Parallel Wang–Landau study of micelle formation*

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1 Introduction

The self-assembly process in amphiphilic solutions is a phenomenon of broad interest and vast computational studies of these processes are challenging. We present a framework for highly parallel Monte Carlo (MC) computer simulations using the Wang–Landau method, which we apply to a generic coarse-grained model for amphiphilic molecules.

2 Generic model for amphiphilic molecules

The generic model we use is based on models previously employed to study the self-assembly of molecules, see [1] and references therein.

We use three different types of coarse-grained particles, representing polar (P) and hydrophobic (H) parts of a larger chain molecule and the surrounding water (W) molecules. The amphiphilic molecules are built up of a polar head and, in this study, two hydrophobic tail monomers (P–H–H). The interaction between solution particles and tail monomers as well as between head monomers and tail monomers is purely repulsive and modeled by a repulsive soft-core potential, all other non-bonded interactions are of Lennard-Jones type. Bonds are finitely extendible, non-elastic (FENE) in nature.

3 Parallelization of the Wang–Landau sampling

In a single-processor Wang–Landau flat-histogram MC simulation [2], a “walker” samples the conformational space and estimates the density of states \( g(E) \) in a certain energy range between \( E_{\text{min}} \) and \( E_{\text{max}} \). This is done in an iterative way, where the histogram of visited energies \( H(E) \) has to become “flat” in order to proceed to the next iteration.

For large-size systems, this very efficient generalized-ensemble sampling can be enhanced by making use of multiple processors working in parallel. This can be done, for example, by introducing multiple walkers sampling an identical energy range and contributing to the same histogram, or by splitting up the energy range and estimating the density of states for the respective energy intervals by independent walkers [3].

Estimate of the logarithm of density of states for a system containing \( m = 75 \) amphiphilic molecules and a total of \( n = 1000 \) particles. Comparison between result from single run with \( E_{\text{max}} = -4500 \) and the respective walkers from a parallel run. Setup as above, no error bars shown.

4 Performance and Results

In order to get reliable results, we want each sample to perform walks through the whole energy range, i.e., it should walk back and forth through all single energy intervals. For the given problem we find that a splitting into nine energy intervals with an overlap of 75% is a good choice. Hence, the width of each single energy interval is 1/3 of the whole energy range. In the following example, we have a total of 81 walkers, with nine walkers in each energy interval. For conformation exchanges, every walker chooses a walker from a neighboring interval at random.

We test the overall performance on a smaller energy range. The single walker needed \( \approx 1.3 \times 10^7 \) sweeps to complete the Wang–Landau iterations and estimate the density of states \( \ln g(E) \) is shown in the figure, dashed green line). The red symbols in the figure represent the same function composed of the results of seven parallel walkers. The walker in the lowest energy interval completed the iteration after \( 7 \times 10^6 \) sweeps.

Due to the overlap of the energy intervals and the multiple walkers per interval, the statistical precision is also much higher.

In an attempt to improve the latter approach, we now also allow for conformation exchanges between independent walkers.

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References