

Department of Applied and Computational Mathematics and Statistics Colloquium

Markos A. Katsoulakis

Department of Mathematics and Statistics
University of Massachusetts, Amherst

will give a lecture entitled:

Parameter sensitivity and error quantification methods for high-dimensional stochastic dynamics

Abstract

In this talk we discuss goal-oriented and information theory-based sensitivity analysis and parameter identifiability methods for complex high-dimensional dynamics, as well as information-theoretic tools for parameterized coarse-graining of non-equilibrium extended systems.

The combination of proposed methodologies is capable to (a) handle molecular-level models with a *very large number of parameters*, (b) address and mitigate the *high-variance* in statistical estimators, e.g. for sensitivity analysis, in spatially distributed Kinetic Monte Carlo (KMC), (c) tackle *non-equilibrium processes*, typically associated with coupled physiochemical mechanisms, boundary conditions, etc. (such as reaction-diffusion systems), and where even steady states are unknown altogether, e.g. do not have a Gibbs structure. Finally, the path-wise information theory tools, (d) yield a surprisingly simple, tractable and easy-to-implement approach to quantify and rank parameter sensitivities, as well as (e) provide reliable molecular model *parameterizations*, based on fine-scale data and *rational model selection* methods through suitable path-space (dynamics-based) information criteria.

The proposed methods are tested against a wide range of high-dimensional stochastic processes, ranging from complex biochemical reaction networks with hundreds of parameters, to spatially extended Kinetic Monte Carlo models in catalysis and Langevin dynamics of interacting molecules with internal degrees of freedom.



**Monday, December 2, 2013
4:00 p.m. to 5:00 p.m.
127 Hayes-Healy Center**

Colloquium Tea

3:30 p.m. to 4:00 p.m. 154 Hurley Hall