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Numerical Advances in Field Theoretic Simulations of Polymers
ERIN M. LENNON, KIRILL KATSOV, HECTOR D. CENICEROS, CARLOS J. GARCIA-CERVERA, GLENN H. FREDRICKSON, University of California, Santa Barbara — Field theoretic simulations have been very successful in predicting the mesoscopic behavior of polymer self-assembly in the mean-field limit. Nevertheless, studies beyond this approximation have been hindered by the numerical complexities of simulating a fluctuating field theory with a complex Hamiltonian. To address these problems, we have developed a suite of highly efficient numerical methods to study practically arbitrary polymer systems. Moreover, we further propose a thermodynamic integration technique suitable for determining the free energy of such field-based fluctuating systems. Using the standard diblock copolymer as our model system, we quantitatively investigate the effect of fluctuations on the order-disorder transition.

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