Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Particles vs. Fields – Finite-Range Interactions in Polymer Field Theories QIANG WANG, Colorado State University — Recently, we proposed a particle-based, fast off-lattice Monte Carlo (FOMC) simulation that uses the same Hamiltonian as in polymer field theories, which has great advantages over conventional molecular simulations. However, the continuous Gaussian chain model and δ-function interactions widely used in polymer field theories (such as the self-consistent field theory) cannot be directly used in FOMC simulations. We therefore extend the field theories to the discrete Gaussian chain model and finite-range interactions. Taking the microphase separation of diblock copolymers as an example, a finite interaction range increases the order-disorder transition from the well-known result of $\chi N \approx 10.5$, as well as the bulk lamellar period. More importantly, this work allows direct comparisons between the polymer field theories and FOMC simulations without any parameter-fitting to unambiguously and quantitatively reveal the effects of fluctuations and correlations in the system.

Qiang Wang
Colorado State University

Date submitted: 07 Dec 2008 Electronic form version 1.4