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Dissipative particle dynamics incorporating non-Markovian effect

IKUYA KINEFUCHI, YUTA YOSHIMOTO, SHU TAKAGI, Department of Mechanical Engineering, The University of Tokyo — The coarse-graining methodology of molecular simulations is of great importance to analyze large-scale, complex hydrodynamic phenomena. In the present study, we derive the equation of motion for non-Markovian dissipative particle dynamics (NMDPD) by introducing the history effects on the time evolution of the system [Y. Yoshimoto et al., Phys. Rev. E 88, 043305 (2013)]. Our formulation is based on the generalized Langevin equation, which describes the motions of the centers of mass of clusters comprising microscopic particles. The mean, friction, and fluctuating forces in the NMDPD model are directly constructed from an underlying MD system without any scaling procedure. For the validation of our formulation, we construct NMDPD models from high-density Lennard-Jones systems, in which the typical time scales of the coarse-grained particle motions and the fluctuating forces are not fully separable. The NMDPD models reproduce the temperatures, diffusion coefficients, and viscosities of the corresponding MD systems more accurately than the conventional DPD models based on a Markovian approximation. Our results suggest that the NMDPD method is a promising alternative for simulating mesoscale flows where a Markovian approximation is not valid.

Ikuya Kinefuchi
Department of Mechanical Engineering, The University of Tokyo

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