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Electrohydrodynamics of polyelectrolytes using Lattice-Boltzmann simulations without electrostatics OWEN A. HICKEY, JAMES L. HARDEN, University of Ottawa, CHRISTIAN HOLM, University of Stuttgart, GARY W. SLATER, University of Ottawa — In computer simulations of polyelectrolyte electrophoresis, the effects of long-ranged hydrodynamics are often ignored due to the high computational cost. However, the hydrodynamic interactions often play a key role in the physics and can lead to some surprising phenomena. We present hybrid Molecular Dynamics simulation methods to study the electrohydrodynamics of polyelectrolytes using a Lattice-Boltzmann (LB) fluid. By applying a local slip between the monomer beads and the LB fluid we are able to reproduce realistic dynamics for free solution electrophoresis as well as the correct stall force for a polyelectrolyte subject to an electric field. Simulations also demonstrate how a net-neutral object, such as a block polyelectrolyte, can have a non-zero net force due to hydrodynamic interactions and that the force can even be perpendicular to the applied electric field.

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