Abstract Submitted
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Towards Fast, Scalable Hard Particle Monte Carlo Simulations on GPUs JOSHUA A. ANDERSON, M. ERIC IRRGANG, JENS GLASER, ERIC S. HARPER, MICHAEL ENGEL, SHARON C. GLOTZER, University of Michigan — Parallel algorithms for Monte Carlo simulations of thermodynamic ensembles of particles have received little attention because of the inherent serial nature of the statistical sampling. We discuss the implementation of Monte Carlo for arbitrary hard shapes in HOOMD-blue [1], a GPU-accelerated particle simulation tool, to enable million particle simulations in a field where thousands is the norm. In this talk, we discuss our progress on basic parallel algorithms [2], optimizations that maximize GPU performance, and communication patterns for scaling to multiple GPUs. Research applications include colloidal assembly and other uses in materials design, biological aggregation, and operations research. [1] Anderson, Glotzer, arXiv:1308.5587 (2013), http://codeblue.umich.edu/hoomd-blue [2] Anderson, Jankowski, Grubb, Engel, Glotzer, J. Comp. Phys. 254, 27 (2013)

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