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Polymer dynamics in confined flows

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It is well known that even in equilibrium the dynamics of a polymer in solution are affected by hydrodynamics and follow Zimm, rather than Rouse, dynamic scaling. However, due to the difficulties in correctly simulating a polymer in a real solvent, most simulations of polymers in solution have used Langevin dynamics which do not include hydrodynamics. My group has created a package for the open-source molecular dynamics package LAMMPS for simulations of particles in a fluid that includes full hydrodynamics. I will describe some of our studies of polymers in confined environments experiencing different flow fields. In particular, we will focus on polymers in channels with constricting and diverging flows and polymer margination in shear flow near a surface. The inclusion of full hydrodynamics is found to have a profound impact on the non-equilibrium behavior observed in these systems.

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