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A Coarse-Grained Simulation of Rheology of Colloidal Suspensions and Polymer Nano-Composites VICTOR PRYAMITSYN, University of Texas@Austin, VENKAT GANESAN — We extend DPD model to address dynamical properties of suspensions of solid particles in complex fluids. In this approach, the solvent particles (polymer segments) are represented as DPD particles. In contrast, the solute particles are represented as spherical hard particles of appropriate size. To provide proper shear friction and grip of the colloids and solvent we utilize Espanol's extensions over standard DPD model by adding rotational degree of freedom and rotational friction and **non-central** dissipative and random forces. For non-polymeric fluids, our results focus on the equilibrium dynamics and the steady state shear rheological behavior for a range of volume fractions of the suspension, and demonstrate excellent agreement with many published experimental and theoretical results. Moreover, we are also able to track the glass transition of our suspension and associated dynamical signatures in both the diffusivities and the rheological properties of our suspension. For polymeric fluid, we have studied influence of polymer-particle friction and particle concentration on polymer matrix relaxation dynamics, particle diffusion and rheology of the composite. Our results suggest that the simulation approach can be used as a mesoscale model to examine quantitatively the rheological properties of colloidal suspensions in complex fluid solvents such as polymeric melts and solutions, as well as allied dynamical phenomena such as phase ordering in mixtures of block copolymers and particles.

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