

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

“Binless Wang-Landau sampling” - a multicanonical Monte Carlo algorithm without histograms¹ YING WAI LI, MARKUS EISENBACH, National Center for Computational Sciences, Oak Ridge National Laboratory — Inspired by the very successful Wang-Landau (WL) sampling ², we innovated a multicanonical Monte Carlo algorithm to obtain the density of states (DOS) for physical systems with continuous state variables. Unlike the original WL scheme where the DOS is obtained as a numerical array of finite resolution, our algorithm assumes an analytical form for the DOS using a well chosen basis set, with coefficients determined iteratively similar to the WL approach. To avoid undesirable artificial errors caused by the discretization of state variables, we get rid of the use of a histogram for keeping track of the number of visits to energy levels, but store the visited states directly for the fitting of coefficients. This new algorithm has the advantage of producing an analytical expression for the DOS, while the original WL sampling can be readily recovered.

¹This research was supported by the Office of Science of the Department of Energy under contract DE-AC05-00OR22725.

²F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).

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Date submitted: 06 Nov 2015

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