Self-Assembly of Coarse-grained Amphiphilic Molecules Using Parallel Wang-Landau Sampling*

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ABSTRACT

Wang-Landau sampling [1, 2] is a serial Monte Carlo simulation method that has proven to be powerful for studying problems with complex free energy landscapes. A recently developed generic, parallel scheme of this sampling method enhanced its applicability to even larger system and more complicated problems [3]. One example to which it has been successfully applied is the self-assembly of amphiphilic molecules into lipid bilayers, using a coarse-grained model with fixed amphiphilic concentration [4]. This problem is already difficult enough such that the sampling of the complete corresponding phase space was only possible by applying the parallel framework.

However, our current interest is to investigate the membrane-forming processes more fully by allowing *both* the energy and the concentration to vary during the simulation. To attack this problem, we realize the necessity of extending our parallel framework further by adding an additional parallelization dimension: the segmentation of the "lipid concentration space". By employing the computing resource of Stampede (through XSEDE), we are able to perform our 2D (energy and lipid concentration dimensions) parallel simulation on a large virtual grid, which is composed of hundreds of processes. Communications (through MPI) between neighboring processes carry out at certain intervals to ensure the correct statistics. We will show that our simulation goes through phase space successfully and provides valuable insight to the membrane-forming processes. With additional resources we should easily be able to extend the simulation to larger systems by increasing the number of parallel processes.

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Categories and Subject Descriptors

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General Terms

Simulation, Algorithms

Keywords

replica-exchange Wang-Landau, lipid bilayers, phase transition, amphiphilic molecules

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