

Optimized multicanonical simulations: a new proposal based on classical fluctuation theory

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We propose a new recursive procedure to estimate the microcanonical density of states in multicanonical Monte Carlo simulations which relies only on measurements of moments of the energy distribution, avoiding entirely the need for energy histograms. This method yields directly a piecewise analytical approximation to the microcanonical inverse temperature, $\beta(E)$, and allows improved control over the statistics and efficiency of the simulations. We demonstrate its utility in connection with recently proposed schemes for improving the efficiency of multicanonical sampling, either with adjustment of the asymptotic energy distribution or with the replacement of single spin flip dynamics with collective updates.

[1] J. Viana Lopes et al., preprint cond-mat/0603758.