Multiple time scale molecular dynamics of complex fluids

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Molecular dynamics (MD) remains one of the most fruitful methods for the investigation of various properties in fluids. This especially concerns complex liquids, such as water, solvated proteins and other collections of biophysical molecules, which are of interest for modern chemistry and medicine. The characteristic feature of these systems is the coexistence of dynamical processes with vastly different time scales. For instance, in water the intramolecular vibrations of atoms relate to the fastest motion, an intermediate time scale arises from the strong short-range intermolecular interactions, while slow dynamics appears due to the weak long-range van der Waals and Coulombic potentials. A lot of multiple time stepping (MTS) approaches have been devised over the years to speed up the MD computations [1]. However, due to the presence of MTS resonance instabilities, the size of the time step in these approaches is limited to relatively small values.

In the current study we propose a novel MTS technique in order to obviate the limitations on the size of the time step in MD simulations of complex fluids. It presents a nontrivial combination of the decomposition operator method with a specific extrapolation of intermolecular interactions complemented by an extended isokinetic Nosé-Hoover chain approach in the presence of translational and orientational degrees of freedom. While the existing multiscale algorithms can increase the outer size of the time step from 5 fs to 100 fs, it is shown on the basis of MD simulations of water that the new technique allows one to significantly overcome this limitation. In particular, now giant time steps of order 500 fs up to 5 ps can be used for studying equilibrium and conformational properties without loss of precision.

The new approach can be applied to more complex models of fluids and their mixtures. It can also be jointed with the integral equation method to further increase the efficiency of the calculations.

[1] I. P. Omelyan, J. Chem. Phys. 131, 104101 (2009).