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Simulating nanoscale particle suspensions using a coupled lattice-Boltzmann and Langevin-dynamics method: application to particle transport in cellular blood flow. ZIXIANG LIU, YUANZHENG ZHU, Georgia Institute of Technology, REKHA RAO, JONATHAN CLAUSEN, Sandia National Laboratories, CYRUS AIDUN, Georgia Institute of Technology — A novel computational approach coupling the lattice-Boltzmann (LB) method and a Langevin-dynamics (LD) approach has been developed to simulate nanoscale particle (NP) suspensions in the presence of both thermal fluctuation and many-body hydrodynamic interactions (HI). The Brownian motion of NPs is explicitly driven by the stochastic force term in the LD. The LB method is coupled with the LD in a two-way fashion through a discrete forcing source distribution term in the LB method. The validity and accuracy of this LB-LD approach is demonstrated through several verification problems, including velocity relaxation of an isolated particle, self-diffusion of a Brownian particle, and relaxation of a polymer chain. Good agreement between simulation and theory is observed. The verified algorithm is applied to study the migration of NPs in cellular blood flow within microvasculature. For NPs of diameter 1˜100 nm, Brownian diffusion, compared to the red blood cell (RBC)-enhanced diffusion, is shown to be the predominant driver for the NP radial diffusion process. For larger NPs of diameter ˜500 nm, Brownian diffusion and RBC-enhanced diffusion are shown to be comparably significant.

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