

Methodological Developments of Large-Scale Biological Molecular Dynamics Simulations on Blue Gene/P: High-Performance, Scalable Molecular Dynamics Simulation of a Polarizable Force Field Based on the Classical Drude Oscillator in NAMD

Wei Jiang, Benoit Roux

Argonne Leadership Computing Facility, Biosciences Division, Argonne National Laboratory, Argonne, IL 60439

Introduction. Most classical molecular dynamics (MD) simulations employ potential functions that do not account for many-body induced polarization effects explicitly. Such simple potential functions are clearly limited in their ability to provide a realistic and accurate representation of both microscopic and thermodynamic properties. In recent years, intensive efforts have been directed to the development of computational models able to account for induced polarization explicitly for the purpose of generating MD trajectories. Popular approaches include the induced dipole model, the fluctuating charge model, and the classical Drude oscillator model. While intense efforts have been and continue to be devoted to the careful parametrization of force fields based on various realizations of these models, their increased computational cost compared with nonpolarizable models is an issue that needs also to be addressed. For instance, simulations of large-scale systems (millions of atoms) are beyond the capabilities of the MD programs currently equipped to treat induced polarization. In addition to critical technical aspects encountered in large-scale simulations of nonpolarizable models, a number of factors can affect performance regarding the particular polarizable model chosen and its implementation.

Current Work. In the present work, we report the first implementation of a polarizable force field based on the classical Drude oscillator model in the program NAMD. NAMD is a parallel MD code designed for high-performance simulations of large-scale biomolecular systems based on nonpolarizable force fields. NAMD adopts a seminal hybrid of force and spatial decomposition and therefore avoids the limitation of simulation space and poor load balance due to simple spatial decomposition. The Drude model preserves the simple particle-particle Coulomb electrostatic interaction employed in nonpolarizable force fields, and implementation of the Drude model in a high-performance MD program is relatively straightforward. Any latent polarization catastrophe can be controlled by modifying the Drude bond parameters, thus achieving high numerical stability. The high efficiency of NAMD and the simplicity of the Drude oscillator model offer a unique opportunity to achieve high performance in an implementation of induced polarization in large-scale MD simulations.

The new Drude NAMD has been applied to compute the structural properties of large-scale water/dodecane interface, a prototype model related to environment remedies and biological interfacial phenomena. The calculated surface normal density profile and surface tension agree well with experiment. The Drude NAMD also is applied to compute the collective transport properties of salt solution of physiological concentrations. Solution of physiological concentration presents a challenging system because of its “intermediate” concentration, which raises serious statistical difficulties. With Drude NAMD, we performed an unprecedentedly large-scale computation of polarizable model. We observed excellent agreement between

experiment and Drude model. In contrast, traditional nonpolarizable model overestimate the electric conductivity and ion diffusion by a factor of 2.5.

Conclusion. The first implementation of a polarizable force field in the high-performance MD simulation program NAMD is presented. The implementation preserves the outstanding scalability of NAMD. The model should be applicable to general all-atom, large-scale simulations. Test simulations demonstrate that the present implementation is numerically stable and is consistent with previous results from CHARMM. The first large-scale application has been performed on an ionic solution of physiological concentration, and transport properties in agreement with experiment have been obtained. Simulations of proteins, membranes, and nucleic acid based on the Drude polarizable force field with NAMD are under way.

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