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Solving Multiscale Polymer Field Theory Simulations with Lattice Boltzmann Equation HSIEH CHEN, YONGJOO KIM, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — A new Lattice Boltzmann (LB) approach is introduced to solve for the modified diffusion equations in polymer field theory. This method bridges two desired properties from different numerical techniques, namely: (i) it is robust and stable as the pseudo-spectral method, and (ii) it is flexible and allows for grid refinement and arbitrary boundary conditions. While the LB method is not as accurate as the pseudo-spectral method, full self-consistent field theoretic (SCFT) simulations of block copolymers on graphoepitaxial templates yield indistinguishable results from pseudo-spectral calculations. Furthermore, we were able to achieve speedups of about 100x compared to single CPU core implementations by using graphics processing units (GPUs). We expect this method to be very useful in truly multi-scale studies where small length scale details have to be resolved, such as in strongly segregating block copolymer blends, nanoparticle-polymer interfaces, or polymer wetting phenomena.

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