



The University of Chicago  
Department of Statistics

Seminar Series

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## **Modeling Macromolecular Dynamics from Simulations**

**WEDNESDAY, May 2, 2007 at 12:00 PM**  
**110 Eckhart Hall, 5734 S. University Avenue**

### **ABSTRACT**

Many important processes in biology occur at the molecular scale. A detailed understanding of these processes can lead to significant advances in the medical and life sciences – for example, many diseases are caused by protein aggregation or misfolding. One approach to studying these systems is to use physically-based computational simulations to model the interactions and movement of the molecules. While molecular simulations are computationally expensive, it is now possible to simulate many independent molecular dynamics trajectories in a parallel fashion by using distributed computing methods such as Folding@Home.

The analysis of these large, high-dimensional, data sets presents new computational challenges. In this seminar, I will discuss a novel approach to analyzing large ensembles of molecular dynamics trajectories to generate a compact model of the dynamics. This model groups conformations into discrete states and describes the dynamics as Markovian, or history-independent, transitions between the states. I will discuss why the Markovian state model (MSM) is suitable for macromolecular dynamics, and how it can be used to answer many interesting and relevant questions about the molecular system. I will also discuss many of the computational and statistical challenges in building such a model, such as how to appropriately cluster conformations, determine the statistical reliability, and efficiently design new simulations.

Bio: Nina Singhal Hinrichs is a Ph.D. student in Computer Science at Stanford University. She received her B.S. degree in Chemical Engineering and Mathematics from MIT in 2001. Her current research interests involve applying computational and statistical techniques to understand molecular dynamics trajectories.

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