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Pseudo-Random Number Generation for Brownian Dynamics and Dissipative Particle Dynamics Simulations on GPU Devices CAROLYN PHILLIPS, JOSHUA ANDERSON, SHARON GLOTZER, University of Michigan — Brownian Dynamics (BD) and Dissipative Particle Dynamics (DPD) are implicit solvent methods commonly used in models of soft matter and biomolecular systems. The interaction of the numerous solvent particles with larger particles is coarse-grained as a Langevin thermostat is applied to individual particles or to particle pairs. The Langevin thermostat requires a pseudo-random number generator (PRNG) to generate the stochastic force applied to each particle or pair of neighboring particles during each time step. In a GPU parallel computing environment, small batches of random numbers must be generated over thousands of threads and millions of kernel calls. We introduce a PRNG scheme, in which a micro-stream of pseudorandom numbers is generated in each thread and kernel call. These high quality, statistically robust micro-streams are more computationally efficient than other PRNG schemes in memory-bound kernels, and uniquely enable the DPD simulation method . This scheme has been implemented in HOOMD-blue, a GPU-accelerated open-source general purpose molecular dynamics simulation package. By enabling BD and DPD to be performed in HOOMD-blue, a broad range of mesoscale coarse-grained simulations can now be accelerated in a massively parallel architecture.

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