Title:	Polymer Translocation Through Conical Pores
Authors:	Sharma, Andri
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Abstract:	Abstract In 1996, Kasianowicz et al. [1], studied the translocation of a RNA molecule through an α−hemolycin pore. It was observed that the ionic current gets blocked whenever the RNA molecule passes through the pore. Since this landmark experiment, considerable efforts have been made in understanding the transport phenomena of macromolecules through biological nanopores. One of the most investigated aspect is the fabrication of various types of nanopores to enable rapid DNA sequencing. Computer simulation studies using coarse-grained models with varying complexities, have greatly enhanced our understanding of the translocation process through various kinds of channels. The goal of this thesis is to understand the translocation of a polymer through an extended conical shaped pore with attractive surface interactions and a driving force which varies spatially inside the channel, using coarse grained molecular dynamics simulations. We consider both flexible, and semiflexible polymers. In our study, the polymer is modelled as a coarse-grained bead-spring chain, where non-bonded monomers interact via a short ranged repulsive Lennard-Jones (rLJ) potential. The consecutive monomers of the chain is bonded via a harmonic potential. To model a semiflexible polymer, an additional bend- ing potential is introduced between consecutive bonds. The semiflexibility of the polymer is controlled by tuning its persistence length. The attractive surface interaction between the polymer and the conical channel is given by the standard Lennard-Jones interaction. The system is in a heat bath modelled as a Langevin thermostat. Verlet algorithm is used to solve the Langevin equation of motion to update the positions and the velocities of the polymer beads. All the simulations are performed using LAMMPS software [2]. For each set of simulation parameters, the results presented are averaged over 1500 − 2000 independent samples. As a first problem, we study the translocation process when the polymer enters the pore from the narrow entrance and exits from the wider end of the conical channel [3]. We refer to this as “Forward Translocation”. We find that the channel gives rise to non- vimonotonic features in the total translocation time as a function of the apex angle of the channel. We also obtained the waiting time distributions of individual monomer beads in- side the channel and found unique features that depend strongly on the driving force and the surface interactions. Polymer stiffness results in longer translocation times for all an- gles of the channel which is consistent with earlier reports [4, 5]. Further, non-monotonic features in the translocation time as a function of the channel angle changes substantially as the polymer becomes stiffer, which is also reflected in the changing features of the waiting time distributions. The total translocation time τ decreases with increasing force strength as expected. Furthermore, with increasing forces, the non-monotonic features also reduce significantly. A break up of the total translocation time into a filling, transfer and escape time provides valuable insight on the translocation dynamics. We construct a free energy description of the system incorporating entropic and energetic contributions in the low force regime to explain the simulation results. In the second problem, we study the translocation process with the entrance and the exit ends interchanged[6]. Now the polymer enters the pore from the wider side and exit from the narrow end. We call this as “Reverse Translocation”. We again obtain the total translocation time and the waiting time distributions, and compare them with the results obtained in the “Forward Translocation” case. We find striking differences between the two cases which we discuss in detail. Comparison of our simulation with experimental results [7] shows a good agreement. We have also obtained the conditions for directional independence of the translocation process so that results for the forward translocation process overlaps with that of the reverse case. It is found that ratio of pore and polymer lengths plays an important role in distinguishing the directional-dependent translocation processes. We find that the two process appears to be same under two circumstances (a) for a very rigid polymer chain, and (b) for a very long polymer chain. As a third problem, we study the effect of different pore-polymer interactions as a function of pore length on the translocation of different polymers. The transition in the viibehavior of average translocation time with pore and polymer length is studied. For an extended pore with pore apex angle zero (i.e., a cylindrical pore), we find that the average translocation time scales nicely with the pore and the polymer lengths with same set of exponents for all ranges of the force considered in our study. However, for a conical pore, the average translocation time shows different behaviour for shorter and longer pore lengths and we do not observe a scaling behavior. viii
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