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Improved Angular-Momentum Verlet Algorithm for Rigid Molecules

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Summary

There has been increased interest to understand through computer simulation the dynamics of micro-droplets; for example, the coalescence and/or disruption of water droplets as a fundamental process of the cloud formation for the earth climate estimation, the formation and size-controlling mechanism of the ink-droplet for advanced ink-jet printer. Since long-time simulations of such water droplets at atomistic scale are required, we often choose the rigid-body type inter-atomic potential as the TIP4P. In the present paper, we propose the improved angular-momentum Verlet (IAMV) method for the time evolution of the rigid molecules, by enforcing complete time-reversibility to the AMV method [1].

The AMV method for rigid molecules is unique in that it is very simple as compared to the symplectic-type methods. The total energy drift in the case of rigid-CH4 becomes much smaller than that obtained with the leap-frog and Gear predictor-corrector methods. Nevertheless, when we performed the dynamic simulation of a water droplet with the TIP4P potential, we could not ignore the energy drift during the simulation. We find that it was caused largely by the incompleteness of the time-reversibility of the AMV method. In our IAMV method, an additional procedure to numerically solve a non-linear function is installed to the AMV method to enforce the complete time-reversibility. The additional procedure requires little computation load.

In the case of a water droplet composed of 1688 rigid-H2O with the TIP4P potential, we can take longer time step (about 3 or 4 times) compared that using the AMV method. Such an improvement will be helpful to realize large-scale, dynamic simulations of droplets.