we investigate the role of multiple scales onto diffusion-weighted signals.

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**MS245**

**Hermite Functions in Modeling Diffusion MRI Data: From Applications to Fundamentals**

Properties of Hermite functions make them ideally-suited to problems of modeling diffusion-weighted (DW) magnetic resonance (MR) signals and estimating propagators. We illustrate the utility of Hermite functions to characterize the anisotropy and diffusion-time dependence of the diffusion process. The ability of the model to represent different signal profiles suggests that the approach could be used even when no information regarding the underlying microstructure is availablea desirable characteristic for imaging applications.

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**MS245**

**Diffusion Dynamics in Porous Media**

Diffusion is known to cause multiple relaxation peaks in NMR relaxation behavior. However, in real porous materials, pore size distribution also results in multiple or broad relaxation times. We have devised a two-dimensional NMR method in order to distinguish these two scenarios. Using analytical and numerical solutions of the diffusion dynamics and numerical simulation we have demonstrated this effect and found it consistent with experimental results.

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**MS246**

**Evaluating Noise in Complex Networks**

As in all computations involving real-world systems, the results of network analysis are affected by experimental, subjection and computational choices. However, network analysis algorithms are primarily based on graph theory and therefore assume the inputs to be exact. In this talk, we will demonstrate how user choices and computational limitations can affect network analysis results and discuss how concepts from numerical analysis such as conditioning and stability can be extended to evaluate the effect of noise in this domain.

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**MS246**

**On the Resilience of Graph Clusterings**

Are clusters found by popular graph clustering algorithms significant? One way to answer this is by measuring cluster resilience as follows: repeatedly perturb the input graph by adding one edge, and for each new edge recluster the vertices and calculate the distance between the original and modified clustering. We hypothesize that the distribution of distances contains information about the stability of clusters in the original graph and present applications of this technique to synthetic and real-world graphs.

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**MS246**

**Quantification of Uncertainty in Network Summary Statistics**

It is common in the analysis of network data to present a network graph and then cite various summary statistics thereof (e.g., degree distribution, clustering coefficient, conductance, etc.). However, most real-world networks derive from low-level measurements that are noisy. Surprisingly, there has been little effort to date aimed at quantifying the uncertainty induced in network summary statistics by noise in the underlying measurements. I will discuss work being done in my group towards this goal.

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