Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Highly scalable many-GPU simulations of soft matter systems using HOOMD-blue JENS GLASER, Dept. of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, JOSHUA ANDERSON, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor, DAVID MORSE, Dept. of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis — We present a new version of the highly optimized, versatile and easy to use molecular dynamics software HOOMD-blue [1] running on tens to hundreds of GPUs. By taking advantage of a refined version of Plimpton's communication scheme [2] fully implemented on the GPU and of standard MPI software, we demonstrate excellent strong scaling in simulations that have as few as 20,000 particles per GPU. This opens up the possibility of carrying out extremely performant multi-million particle simulations on GPU-based clusters and supercomputers, which are becoming increasingly available to the scientific community.

[1] Anderson, J., Lorenz, C., & Travesset, A. (2008), J. Comp. Phys., 227, 5342-5359.
[2] Plimpton, S. (1995), J. Comp. Phys., 117, 1-19.

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Date submitted: 20 Dec 2012 Electronic form version 1.4