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Direct Numerical Simulations of Colloidal Dispersions under External Force

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There have been proposed several numerical methods applicable to colloidal dispersions. Recently, it has been shown that the use of diffuse colloid/fluid interfaces with non-zero thickness $\xi$ much improves the efficiencies of the simulations [1, 2]. Along with this line, we developed a method for direct numerical simulations (DNS) of electro-hydrodynamic phenomena in charged colloidal dispersions [KAPSEL:http://www-tph.cheme.kyoto-u.ac.jp/kapsel/] [3]. This method enables us to compute the time evolutions of colloidal particles, ions, and host fluids simultaneously by solving Newton, advection-diffusion, and Navier-Stokes equations so that the electro-hydrodynamic couplings can be fully taken into account [4]. The electrophoretic mobilities of charged spherical particles are calculated in several situations. The comparisons with approximation theories show quantitative agreements for dilute dispersions without any empirical parameters; however, our simulation predicts notable deviations in the case of dense dispersions [5].

We recently modified our DNS code for particle dispersions to take into account the effect of Brownian motions of the particles. The new code has been applied to several cases where coupling between hydrodynamic interaction and the thermal fluctuation becomes important (left figure) [6]. DNS simulations have been performed for several systems under external fields. Striking examples include chain formations of likely charged particles due to the application of
Left: A snapshot of a fluctuating polymer chain of N=10. Right: Shear viscosity vs. shear rate for a Brownian particle dispersion. The colloid volume fractions are 0.51, 0.41, and 0.2 for phi = 3, 2, and 1, respectively. Clear shear thickening behavior is observed for high volume fraction cases when shear rate is increased.

external electric fields. The mechanism behind this phenomena has been analyzed. Also a clear tendency of the shear thickening behavior of colloidal dispersions has been obtained when we apply shear flow to the system (right figure) [7]. The origin of the thickening will be discussed.

References


