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Mesoscopic Simulation Methods for Polymer Dynamics

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We assess the accuracy and efficiency of mesoscopic simulation methods, namely Brownian Dynamics (BD), Stochastic Rotation Dynamics (SRD) and Dissipative Particle Dynamics (DPD), for polymers in solution at equilibrium and in flows in microfluidic geometries. Both SRD and DPD use solvent particles to carry momentum, and so account automatically for hydrodynamic interactions both within isolated polymer coils, and with other polymer molecules and with nearby solid boundaries. We assess quantitatively the effects of artificial particle inertia and fluid compressibility and show that they can be made small with appropriate choice of simulation parameters. We then use these methods to study flow-induced migration of polymer chains produced by: 1) hydrodynamic interactions, 2) streamline curvature or stress-gradients, and 3) convection of wall depletion zones. We show that huge concentration gradients can be produced by these mechanisms in microfluidic geometries that can be exploited for separation of polymers by size in periodic contraction-expansion geometries. We also assess the range of conditions for which BD, SRD or DPD is preferable for mesoscopic simulations. Finally, we show how such methods can be used to simulate quantitatively the swimming of micro-organisms such as *E. coli*.

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