Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Wang-Landau sampling for homopolymer collapse DANIEL T. SEATON, STEVEN J. MITCHELL, DAVID P. LANDAU, University of Georgia — We explore the behavior of a continuum-homopolymer model using the Wang-Landau algorithm, concentrating on phase transitions such as the coil-globule and solid-liquid transitions. Using the density of states generated by the Wang-Landau algorithm, we calculate various thermodynamic quantities, e.g., the internal energy and specific heat. We also study how algorithmic parameters, such as sampling boundaries (maximum and minimum energies for random walks) and the final value of the modification factor, affect these quantities. In particular, we observe how the sampling boundaries can significantly alter the transition behavior. Our results are compared with two recent studies that yielded contradictory results, one using the bond-fluctuation model and the other using a continuum model similar to our own. We find that the transitions seen in our model are much more similar to those in the bond-fluctuation study. The careful analysis of the effects of algorithmic parameters on thermodynamic quantities should be relevant to the study of other polymeric/protein models.

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Date submitted: 27 Nov 2007 Electronic form version 1.4