Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Computational Methods for Enhanced Conformational Kinetics
IOAN ANDRICIOAEI, University of Michigan — We present and analyze two general method to calculate time-correlation functions from molecular dynamics on scaled potentials or from molecular dynamics with artificial momenta distributions. They are useful for complex systems whose simulations are affected by broken ergodicity. Depending on the value of the scaling factor or of the details of the momentum distributions, correlation functions can be accurately calculated for times that can be orders of magnitude longer than those accessible to current molecular dynamics simulations. We show that the exact value of the correlation functions of the original system can be obtained, in principle, using an action-reweighting scheme based on a stochastic path-integral formalism. Tests on model systems and peptides are exemplified. We also show that free energy profiles using Jarzynski's identity can be more effectively calculated within this scheme.

Ioan Andricioaei
University of Michigan

Date submitted: 30 Nov 2005 Electronic form version 1.4