Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

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 enable efficient multi-scale simulations, we propose the use of systematically coarse-grained field theories that can be simulated on coarse computational lattices while accurately incorporating the effects of important sub-lattice-scale physics. We present a rigorous formalism for generating such coarse-grained theories from data obtained from small-scale fine-grained simulations, and demonstrate our methodology's effectiveness for a representative polymer solution model.

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Date submitted: 01 Nov 2010 Electronic form version 1.4