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HOOMD-blue, general-purpose many-body dynamics on the GPU JOSHUA ANDERSON, AARON KEYS, CAROLYN PHILLIPS, TRUNG DAC NGUYEN, SHARON GLOTZER, Dept. of Chemical Engineering, University of Michigan, Ann Arbor — We present HOOMD-blue, a new, open source code for performing molecular dynamics and related many-body dynamics simulations on graphics processing units (GPUs). All calculations are fully implemented on the GPU, enabling large performance speedups over traditional CPUs. On typical benchmarks, HOOMD-blue is about 60 times faster on a current generation GPU compared to running on a single CPU core. Next generation chips are due for release in early 2010 and are expected to nearly double performance. Efficient execution is achieved without any lack of generality and thus a wide variety of capabilities are present in the code, including standard bond, pair, angle, dihedral and improper potentials, along with the common NPT, NVE, NVT, and Brownian dynamics integration routines. The code is object-oriented, well documented, and easy to modify. We are constantly adding new features and looking for new developers to contribute to this fast maturing, open-source code [1]. In this talk, we present an overview of HOOMD-blue and give examples of its current and planned capabilities and speed over traditional CPU-based codes. [1] Find HOOMD-blue online at: http://codeblue.umich.edu/hoomd-blue/

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