Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

**Towards a Discrete Element Method (DEM) for modeling anisotropic, nano- and colloidal scale particles in Molecular Dynamics (MD)** RYAN MARSON, MATTHEW SPELLINGS, JOSHUA ANDERSON, SHARON GLOTZER, Univ of Michigan - Ann Arbor — Faceted shapes, such as polyhedra, are commonly created in experimental systems of nanoscale, colloidal, and granular particles. Many interesting physical phenomena, like crystalline nucleation and growth, vacancy motion, and glassy dynamics, are challenging to model in these systems because they require detailed dynamical information at the individual particle level. Within the granular materials community the Discrete Element Method has been used extensively to model systems of anisotropic particles under gravity, with friction. We report the first implementation of DEM MD intended for thermodynamic nanoscale simulation. Our method is implemented in parallel on the GPU within the HOOMD-Blue framework. By decomposing the force calculation into its components, this implementation can take advantage of massive data parallelism, enabling optimal use of the GPU for even relatively small systems while achieving a speedup of 60 times over a single CPU core. This method is a natural extension of classical molecular dynamics into the realm of faceted particles, and allows simulation of disparate size scales ranging from the nanoscale to granular particulates, all within the same framework.

Ryan Marson
Univ of Michigan - Ann Arbor

Date submitted: 15 Nov 2013 Electronic form version 1.4