Project DPD II: Dynamics

A simple model for DNA translocation through membranes

This project is designed to provide students with an understanding of phase separation driven by enthalpy. Students will utilize LAMMPS codes and Python scripts to generate and analyze data. In this phase, they will explore the role of chemical composition behind the functioning of the microscopic systems, learn various computational methods to characterize them, and assess their relevance within the context of experimental data.

Introduction

The diffusion of polymers through confined environments is a fundamental process in soft matter physics, biophysics, and materials science. When polymers move through narrow channels, pores, or membranes, their dynamics are significantly influenced by geometric constraints, interactions with the surrounding medium, and entropic effects.

In confined spaces, polymer diffusion can deviate from classical Brownian motion, often exhibiting sub-diffusive behavior at short timescales due to entanglements, steric hindrance, or interactions with the walls. Over longer timescales, the diffusion may transition to normal diffusion once the polymer overcomes these constraints. In biological systems, such as DNA passing through nanopores or proteins navigating cellular environments, confinement-driven diffusion plays a critical role in cellular transport and gene regulation.

In simulations and experiments, factors such as polymer flexibility, chain length, solvent interactions, and external forces are studied to understand how confinement affects polymer mobility. This knowledge is essential for designing nanoporous materials, drug delivery systems, and filtration membranes.

Many studies have investigated the effect of colloidal particle shape and size on their dynamics. The dynamical properties of colloidal particles play a crucial role in various natural and industrial processes. The diffusivity of these particles also depends on the geometry of the system. For instance, in the presence of interconnected narrow channels, a particle may exhibit sub-diffusive motion at short timescales and transition to diffusive behavior at longer timescales, where its diffusivity can be approximated by a one-dimensional diffusion model.

In the case of active particle diffusion, where particles propel themselves, the geometry of confinement becomes a critical factor. However, various passive mechanisms can also drive particle diffusivity; one example is the escape of DNA molecules through eukaryotic cell membranes.

In this project, students will simulate the passive escape of polymers through a membrane, driven by enthalpy. The simulation box is divided into two regions by a rigid, immovable wall with a narrow opening. Initially, polymers are confined to one region and can escape into the other. The effect of enthalpy is introduced by adjusting the force constant between the polymers and solvent beads so that the initial configuration of the polymers in one region is energetically unfavorable. As the polymers escape through the membrane, they transition into a more energetically favorable state.

Students will systematically vary the interactions between the polymers and the solvent in both regions and analyze their impact on the polymer escape rate.

The aim of the project is to investigate the system within the context of several of the following questions:

- How can enthalpic forces affect the dynamics of polymers across the narrow channel?
- What is the role of the membrane wall in the escape of polymers?
- Can we direct the motion of large molecules, such as polymers, using a chemical gradient?
- What is the effect of polymer conformations on dynamics through the narrow channel?
- How does confinement volume affect the escape rate?
- What is the effect of polymer-polymer interactions on the escape rate?
- Can we design a polymer with multiple segments that can escape quickly through a chemical gradient, and what challenges might arise?

Project tasks

These are some general information within the context of project tasks:

- Create a substrate using the given python script, which is a hexagonal flat structure with its plane-normal parallel to x-axis (see tables for the specification).
- Edit the given LAMMPS input script following the given table and run the simulations.
- For each output, analyze the binned particle distribution data and compute the average number of polymer beads within or outside of the region enclosed by the barriers with narrow opening(n_c). Division of the quantity with the number of beads within a single polymer molecule, is your desired number of polymers escaped through the enclosure.

Symbols: Before further going with the simulation details, here students are being introduced with various symbols to make things easier to perceive.

