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Construction of interaction models of dissipative particle dynamics by coarse-graining Lennard-Jones fluids: Evaluation of non-Markovian formulation YUTA YOSHIMOTO, TOSHIKI MIMA, The University of Tokyo, AKINORI FUKUSHIMA, Tohoku University, IKUYA KINEFUCHI, The University of Tokyo, TAKASHI TOKUMASU, Tohoku University, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo — The application of molecular dynamics (MD) simulation to mesoscale (10-100 nm) flow analysis is computationally expensive at present. Dissipative particle dynamics (DPD) simulation is a powerful candidate for the alternative method because the DPD interaction, which has a soft potential between mesoscopic particles, enables larger space and longer time simulation. In the present study, we develop the method of bottom-up construction of non-Markovian DPD (NMDPD) models by means of MD simulations. We focus on the center of mass of the cluster containing Lennard-Jones particles, and extract the effective forces exerted on the clusters. Moreover, we sample the spectra of fluctuating forces acted on the clusters in the MD system, and find that the white noise used in the conventional DPD simulations should be replaced by colored noise. In order to reproduce the spectra, finite impulse response filters are employed in NMDPD simulations. Finally we evaluate the NMDPD models by comparing the simulation results with the MD counterparts.

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