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HOOMD-blue – scaling up from one desktop GPU to Titan
JENS GLASER, JOSHUA A. ANDERSON, SHARON C. GLOTZER, Department of Chemical Engineering, University of Michigan — Scaling molecular dynamics simulations from one to many GPUs presents unique challenges. Due to the high parallel efficiency of a single GPU, communication processes become a bottleneck when multiple GPUs are combined in parallel and limit scaling. We show how the fastest general-purpose molecular dynamics code currently available for single GPUs, HOOMD-blue [1,2], has been extended using spatial domain decomposition to run efficiently on tens or hundreds of GPUs. A key to parallel efficiency is a highly optimized communication pattern using locally load-balancing algorithms fully implemented on the GPU. We will discuss comparisons to other state-of-the-art codes (LAMMPS) and present preliminary benchmarks on the Titan super computer. [1] http://arxiv.org/pdf/1308.5587 [2] http://codeblue.umich.edu/hoomd-blue

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