

Abstract Submitted
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An Efficient Algorithm to Calculate Density of State in Large Systems: Generalized Ensemble Means and Compression-Variable Transformation¹ XIN ZHOU, T7, Los Alamos National Laboratory — We present a high efficient algorithm to calculate density of state (DOS, or its logarithm, $S(U)$) of large systems in any macroscopic variable U . The algorithm calculate the ensemble means and fluctuations of U in a series of generalized ensembles to form $S(U)$ and its derivative in some adaptively generated U_i , then interpolate whole the $S(U)$ curve within the required accuracy. We also apply a compression transformation in the U space to focus the most computation cost on extrapolating $S(U)$ in new U region. The algorithm is found to be order of $O(N^{1/2})$ (or faster) as the increasing system size N , which is far faster than all current available methods (at least $O(N^{3/2})$). The algorithm satisfies the detailed-balance condition in whole simulations by averaging the ensemble means in each segment of simulation by using their errors as weight, so that it has great numerical stability. The method can be compined with the parallel tempering (PT) algorithm to simulate the low-temperature properties of large complex fluids and decrease the number of the needed replica in original PT, $O(N^{1/2})$, to one in each macroscopic phase. The validity of the new approaches are demonstrated by presenting the simulated results of Lennard-Jone liquids with different size N . The approaches even generate DOS of each super-saturated macroscopic phase in the unstable liquid/solid coexistence region, respectively, which provides much more information to understant the phase coexistence and transitions.

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