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A comparison of lattice-Boltzmann and Brownian dynamics simulations of dilute polymer solutions TONY LADD, RAHUL KEKRE, JASON BUTLER, University of Florida — We have compared lattice-Boltzmann and Brownian dynamics simulations of a single flexible polymer, in isolation and in confined geometries. In the case of the isolated chain we find agreement to within 1% in the diffusion coefficient and the Rouse mode relaxation times. We have obtained good agreement for the concentration profiles in a bounded shear flow, but the Brownian dynamics simulations currently use a superposition of the hydrodynamic fields generated by the walls. We expect to know the effects of the inter-wall correction by the time of the meeting. We have gone to some lengths to match the conditions of both simulations as closely as possible. We use identical potential parameters and correct for the differences between the periodic boundaries used in the LB simulations and the unbounded domains used in the BD simulations. We use very long runs, of the order of 10000 times the longest relaxation time, to reduce the statistical uncertainties to less than 0.1%. We find excellent agreement in the relaxation times over a wide range of temperatures and fluid viscosity. The most quantitative agreement is achieved in the weak coupling limit, where the hydrodynamic radius of the monomers is less than one quarter of the lattice spacing.

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