



The University of Chicago  
Departments of Computer Science,  
Mathematics, and Statistics

## Scientific and Statistical Computing Seminar

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**AARON DINNER**

The Dinner Group  
The University of Chicago

### Enhanced Sampling Algorithms for Molecular Systems Far from Equilibrium

**FRIDAY, February 24, 2012, at 3:30 PM**

133 Eckhart Hall, 5734 S. University Avenue.

### ABSTRACT

Most computational approaches for boosting the exploration of the phase space of a model of a molecular system rely on microscopic reversibility. However, there are many systems of fundamental and applied interest that do not satisfy detailed balance. I will discuss a number of approaches that we have developed over the last five years to obtain both the steady-state and transient statistics of rare events in nonequilibrium systems.

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