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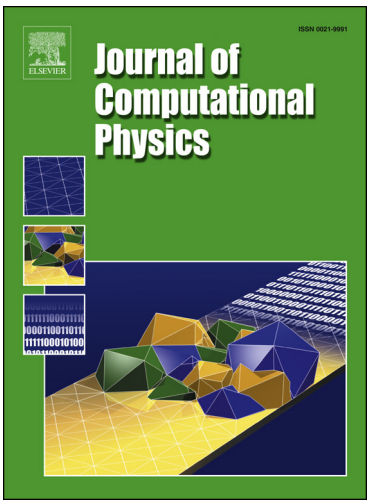

Anisotropic single-particle dissipative particle dynamics model

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Anisotropic single-particle dissipative particle dynamics model

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Abstract

We have developed a new single-particle dissipative particle dynamics (DPD) model for anisotropic particles with different shapes, e.g., prolate or oblate spheroids. In particular, the conservative and dissipative interactions between anisotropic single DPD particles are formulated using a linear mapping from the isotropic model of spherical particles. The proper mapping operator is constructed between each interacting pair of particles at every time step. Correspondingly, the random forces are properly formulated to satisfy the fluctuation-dissipation theorem (FDT). Notably, the model exactly conserves both linear and angular momentum. We demonstrate the proposed model's accuracy and efficiency by applying it for modeling colloidal ellipsoids. Specifically, we show it efficiently captures the static properties of suspensions of colloidal ellipsoids. The isotropic-nematic transition in an ellipsoidal suspension is reproduced by increasing its volume fraction or the aspect ratio of ellipsoid particles. Moreover, the hydrodynamics and diffusion of a single colloidal ellipsoid (prolate or oblate with moderate aspect ratios) are accurately captured. The calculated drag force on the ellipsoid and its diffusion coefficients (both translational and rotational) agree quantitatively with the theoretical predictions in the Stokes limit.

Key words:
Dissipative Particle Dynamics; Single-particle Dissipative Particle Dynamics; Colloid Suspension; Ellipsoidal Particle

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