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Performance of replica-exchange Wang-Landau sampling for the study of spin systems YING WAI LI, MARKUS EISENBACH, Oak Ridge National Laboratory, U.S.A., THOMAS VOGEL, Los Alamos National Laboratory, U.S.A., THOMAS WÜST, Swiss Federal Research Institute WSL, Switzerland, DAVID P. LANDAU, University of Georgia, U.S.A. — The recently proposed replica-exchange Wang-Landau sampling (REWL)[1] is a novel, massively parallel Monte Carlo method which allows for the parallelization of Wang-Landau sampling based on a replica-exchange framework. The robustness of the scheme is demonstrated by its broad applicability on a variety of spin systems: from the simplest models with discrete or continuous energy domains, to complex systems captured by large-scale first principles density functional theory calculations. The accuracy of REWL is studied by comparing the thermodynamic properties with exact solutions and results obtained by the original, serial Wang-Landau sampling. The principles for the speed-up, the strong and weak scaling behavior of REWL are also investigated when different parameter settings are employed. We will show, with the aid of selected spin systems, that the method accelerates the simulations significantly with a possible improved accuracy.[2]

[1]Phys. Rev. Lett. **110**, 210603 (2013)

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