Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Parallel Verlet Neighbor List Algorithm for GPU-Optimized MD Simulations SAMUEL CHO, Departments of Physics and Computer Science, Wake Forest University — How biomolecules fold and assemble into well-defined structures that correspond to cellular functions is a fundamental problem in biophysics. Molecular dynamics (MD) simulations provide a molecular-resolution physical description of the folding and assembly processes, but the computational demands of the algorithms restrict the size and the timescales one can simulate. In a recent study, we introduced a parallel neighbor list algorithm that was specifically optimized for MD simulations on GPUs. We now analyze the performance of our MD simulation code that incorporates the algorithm, and we observe that the force calculations and the evaluation of the neighbor list and pair lists constitute a majority of the overall execution time. The overall speedup of the GPU-optimized MD simulations as compared to the CPU-optimized version is N-dependent and $\sim$ 30x for the full 70s ribosome (10,219 beads). The pair and neighbor list evaluations have performance speedups of $\sim$ 25x and $\sim$ 55x, respectively. We then make direct comparisons with the performance of our MD simulation code with that of the SOP model implemented in the simulation code of HOOMD, a leading general particle dynamics simulation package that is specifically optimized for GPUs.

Samuel Cho
Departments of Physics and Computer Science, Wake Forest University

Date submitted: 03 Dec 2012 Electronic form version 1.4