TEMPLE UNIVERSITY
Department of Mathematics

Applied Mathematics and Scientific Computing Seminar

Room 617 Wachman Hall

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Using Molecular Simulation and Kinetic Network Models to Study Protein Folding

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Abstract.

In this talk I will present a very broad and non-rigorous overview of molecular simulation methods and how we can use them to study protein folding. First, I will introduce some basic biological concepts of proteins, their folding, and why these processes are so important to model computationally. Next, I will discuss the use and implementation of molecular simulation methods for studying the structure of dynamics of large macromolecules like proteins. The remainder of the talk will focus on the use of so-called Markov State Model (MSM) approaches to study protein folding. These models, originally devised in the applied math community, have made a big impact in our field. MSMs are kinetic network models that describe molecular dynamics as a set of transition rates between discrete conformational states. MSMs can be used to model dynamics on long timescales from ensembles of much shorter trajectories. A key problem we face is efficiently and accurately constructing such models from large numbers of simulation trajectories. I will discuss current approaches to solving this problem, along with some recent examples of applications.