Algorithmic enhancements to boost the performance of general purpose molecular dynamics on data-parallel architectures

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HOOMD is an established open-source package that performs general purpose molecular dynamics on NVIDIA graphics processing units (GPUs). Running on the GTX 285 GPU, its current performance is fifty to sixty times faster than a single AMD Opteron CPU core. This level is up almost by a factor of two from the performance levels initially reported a year and a half ago. Some of the increase is due to a new, faster hardware generation, but much is also from significant algorithmic improvements. First, memory prefetching is now used in many of the computations. Second, the neighborlist computation has been rewritten with a much better memory access pattern and to maximize the latency hiding ability of the GPU. Third, the only step remaining on the CPU in the initial publication, binning the particles, has been efficiently implemented on the GPU. With the performance HOOMD provides, running it on a single inexpensive GPU is a viable alternative to traditional MD software running on a distributed memory cluster.