



THE UNIVERSITY OF CHICAGO

Department of Statistics

SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

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A Relative Entropy Formulation of Diffusive Molecular Dynamics

THURSDAY, April 23, 2015 at 4:30 PM
133 Eckhart Hall, 5734 S. University Avenue

ABSTRACT

Diffusive Molecular Dynamics (DMD) is a novel approach to problems in molecular dynamics that aims to reach the diffusive time scale of milliseconds and beyond. To accomplish this, DMD “averages out” the vibrational time scale of femtoseconds and evolves probability densities at atomistic sites. This requires the approximation of a probability distribution in an extended state space by a synthetic approximate distribution, which can easily be sampled. We will present an analysis that this approximation can be interpreted as a minimization of the relative entropy distance between distributions. This has consequences for the implementation of the algorithm, and it allows for flexibility in future applications. This is joint work with Mitchell Luskin (University of Minnesota) and David Srolovitz (University of Pennsylvania).

Organizers:

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