Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Fields Help Particles – Fast Off-Lattice Monte Carlo Simulations of Soft Materials YUHUA YIN, QIANG WANG, Colorado State University — Conventional molecular simulations of multi-chain systems are hindered by "hard" excluded-volume interactions (e.g., the Lennard-Jones potential in off-lattice simulations and the self- and mutual-avoiding walks in lattice simulations). Although such interactions are necessary for obtaining realistic dynamics, they significantly slow down the chain relaxation towards equilibrium configurations and efficient sampling of the configurational space. The idea of fast off-lattice Monte Carlo (FOMC) simulations is to perform particle-based Monte Carlo simulations in continuum with a Hamiltonian commonly used in polymer field theories, where individual polymer segments are modeled as "soft" particles whose interaction energy is finite when they overlap. This leads to much faster chain relaxation and better sampling of the configurational space. Furthermore, using the same Hamiltonian in both polymer field theories and FOMC simulations enables quantitative comparisons between them without any parameter-fitting to unambiguously reveal the effects of fluctuations and correlations in the system. Here we demonstrate these great advantages of FOMC simulations using several model systems.

Yuhua Yin
Colorado State University

Date submitted: 26 Nov 2008 Electronic form version 1.4