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Molecular Dynamics of Polymer Systems on Graphic Processing Units (GPUs)[1] JOSHUA ANDERSON, Iowa State University and Ames Laboratory, CHRIS LORENZ, Kings College London, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Molecular dynamics (MD) is a powerful, but computationally intensive, simulation technique capable of modeling a wide range of systems in and out of thermodynamic equilibrium. Using traditional computers, simulations large enough to explore the phases of polymer systems require the use of expensive distributed memory clusters. Graphics Processing Units now offer an unprecedented amount of computing power for general purpose applications. They are inexpensive ($500) and can be added to almost any standard desktop system. MD algorithms are adapted to execute on a single GPU, which is able to attain the same performance as 32 processor cores on a cluster. It is possible for a single system to host up to 4 GPUs, putting the power of a 128 processor core cluster on the desktop. This performance is illustrated in a variety of polymer systems such as low density micellar phases with cubic symmetry, high density lamellar and nanocomposite gyroid systems. GPUs offer unprecedented opportunities for the simulation of polymer systems.

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