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Manipulating the Dynamics of Confined Polymers

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The dynamics of a polymer in solution are affected by hydrodynamics. It has often been assumed that these effects are mostly long range and therefore should be less significant in confined environments. However, there are a growing number of experiments on polymers in micro- and nano-fluidic devices where the hydrodynamic flow field is an essential part of the nonequilibrium dynamics of the system and cannot be ignored. My group has created, and maintains, a package for the open-source molecular dynamics package LAMMPS for simulations of particles in a fluid that includes full hydrodynamics which we use to study these systems. We demonstrate how the interaction between a polymer and fluid flow in a nano-fluidic device can be used to unfold and stretch out a polymer's configuration. This, in-turn can be exploited to maximize the probability of single-file translocation. In contrast, in a different configuration, we show how the flow around a pushed polymer can result in a compacted configuration and coexistence between a jammed and unjammed state for a long polymer.

Keyword-1

polymer

Keyword-2

simulation

Keyword-3

hydrodynamics

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