

Bridging coarse-grained models by jump-in-sample simulations

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We present an efficient method to construct coarse-grained (CG) models from models of finer resolution. The method estimates the free energies in a generated sample of the CG conformational space and then fits the entire effective potential surface in the high-dimensional CG conformational space. A jump-in-sample algorithm that uses a random jumping walk in the CG sample is used to iteratively estimate the free energies. We test the method in a tetrahedral molecular fluid where we construct the intermolecular effective potential and evaluate the CG molecular model. Our algorithm for calculating the free energy involves an improved Wang-Landau (WL) algorithm, which not only works more efficiently than the standard WL algorithm, but also can work in high-dimensional spaces. © 2008 American Institute of Physics. [DOI: 10.1063/1.2912561]

I. INTRODUCTION

Computational simulations including Monte Carlo (MC) and molecular dynamics (MD) simulations have been standard tools for providing equilibrium and dynamical properties of systems in materials science, chemistry, physics, and biology. The fundamental limitation of these simulations is that the accessible time and spatial scales are too small to study many interesting macroscopic phenomena and processes. Recent attempts to overcome this limitation include the enhanced sampling techniques^{1–9} for achieving more complete equilibrium samples, the slow-dynamic techniques^{10–17} for long-time kinetics or dynamics, and many kinds of multiscale methods^{18–21} for studying systems involving large-spatial and sometimes also large-time scales. The coarse-graining method, which averages some degrees of freedom of the original system, is one of the multiscale techniques. For example, in the simulations of polymers, some bonded atoms may be mapped into superatoms that interact through an effective potential,^{18,22–25} such that larger systems can be simulated. This coarse-graining method of lumping atoms together is found to not only quantitatively reproduce the equilibrium properties of the polymers, but also to qualitatively (even semiquantitatively) reproduce the kinetics and/or dynamics of the original systems.

The coarse-graining method can be formally described as follows. We have an original atomic system with N atoms, whose potential energy is $V(\mathbf{R}^N)$, and \mathbf{R}^N is the $3N$ -dimensional conformation vector. By lumping some of the atoms into superatoms, we have a coarse-grained (CG) model with n superatoms, $n < N$. The CG model has an effective potential $V_{\text{eff}}(\mathbf{X}^n)$ in a CG-variable space \mathbf{X}^n , where \mathbf{X}^n is the $3n$ -dimensional conformation vector. The position

of a superatom is usually defined as the position of the center-of-mass of the corresponding group of atoms $\mathbf{X}_i = (1/M_i) \sum_a m_a \mathbf{R}_{ia}$, where $M_i = \sum_a m_a$ and m_a and \mathbf{R}_{ia} are the mass and position of the a th atom of the i th superatom, respectively. Thus, the original atomic conformation \mathbf{R}^N can be rewritten as the CG conformation \mathbf{X}^n and the remaining \mathbf{Y}^{N-n} coordinates under a linear transformation. The CG variables x and the corresponding effective potential $V_{\text{eff}}(x)$ form a complete CG model of the original system. To reproduce the thermodynamics of the original system, the effective potential should be equal to the Landau free energy $F(x)$,

$$F(x) = -k_B T \ln \int e^{-\beta V(\mathbf{r})} \delta(x - x(\mathbf{r})) d\mathbf{r}, \quad (1)$$

where $\beta = 1/(k_B T)$. However, $F(x)$ is often hard to obtain in the $3n$ -dimensional space x , if n is large. Canonically, we presume some formula for the effective potential with a few free parameters, then determine these parameters by requiring that the CG model reproduces some important thermodynamic properties of the original system. The most commonly used thermodynamic properties are the equation of states and the radial distribution function (RDF). These properties of the original system can be obtained either from atomistic simulations of the original system or from experiments.

We aim to improve this method for generating the effective potentials of the CG models for the following reasons. (1) The choice of the thermodynamic properties is arbitrary. Usually, only a few properties are used in the construction of the CG models, thus the fitted effective potentials depend on the particular choice. (2) These fitted properties are the result of macroscopic (i.e., ensemble) averaging. Thus the effective potential might not correctly reproduce the microscopic distribution of the corresponding physical variables. (3) These thermodynamic properties result mainly from important (stable) conformations and thus the CG model might not characterize interesting transition regions. In principle, we do

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