LARGE SCALE SIMULATIONS OF COLLOIDAL SUSPENSIONS

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Our group has developed a method for efficient computation of hydrodynamic interactions in concentrated suspensions at low Reynolds numbers. This method follows the formulation of the Stokesian dynamics approach with a far field multipole expansion for the many body effects combined with a near field lubrication correction based on exact two body resistance functions. In contrast to the $O(N^2, N^3)$ cost of the classic algorithm, an $O(N \ln N)$ computational algorithm was developed where N is the number of particles. The new algorithm is based on a particle mesh Ewald approach whereby near field interactions are evaluated directly and far field interactions are computed using a grid based velocity computed with FFT's. Simulations for non-Brownian suspensions have been conducted for dynamic simulations with up to 64,000 particles and Monte Carlo realizations with up to 1 million particles. Simulations for Brownian suspensions (with accurate hydrodynamic interactions) have been conducted for up to 27,000 particles. These latter simulations employ an iterative algorithm for computing matrix square roots for matrices of rank up to $O(10^5)$. All simulations employ efficient preconditioned GMRES iterative solvers.

The algorithm has been extended to investigate systems of anisotropic particles. Numerical simulations have been conducted for the rheology of concentrated suspensions of non-Brownian platelike particles. Platelike particles are modeled as rigid planer assembledges of spherical particles. Simulations are conducted for systems with 64 to 512 platelets involving up to 104 individual spheres. The suspension rheology and suspension microstructure is documented over a wide range of volume fraction and particle aspect ratio. Details of the suspension microstructure include strong flow induced orientation ordering and formation of large particle clusters. The extension of the method for Brownian simulation of constrained particle assembledges is discussed.