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Generic parallel Wang-Landau sampling for complex systems YING WAI LI, National Center for Computational Sciences, Oak Ridge National Laboratory, U.S.A., THOMAS VOGEL, DAVID P. LANDAU, Center for Simulational Physics, University of Georgia, U.S.A., THOMAS WÜST, Swiss Federal Research Institute WSL, Switzerland — We introduce a parallel realization for Wang-Landau sampling in Monte Carlo simulations based on a replica-exchange framework. The key idea is to split the entire energy range of the system under consideration into several smaller, overlapping sub intervals. The survey of configurational phase space can then be distributed over multiple processors, with exchanges of random walkers taking place in the overlapping energy windows. To demonstrate the robustness and advantages of this parallel scheme for the simulations of complex systems, we have applied it to protein adsorption problems using the HP lattice protein model¹. The method gives significant speed-up and achieves strong scaling on small computer architectures like multi-core processors, with a possible improvement in accuracy. We believe that it could be potentially beneficial for large-scale petaflop machines.

¹K. A. Dill, Biochemistry **24**, 1501 (1985).

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