Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Accelerating Atomistic Molecular Dynamics Simulation in Entropic Systems XIN ZHOU, Los Alamos National Laboratory — The time scale of the traditional atomistic molecular dynamics simulations is too short to study wide slow dynamics of complex systems. Hyperdynamics method developed by A. F. Voter in studying of solids can not use directly in entropic systems such as fluids, biopolymers etc. By applying suitable order parameters with the symmetry of the studied systems and the characteristics of short trajectory, we build the condition of extending the hyperdynamics into fluids and algorithms. We test our results in a few modeling systems and expect the methods is used generally in simulating atomistically slow dynamics of complex fluids and biopolymers.

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Date submitted: 28 Nov 2005 Electronic form version 1.4