MAR15-2014-020200

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Dynamical coarse grained models with realistic time dependence

HANS ANDERSEN, Department of Chemistry, Stanford University

Coarse grained (CG) models of molecular systems, with fewer mechanical degrees of freedom than an all-atom model, are used extensively in chemical physics. It is generally accepted that a coarse grained model that accurately describes equilibrium structural properties (as a result of having a well constructed CG potential energy function) does not necessarily exhibit appropriate dynamical behavior when simulated using conservative Hamiltonian dynamics for the CG degrees of freedom on the CG potential energy surface. Attempts to develop accurate CG dynamic models usually focus on replacing Hamiltonian motion by stochastic but Markovian dynamics on that surface, such as Langevin or Brownian dynamics. However, depending on the nature of the system and the extent of the coarse graining, a Markovian dynamics for the CG degrees of freedom may not be appropriate. We consider the problem of constructing dynamic CG models within the context of the Multi-Scale Coarse Graining (MS-CG) method of Voth and coworkers. We propose a method of converting an MS-CG model into a dynamic CG model by adding degrees of freedom to it in the form of a small number of fictitious particles that interact with the CG degrees of freedom in simple ways and that are subject to Langevin forces. The dynamic models are members of a class of nonlinear systems interacting with special heat baths that was studied by Zwanzig [R. Zwanzig, J. Stat. Phys. 9, 215 (1973)]. The dynamic models generate a non-Markovian dynamics for the CG degrees of freedom, but they can be easily simulated using standard molecular dynamics simulation programs. We present tests of this method on a series of simple examples that demonstrate that the method provides realistic dynamical CG models that have non-Markovian or close to Markovian behavior that is consistent with the actual dynamical behavior of the all-atom system used to construct the CG model. The dynamic CG models have computational requirements that are similar to those of the corresponding MS-CG model and are good candidates for CG modeling of very large systems.