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Dissipative Particle Dynamics Simulations at Extreme Scale: GPU Algorithms, Implementation and Applications[1] YU-HANG TANG, GEORGE KARNIADAKIS, Brown Univ, CRUNCH TEAM — We present a scalable dissipative particle dynamics simulation code, fully implemented on the Graphics Processing Units (GPUs) using a hybrid CUDA/MPI programming model, which achieves 10-30 times speedup on a single GPU over 16 CPU cores and almost linear weak scaling across a thousand nodes. A unified framework is developed within which the efficient generation of the neighbor list and maintaining particle data locality are addressed. Our algorithm generates strictly ordered neighbor lists in parallel, while the construction is deterministic and makes no use of atomic operations or sorting. Such neighbor list leads to optimal data loading efficiency when combined with a two-level particle reordering scheme. A faster *in situ* generation scheme for Gaussian random numbers is proposed using precomputed binary signatures. We designed custom transcendental functions that are fast and accurate for evaluating the pairwise interaction. Computer benchmarks demonstrate the speedup of our implementation over the CPU implementation as well as strong and weak scalability. A large-scale simulation of spontaneous vesicle formation consisting of 128 million particles was conducted to illustrate the practicality of our code in real-world applications.

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