Abstract Submitted
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Replica-exchange Wang-Landau simulations of the H0P model of protein folding[1] GUANGJIE SHI, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia, THOMAS WÜST, Scientific IT Services, ETH Zurich IT Services, YING WAI LI LI, Oak Ridge National Laboratory — The hydrophobic-polar (HP) model has served as a coarse-grained lattice protein folding model attracting scientists from various disciplines. However, simplification into H and P monomers may yield high ground state degeneracies which stands in contrast to the generally unique native states of natural proteins. We propose a simple modification, by introducing a new type of "neutral" monomer, 0, i.e. neither hydrophobic nor polar, rendering the model more realistic without increasing the difficulties of sampling significantly. With the newly developed parallel Wang-Landau (replica exchange Wang-Landau) scheme[2] and an innovative method of estimating the ground state degeneracies,[3] we investigated some widely studied HP proteins and their H0P counterparts. Dramatic differences in ground state and thermodynamic properties have been observed, e.g. the estimation of ground state degeneracy for the 46mer is 460,000 for the HP version and only 20 for the H0P mapping. Similarly, the specific heat and structural properties: radius of gyration and etc. show more pronounced signals associated with folding.

[1]Supported by NSF.
[2]T. Vogel, Y. W. Li, T. Wüst, and D. P. Landau, Phys. Rev. Lett., 110, 210603 (2013)
[3]G. Shi, T. Vogel, T. Wüst, Y. W. Li, and D. P. Landau, Phys. Rev. E 90, 033307

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