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New algorithms for field-theoretic block copolymer simulations: Progress on using adaptive-mesh refinement and sparse matrix solvers in SCFT calculations SCOTT SIDES, BEN JAMROZ, ROBERT CROCKETT, ALEXANDER PLETZER, Tech-X Research — Self-consistent field theory (SCFT) for dense polymer melts has been highly successful in describing complex morphologies in block copolymers. Field-theoretic simulations such as these are able to access large length and time scales that are difficult or impossible for particle-based simulations such as molecular dynamics. The modified diffusion equations that arise as a consequence of the coarse-graining procedure in the SCF theory can be efficiently solved with a pseudo-spectral (PS) method that uses fast-Fourier transforms on uniform Cartesian grids. However, PS methods can be difficult to apply in many block copolymer SCFT simulations (eg. confinement, interface adsorption) in which small spatial regions might require finer resolution than most of the simulation grid. Progress on using new solver algorithms to address these problems will be presented. The Tech-X Chompst project aims at marrying the best of adaptive mesh refinement with linear matrix solver algorithms. The Tech-X code PolySwift++ is an SCFT simulation platform that leverages ongoing development in coupling Chombo, a package for solving PDEs via block-structured AMR calculations and embedded boundaries, with PETSc, a toolkit that includes a large assortment of sparse linear solvers.

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