

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Long-Range Hydrodynamic Interactions Implemented into LAMMPS (Parallel MD)** FRANCES MACKAY, COLIN DENNISTON, University of Western Ontario — We use an explicit solvent method to study the interaction between particles and a fluid. Similar to the Particle-Mesh-Ewald schemes for electrostatics, the long range hydrodynamic interactions are treated by interpolating the particle density onto a mesh. This is then coupled to the fluid, which we model using a thermal lattice Boltzmann scheme. Mass and momentum conserving noise in the lattice Boltzmann fluid scheme provides a thermostat for both the fluid and the particles. This work has been fully parallelized and implemented into LAMMPS, an open-source molecular dynamics code. We demonstrate the scheme with some examples from colloidal physics and flow over rough surfaces.

Frances Mackay  
University of Western Ontario

Date submitted: 26 Nov 2008

Electronic form version 1.4