

1033-37-94

Zachariah Sinkala* (zsinkala@mtsu.edu), Department of Mathematical Sciences, Box 34, Middle Tennessee State University, Murfreesboro, TN 37132, and **Terrance Quinn, Abdul Khaliq, Mary Farone, Anthony Farone** and **Paul Kline**. *Simulation of the Dynamics of Protein Chains using Metropolis Algorithm*. Preliminary report.

The Metropolis implementation of the multicanonical replica-exchange algorithm has been developed to study the equilibrium thermodynamics of many-body systems. Choosing small trial moves, the trajectories obtained applying this algorithm agree with those obtained by Langevin's dynamics. Applying this procedure to a simplified protein model, it is possible to show that the setting a threshold angle on the movement of the dihedrals of the protein backbone in a single step the algorithm step, the mean quantities associated with the off-equilibrium dynamics are well reproduced, while the good description of higher moments requires smaller moves. An important result is that the time duration of the algorithm step depends linearly on the temperature, something which should be accounted for when doing simulations at different temperatures. (Received September 05, 2007)