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Multi-fluid simulations of polymer dynamics DOUGLAS TREE, KRIS DELANEY, GLENN FREDRICKSON, Univ of California - Santa Barbara — In many industrially important polymeric materials, a discrepancy exists between the time scale intrinsic to the system and processing time scales. As a consequence, models which go beyond equilibrium thermodynamics are required to understand the evolution of the microstructure of such materials. Building a tractable model to address such a system becomes especially challenging when process dynamics coexist with complex thermodynamic behavior such as micro- or macro-phase separation. Indeed, in many traditional simulation schemes (e.g. Brownian or molecular dynamics or dynamic field theories), cost constraints become prohibitive for 3D dynamic simulations as length and time scales increase. To address such problems, we explore a framework of meso-scale dynamic phase field models originally proposed by Brochard and de Gennes. Expanding on the "two-fluid" formalism of Doi and Onuki, we find that such models are capable of incorporating many phenomena relevant for industrially important polymer materials, including phase separation dynamics and viscoelastic fluid flow. In addition, we explore numerical methods capable of solving such models, with the goal of developing a framework for inexpensive "multi-fluid" simulations of polymer dynamics.

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