



PURDUE UNIVERSITY

Department of Mathematics Colloquium

Speaker: Professor Eric Vanden-Eijnden, Courant Institute of Mathematical Sciences, NYU

Title: "Transition Pathways in Complex Systems: Application of the Finite-temperature Strong Method to the Alanine Dipeptide"

Date: Tuesday, April 11, 2006

Time: 4:30 P.M.

Place: MATH 175

Abstract

I will discuss the theoretical background and algorithmic details of the finite-temperature string method, as well as the application of the method to the study of isomerization reaction of the alanine dipeptide, both in vacuum and in explicit solvent. It will be shown that the method allows one to identify directly (i.e. without computing reactive trajectories before hand) the isocommittor surfaces, which are approximated by hyperplanes, in the region of configuration space where the most probable reactive trajectories are concentrated. These isocommittor surfaces constitute the best reaction coordinate to describe the reaction, obtain its rate and compute its associated free energy. The results on alanine dipeptide will be verified subsequently by computing directly the committor distribution on the hyperplanes that define the transition state region.

Refreshments will be served in the Math Library Lounge, 4:00 P.M.