**TEMPLE UNIVERSITY**
Department of Mathematics

# Applied Mathematics and Scientific Computing Seminar

Room 617 Wachman Hall

Wednesday, 18 February 2015, 4:00 p.m.

## Markov State Models of Biomolecular Dynamics in Theory and Practice

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**Abstract.**

In this talk, I will discuss Markov State Model (MSM) approaches to studying the molecular dynamics of biomolecules, particular protein folding. MSMs are kinetic network models that describe molecular dynamics as a set of transition rates between discrete conformational states. I will discuss the background and theory of these models, as well as applications of MSMs to constructing models of protein folding from large numbers of simulation trajectories. MSMs can be used to model dynamics on long timescales from ensembles of much shorter simulation trajectories. They can also be used to extract "human-readable" information about folding mechanisms that would be hard to obtain by other methods.