A new Monte Carlo approach for exact calculation of polymer translocation time through a channel

MICHEL G. GAUTHIER, GARY W. SLATER, University of Ottawa — Molecular Dynamics simulations are useful to study the impact of hydrodynamic interactions on the translocation process, but this technique requires large computer resources (both time and memory) which limit the size of the systems that we can study. We propose a new Monte Carlo algorithm that integrates various effects such entropic forces, external force fields frictional effects, and polymer-channel interactions. Our novel approach allows us to study the polymer as a single Brownian particle diffusing on a one-dimensional lattice in a non-constant force field. The calculation technique we suggest gives us the exact value of the translocation time via the resolution of a simple system of linear equations. This Monte Carlo approach can be used to obtain scaling laws of polymer translocation through a channel much faster than by using fluctuating-bond simulation models.