Simulating the rheology of complex fluids using Smoothed Particle Hydrodynamics

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ABSTRACT

Complex fluids can be found in a wide range of industrial applications, such as dense slurry transport, colloidal suspensions and suspended biomass particles. Complex fluids often display non-Newtonian rheology which has important consequences for the design of transport systems. The rheological properties of the system cannot not always be obtained from experiments or theory alone, especially for dense systems with non-uniformly shaped impurities.

In the present work, we use Smoothed Particle Hydrodynamics (SPH) for the direct simulation of complex fluids in order to derive relevant transport properties. SPH is a meshless method which allows the simultaneous solution of the carrier fluid (SPH particles following Navier-Stokes equations) and impurities (following rigid body equations). The particle interactions are based on Newton's Third Law, so both linear and angular momentum are conserved in the simulation.

Key features in the SPH simulator that are required for small scale simulations of complex fluids are: (1) an unrestricted number of free-floating rigid bodies, (2) a collision model to account for collisions between the rigid bodies, (3) thermal fluctuations in order to capture mesoscale dynamics [1]. All features are incorporated in an SPH code with distributed memory running on multiple nodes [2]. The implementation of the collision model and the thermal fluctuations, in particular, required special attention with regards to communication of information in a distributed memory system.

The first application is the case of dense slurry transport in a Taylor-Couette flow, similar to the model described by [3]. The simulation can be seen as a computer model of a classic rheometer experiment that is commonly used to determine the viscosity of a complex fluid. The dense slurry is modelled as a collection of hard spheres suspended in a continuous fluid. The effective viscosity, measured in a suite of simulations at varying particle concentrations, appears to be in good agreement with Einstein's estimate for small volume fractions [4]. In comparison with the analytical estimate, the SPH simulation technique offers the possibility to study high particle concentrations and particle geometries of arbitrary shapes (within the limit of the available SPH particle resolution), such as fibres, ellipsoids, and wood chips. A second example where the present simulation method has been applied is in the simulation of dilute polymer solutions, where each polymer molecule is modelled as a collection of beads and springs. The effective viscosity, derived from these simulations for a range of polymer concentrations, reflects the shear thinning behaviour also observed in experiments.

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