Advanced Scientific Computing Research
FY 2006 Accomplishment

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

P. Randall Schunk *, Sandia National Laboratories
Lisa A. Mondy, Sandia National Laboratories
Alan L. Graham, Los Alamos National Laboratory

Summary

The main objective of the research is to develop a robust numerical simulation capability for flows of particles suspended in a liquid that incorporates effects spanning diverse time and length scales. Linking recent progress in molecular and nano-scale science to progress in the ability to accurately model suspension flows at the macroscale is an important challenge for many energy-related technologies. By deploying a unique approach that allows for Lagrangian mechanics in the particles to be coupled to an incompressible flow solver, we have examined mathematical coupling methods at the particle scale which accurately account for hydrodynamic effects under near-contact and full-contact conditions.

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. 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.

Using the DLM approach, we have examined the effects of mechanical properties of the particles in near contact conditions. Specifically, we have built two-particle models, each particle composed of a

* (505) 844-5992, prshun@sandia.gov

core material and an outer shell, and subjected them to various flow configurations that lead to close contact.

The figure below illustrates 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 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). In particle squeezing configurations 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.

Acknowledgments
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. Funded at Los Alamos by the Department of Energy under contract W-7405-ENG-36.

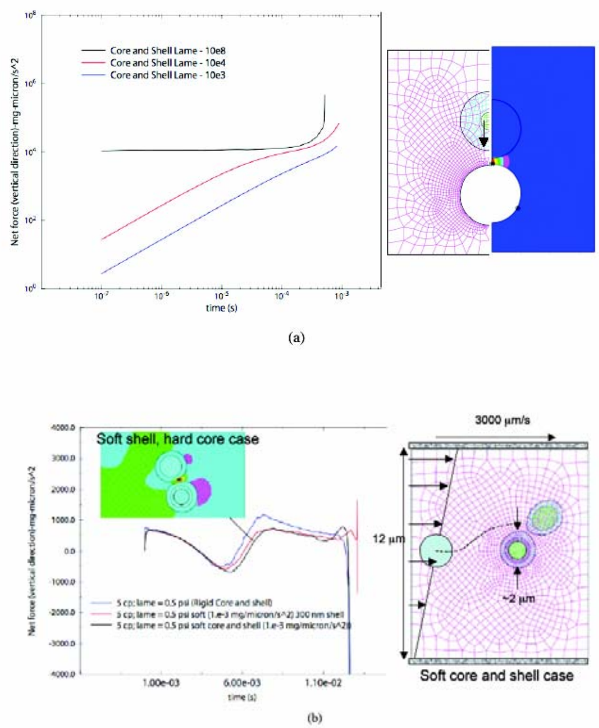

Figure 1. *Sample overset grid (DLM) simulations of soft particle interactions in (a) squeezing flow (top particle impressed with prescribed motion toward a fixed second particle in an axisymmetric geometry) and (b) in a confined shearing flow. Particle sizes in both cases are about 2 microns (with some variation due to the shell thickness).*

For further information on this subject contact:
Dr. Anil Deane, Program Manager
Mathematical, Information, and Computational Sciences Division
Office of Advanced Scientific Computing Research
Phone: 301-903-1465
deane@mics.doe.gov