A Coarse-Grained Simulation of Rheology of Colloidal Suspensions and Polymer Nano-Composites

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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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Date submitted: 01 Dec 2004
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