MULTISCALE, NEAR-CONTACT BOUNDARY ELEMENT SIMULATIONS

Shihai Feng[*], Marc Ingber[+], Antonio Redondo[*], Howard Brenner[#], and Alan Graham[*]

[*]Los Alamos National Laboratory
Los Alamos, NM 87544, USA
graham@lanl.gov

[+]University of New Mexico
Albuquerque, NM 87131, USA

[#]Massachusetts Institute of Technology
Cambridge, MA 02139, USA

In concentrated model suspensions of smooth, neutrally-buoyant spheres in Newtonian liquids, continuum theories predict that particles can reach separation distances of less than 10^{-9} particle radii. For many suspensions these separation distances would be of molecular dimensions. Under these circumstances, the continuum approximations break down. In this study we describe a new methodology for coupling coarse grain molecular dynamics in the near contact region with continuum-level simulations in the bulk suspensions. First we show how the results of this new computational algorithm converge to exact hydrodynamic solutions. Then a new multiscale integration technique is properly constrained and used for linking the molecular dynamics with the hydrodynamics is described. This multiscale analysis introduces an absolute length scale in the otherwise scaleable hydrodynamic calculations. The results of these preliminary calculations will describe under what conditions these non-continuum effects appreciably effect suspension behavior.

Keywords: molecular dynamics, suspensions, multiscale