Abstract Submitted
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Highly parallel computational study of amphiphilic molecules using the Wang–Landau method[1] THOMAS VOGEL, DAVID LANDAU, The Center for Simulational Physics, University of Georgia, Athens, GA, 30602, U.S.A. — The self-assembly process in amphiphilic solutions is a phenomenon of broad interest. Molecular dynamics simulations generally used to study micelle formation or lipid layer assembly in an explicit solvent are limited in time scale. Vast studies of structure formation processes via standard Markov-chain based Monte Carlo simulations are challenging, but the Wang–Landau method [1] provides a way to efficiently study such systems in a generalized thermodynamic ensemble. This makes it possible, for example, to get results over a broad temperature range from a single simulation. In an attempt to develop highly parallel applications using this method, we study the thermodynamic behavior of a generic coarse-grained model for amphiphilic molecules [2] as well as of a new coarse-grained lipid model specifically designed for dimyristoyl phosphatidylcholine (DMPC) [3]. Here, we focus on the design and the performance of our parallel Wang–Landau simulation on multi-CPU and GPU systems.

[1] F. Wang and D.P. Landau, Phys. Rev. Lett. **86**, 2050 (2001)
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