Almost exact multiple time scale molecular dynamics

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The vast majority of systems in physics, chemistry, and biology are characterized by the coexistence of dynamical processes with different time scales. Molecular dynamics (MD) is a powerful tool which is widely used to study various phenomena in such systems. In view of the restricted capabilities of computers, the main factor responsible for further progress in MD modeling is the increase of efficiency of integrating schemes. A lot of multiple time stepping (MTS) techniques have been devised over the years to improve the efficacy of MD simulations. Despite the previous achievements, all the known MTS algorithms are precise only to the second order in the time steps. This means that only modest accuracy of the computations can be reached.

In the present investigation we propose a novel MTS method for the integration of motion in MD simulations of many-particle systems. It combines special phase-space transformations with a high-accuracy reversible factorization of the time evolution propagator into analytically solvable parts related to different time scales. This allows one to overcome principal limitations imposed on efficiency of the simulations in standard MTS algorithms. Comparison with the well-recognized previous MTS approaches has shown, in particular, that the new method is able to substantially increase the precision of the integration incurring nearly the same computational efforts. This makes the MD calculations almost exact already at typical sizes of the time steps.

Our method is quite general and can be applied to various areas including hybrid Monte Carlo and *ab initio* MD simulations. It can also be extended to more complicated non-Hamiltonian systems and statistical ensembles with additional degrees of freedom and arbitrary numbers of time scales.

1. I. P. Omelyan, Phys. Rev. E **78**, 026702 (2008).
2. I. P. Omelyan, J. Chem. Phys. **127**, 044102 (2007).