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Simulation of driven self assembly of complex polymeric systems across multiple length scales

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The self assembly of macromolecular systems is often driven or facilitated by the application of external fields, including flow, voltage, or confinement. The structures that arise when external fields are applied often depend on the history of the sample, and it is therefore important to develop theoretical and computational methods capable of describing the order formation process across multiple length and time scales. Over the past several years we have developed several new classes of multiscale modeling techniques for study of the structure and properties of polymeric materials under external fields, including confinement or flows. For systems at equilibrium, these systems permit precise calculation of the free energy. For systems beyond equilibrium, these methods include the effects of fluctuating hydrodynamic interactions (for dilute and semidilute systems) and the effects of constraining molecules (for concentrated melts). These models and methods can be used to investigate the equilibrium structure and relaxation of a variety of fluids, including solutions of biological macromolecules. The usefulness and limitations of our proposed approach will be discussed in the context of three applications. The first application is concerned with the elongation and presentation of long DNA molecules in nanofluidic channels. A multiscale model, that includes fluctuating hydrodynamic interactions, has been used to design a gene mapping device and to interpret experimental data pertaining to the structure and dynamics of confined chromosome-length DNA. The second application is concerned with the study of liquid-crystal based biosensors. A multiscale model has been used to design a liquid-crystal based device in which nanoscale particles suspended in a liquid crystal self assemble into highly regular structures, including chains, upon exposure to proteins or virions. The third application focuses on the formation of ordered block copolymer structures on nanopatterned substrates. Results from mesoscopic multiple length and time scale simulations will be presented to explain the effects of surfaces and different types of confining walls on the free energy of a variety of morphologies.