

224d Spanning Time and Length Scales in Simulations of Polymer Solutions

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An efficient method of simulating polymer solutions has been implemented by combining the fluctuating lattice-Boltzmann method with micromechanical models of the polymer molecules. In this algorithm, thermal fluctuations are added to the fluid rather than the polymer and the polymer point-beads interact with the lattice-Boltzmann fluid model through a frictional coupling. Therefore, the hydrodynamic interactions between the monomers develop in time and space from purely local interactions and the computation scales linearly with the number and length of the biopolymers. This approach enables simulation of the dynamics over an unprecedented range of scales – recent work shows that it is feasible to calculate the dynamics of a hydrodynamically interacting polymer with 1024 beads. We demonstrate the capabilities of the technique on some problems of relevance to microfluidic flows, including the net migration of polymers under confinement and the separation of biopolymers using entropic trapping mechanisms. These problems take advantage of an additional benefit of the fluctuating lattice-Boltzmann approach - bounding walls can be incorporated within the simulations at no additional numerical cost.