Fluctuations in Confined Homopolymers Studied by Fast Off-Lattice Monte Carlo Simulations YUHUA YIN, QIANG WANG — The conventional molecular simulations of many-chain systems are hindered by explicit excluded-volume interactions and expensive pair-potential calculations. The former greatly reduces the chain relaxation towards equilibrium configurations and the efficiency of sampling the configurational space, while the latter becomes computationally very expensive for concentrated polymeric systems. Fast off-lattice Monte Carlo (FOMC) simulations overcome these limitations, where individual polymer segments are modeled as volumeless points with the excluded-volume interactions modeled by either solvent quality, Helfand compressibility, or incompressibility constraint commonly used in polymer field theories. By dividing the simulation box into cells and assigning polymer segments to a cell, the short-range interactions can be readily evaluated without expensive pair-potential calculations. To demonstrate the great advantages of FOMC simulations, we have studied homopolymers confined between two parallel surfaces, and compared the results with self-consistent field calculations and field-theoretic simulations (FTS). Since FOMC simulation is particle-based, it avoids the unsolved ?sign problem? encountered in FTS. For the systems we have studied, FOMC simulations can sample the whole spectrum of fluctuations and are several orders of magnitude faster (more efficient) than FTS.

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