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Rigid body constraints in HOOMD-Blue, a general purpose molecular dynamics code on graphics processing units TRUNG D. NGUYEN, CAROLYN L. PHILLIPS, JOSHUA A. ANDERSON, SHARON C. GLOTZER, University of Michigan, Ann Arbor — Rigid body constraints are commonly used in a wide range of molecular modeling applications from the atomistic scale, modeling the bonds in molecules such as water, carbon dioxide, and benzene, to the colloidal scale, modeling macroscopic rods, plates and patchy nanoparticles. While the parallel implementations of rigid constraints for molecular dynamics simulations for distributed memory clusters have poor performance scaling, on shared memory systems, such as multi-core CPUs and many-core graphics processing units (GPUs), rigid body constraints can be parallelized so that significantly better performance is possible. We have designed a massively parallel rigid body constraint algorithm and implemented it in HOOMD-Blue, a GPU-accelerated, open-source, general purpose molecular dynamics simulation package. For typical simulations, the GPU implementation running on a single NVIDIA® GTX 480 card is twice as fast as LAMMPS running on 32 CPU cores. In the HOOMD-blue code package, rigid constraints can be used seamlessly with non-rigid parts of the system and with different integration methods, including NVE, NVT, NPT, and Brownian Dynamics. We have also incorporated the FIRE energy minimization algorithm, reformulated to be applicable to mixed systems of rigid bodies and non-rigid particles.

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