Numerical Coarse-Graining of Polymer Field Theories

MICHAEL VILLET, GLENN FREDRICKSON, University of California, Santa Barbara — Field theoretic models of polymers are widely used to investigate polymer self-assembly, but numerical simulations of these models that include full fluctuation physics are computationally demanding and infrequently conducted. To reduce this computational cost, we propose the use of systematically coarse-grained field theories that can be simulated on a coarsely spaced lattice without truncation of important short-wavelength physics. We present a variational method for numerically executing this coarse-graining, in which fine-grained simulation data is used to parameterize trial coarse-grained models, and results from the application of this method to some model systems.

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