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Using adaptive-mesh refinement in SCFT simulations of surfactant adsorption SCOTT SIDES, Tech-X Research, RAJEEV KUMAR, Oak Ridge National Lab, BEN JAMROZ, ROBERT CROCKETT, ALEX PLETZER, Tech-X Research — Adsorption of surfactants at interfaces is relevant to many applications such as detergents, adhesives, emulsions and ferrofluids. Atomistic simulations of interface adsorption are challenging due to the difficulty of modeling the wide range of length scales in these problems: the thin interface region in equilibrium with a large bulk region that serves as a reservoir for the adsorbed species. Self-consistent field theory (SCFT) has been extremely useful for studying the morphologies of dense block copolymer melts. 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. However, even SCFT methods can be difficult to apply to systems in which small spatial regions might require finer resolution than most of the simulation grid (eg. interface adsorption and confinement). We will present results on interface adsorption simulations using PolySwift++, an object-oriented, polymer SCFT simulation code aided by the Tech-X Chompst library that enables via block-structured AMR calculations with PETSc.

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