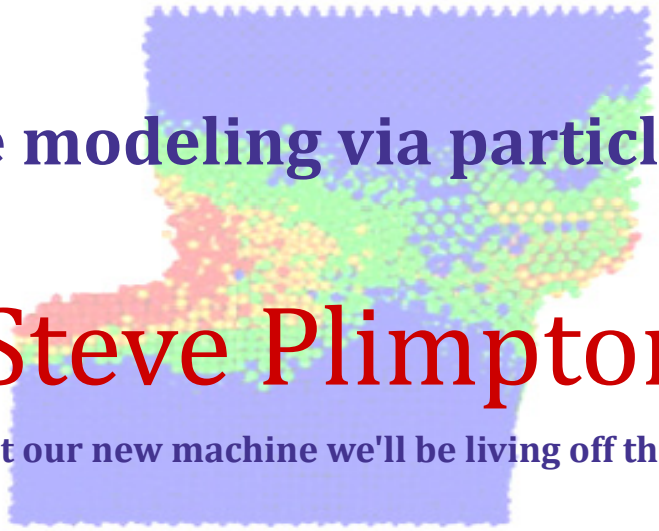
LSU DEPARTMENT OF MECHANICAL ENGINEERING

The Sidney E. Fuchs Seminar Series

3:30-4:30pm, Friday, November 4, 2011

Frank H. Walk Design Presentation Room



Multi-scale modeling via particle methods

by **Steve Plimpton***

"when we get our new machine we'll be living off the fat of the land"

I'll describe two approaches to multi-scale modeling that we have undertaken using our molecular dynamics code LAMMPS. The first is to provide a hierarchy of methods for coarse-graining a model, so that simulations at varying length and timescales can be performed with the same code, hopefully with some overlap. In our case, we have done this to model the rheological properties of solvated nanoparticles, in collaboration with industrial partners. The second approach is to couple particle dynamics to other more meso-scale methods such as kinetic Monte Carlo models for microstructural evolution in solids. This work is more preliminary, but I will illustrate how it can be done. Finally, I'll highlight a trend in all-atom molecular dynamics modeling whereby potentials are growing both more accurate and more expensive over time.

* Steve Plimpton is a staff member at Sandia National Laboratories, a US Department of Energy lab. For many years he was in the Parallel Computational Sciences group. In 2001, he moved to a new Computational Biology group. In 2007, he became part of the Scalable Algorithms group. Steve's work involves implementing and using scientific simulations designed for parallel supercomputers. Often this includes the creation of efficient parallel algorithms. The applications he works on typically use particles, finite elements, or partial differential equations. With collaborators, he also distributes open-source versions of molecular dynamics (LAMMPS), kinetic Monte Carlo (SPPARKS), and MapReduce (MR-MPI) software.

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