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Equivalence of particle and field representation of coarse-grained polymer models KIRILL TITIEVSKY, KENNETH BEERS, Massachusetts Institute of Technology — Particle-based and field theoretic coarse-grained models of heterogeneous polymer melts have been difficult to compare quantitatively because of the differences in state variables and simulation parameters. We reconcile the two approaches by noting that assumptions involved in discretizing a polymer field theory allow each molecule to be treated as several particles connected by spring bonds. In effect, these particles are the grid points on which the fields are discretized. The interaction potentials of the points, therefore, are obtained directly from the energy model (e.g. Flory) used in the field theory. The equilibrium phase behavior of a melt of such coarse-grained chains is calculated by stochastic dynamics or Monte Carlo simulations. Unlike field theory which becomes infeasible away from the mean field limit due to complex terms in the Hamiltonian, our simulations converge for realistic chain lengths because the potentials are smooth and real. Also, unlike in existing particle-based methods, all parameters in our model are explicitly related to experimentally measurable quantities. Our simulations of diblock copolymers, furthermore, are quantitatively consistent with experimental and field theoretic results.

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