



THE UNIVERSITY OF CHICAGO

Department of Statistics

SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

GILLIAN QUEISSER

Goethe-Center for Scientific Computing
Goethe University

Multiscale Modeling and Simulation of Neuronal Processes

THURSDAY, November 20, 2014 at 4:30 PM
133 Eckhart Hall, 5734 S. University Avenue
Host: Ridgway Scott

ABSTRACT

Biological processes are typically active on multiple, coupled scales. Examples are the chemical contacts between brain cells. We present a multiscale model of chemical synapses, that couples the molecular dynamics of cell-adhesion Cadherin molecules interacting with calcium ions and the continuum scale model representing synaptic function and intracellular signaling. For this purpose we developed a tetrahedral volume grid representation of a synapse and neuron used in a Finite Volume discretization of the synaptic model (described by a system of PDEs). On the molecular scale we use molecular dynamics (MD) simulations and couple these to the discrete function space of the PDE-problem, using transfer operators that map between the cartesian space and function space. The three-dimensional non-linear diffusion-reaction system with non-linear interface conditions is solved using parallel multi-grid methods and adaptive grid refinement based on a newly developed a posteriori error estimator. Simulation results demonstrate the methods applied to the model of intercellular coupling between nerve cells and the necessity to employ a multiscale model solved with multi-level solvers.

Organizers:

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