A Unique Approach to Couple Lagrangian Mechanics and an Incompressible Flow Solver

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Discrete multiphase systems exhibit a wealth of behavior that result from a potentially diverse microstructure. At higher concentrations, separations between dispersed phase elements can be on the order of nanometers to microns. Not only can large stress gradients exist in such interstitial regions, the continuum hypothesis itself can break down. This represents a class of problems for which scale coupling is a necessity. Examples of such systems include composite materials at high concentration, suspensions, emulsions, and foams. This work focuses on development of robust numerical simulation capabilities for suspensions of small solid particles in liquids, incorporating effects spanning diverse time and length scales.

We have examined mathematical coupling methods at the particle scale which accurately account for hydrodynamic effects under near-contact and full-contact conditions. In anticipation of supporting a modeling capability that deploys a distributed Lagrange Multiplier approach (DLM) to couple particle and fluid mechanics as a complimentary approach to the more traditional boundary element methods, we have examined the breakdown of continuum finite element/overset Langrangian solid coupling using the computer code Goma originally developed at Sandia National Laboratories [1]. More specifically, we are deploying a unique approach that allows for Lagrangian mechanics in the particles to be coupled in a Newton-Rahpson framework with an incompressible flow solver using the mortar finite element method and distributed Lagrange multiplier constraints.

We have examined two-particle geometries with a user-prescribed particle squeezing flow and compared the integrated particle stress (force) with analytical solutions in a creeping flow regime. We have found (not surprisingly) that agreement is good at separations of order of one particle diameter, but as the gap closes to nanometer length scales the predicted singularity in the lubrication stress (force) is grossly underpredicted. Using the DLM approach, we have also examined the effects of mechanical properties of the particles in near contact conditions brought about in a shearing and squeezing flow. Specifically, we have built two-particle models, each particle composed of a core material and an outer shell, and subjected them to various flow configurations.

The figure below illustrates the nature of the models and the computational experiments we have run. In the rigid-particle case, both core and shell materials are taken to have the same elastic constants, which are set exceedingly large so as to suppress any deformation brought about by hydrodynamic forces. To mimic a typical nanoparticle suspension (or colloidal suspension) we then soften the outer shell material as if it were a grafted polymer brush and examine the effect on the interparticle force imparted in shear flows. Such brushes are essential to the dispersion stability of colloidal suspensions, and their presence may in fact change the course of our ultimate modeling approach due to the mechanical (steric) and chemical (osmotic) repulsion which may prevent rigid core contact in all but extreme flow conditions. Illustrated in the figure are the effects of the shell mechanical properties on the interparticle force during a near-contact event (viz. force component in one direction versus time as one particle approaches another due to an impressed flow). Interestingly, we find that the shell softness reduces the peak force when compared to the rigid case, and further reduction is seen by

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making the particle core soft as well. In a particle squeezing configurations (viz. one particle forced to approach a second on a line between centers, with no rotation) we see that the onset of the precipitous increase in force at near-contact is delayed in time the softer the particle, and that the maximum force is drastically reduced.

In a complimentary study we have begun to build in colloidal forces together with Hertzian contact forces into the molecular dynamics code LAMMPS in order to examine the stability of suspensions, with the ultimate goal to couple in hydrodynamics by one of many candidate techniques. .

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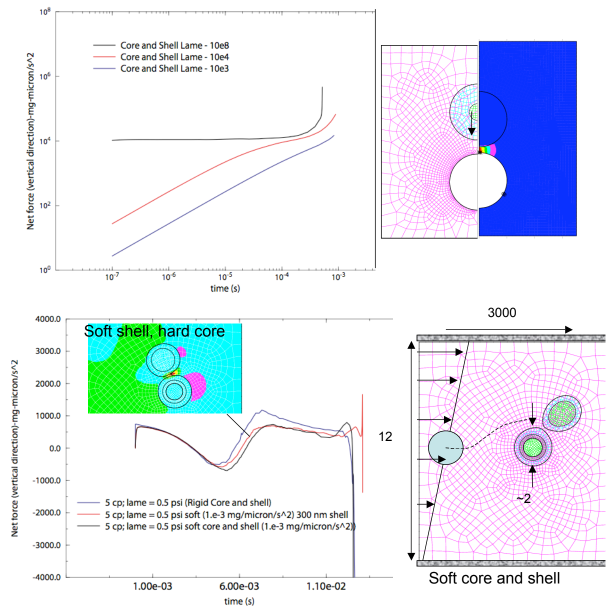

(b

Sample overset grid (DLM) simulations of soft particle interactions in (a) squeezing flow (top particle impressed with prescribed motion toward a fixed second particle in an axisymmetric geometry) and (b) in a confined shearing flow. Particle sizes in both case are about 2 microns (with some variation due to the shell thickness). Fluid viscosity is 5 cP and shell core bulk and shear modulii are varied between 1.x106 psi and 0.5 psi.