Symbols	Meaning	Definition
V	total volume of the box	$length \cdot width \cdot height$
r_o	radius of wall opening	$2.0 \cdot length \cdot width$
N	number of polymers	
n_p	total number of polymer beads	
n_w	total number of water beads	
n_c	total number of escaped beads	
ρ_p	polymer density	total number of polymer beads/total volume
ρ_w	solvent (water) density	total number of water beads/total volume
ρ_t	total density	total number of beads/total volume
s_p	total polymer length	total number of beads in a single polymer
s_A	size of segment type A	number of type A beads
s_B	size of segment type B	number of type B beads
a_B	fraction of segments with type B bead	s_b/s_p
A_{AA}	force constant	between polymer bead A and solvent A
A_{BC}	force constant	between polymer bead B and solvent C
P_{AA}	force constant	between polymer beads A and A
S_{BC}	force constant	between solvent beads B and C
k	spring constant	deciding the fluctuation of membrane wall
C	number of chemical segments	ayer of beads within the confinement

Table 1: List of symbols and their definition.

Simulate the system for the following tables, where students are supposed to produce a single plot for each table.

Study 1 (A_{AA} vs τ)

To study the effect of enthalpic forces students have to change the interaction strength between the polymer beads a and repulsive solvent bead B, in which the polymers are emerged initially.

#	A_{AB}
1	30
2	35
3	40
4	45
5	50

Table 2: Simulation parameters for different systems corresponding to the plot 1. Where independent variable, which are constants, are fixed in the following way, position of wall with opening $5, 0, 0$, position of the pseudo wall, at $15, 0, 0$ (to keep the pressure same across the compartment, where the solvent particles can cross this wall not the polymers mimicking the real condition, e.g, the mechanical contraction of the membrane, which keeps the pressure same across the whole system). Total size of the simulation box is given as $X = 20$, $Y = 10$ and $Z = 10$, $\rho_t = 3.0$, $N = 30$, $s_p = 16$. Number of solvent type A $n_A = 2760$ and type B $n_B = 2760$. There is another layer of wall with the same lattice arrangement added with springs attached to the particles, where the spring have force constant $k = 100$ (almost a hard wall).

Study 2 (k vs τ)

To study the effect of wall properties students are supped to change the force constant for the wall particles, which are vibrating over the substrate, with a simple one dimensional and single vibrational mode,

#	k
1	30
2	40
3	50
4	60
5	70
6	80
7	90
8	100

Table 3: Simulation parameters for different systems corresponding to the plot 2. Where independent variable, which are constants, are fixed in the following way, position of wall with opening $5, 0, 0$, position of the pseudo wall, at $15, 0, 0$. Total size of the simulation box is given as $X = 20$, $Y = 10$ and $Z = 10$, $\rho_t = 3.0$, $N = 30$, $s_p = 16$. Number of solvent type A $n_A = 2760$ and type B $n_B = 2760$.

Study 3 (C vs τ)

To study the effect of chemical gradient, we segment the whole confinement region by filling different kind of beads such that the force constant between the consecutive beads decreases monotonically:

#	C	Δf
3	5	5
4	4	5
5	3	5

Table 4: Simulation parameters for different systems corresponding to the plot 3. Rest of the parameters are as same as in the previous section, however there are C type of solvent B present in the system, such that each type of type B particle have different polymer-bead force constant. Starting from the closest section of compartment, we put $A_{AB1} = 30$, $A_{AB2} = 35$, $A_{AB3} = 40$..., such that $\Delta f = 5$. So as the polymer moves it has more movement towards the narrow wall opening rather than in the opposite direction.

Study 4 (s_p vs τ)

To study the effect of polymer length on the escape time, students are supposed to change the polymer length such that the radius of gyration to box extension remains the same along with ρ_t and ρ_p:

#	s_p	n_B
1	8	2760
2	16	2520
3	24	2280
4	32	2040
5	40	1800

Table 5: Simulation parameters for different systems corresponding to the plot 4. Where independent variable which are constants, are fixed in the following way , $\rho_t = 3.0$, $\rho_p = 0.16$, $a_r = 0.32$, $s_p = 16$.

Study 5 (V vs τ)

To study the effect of V on the escape time of polymers one need to increase the volume while keeping the ratio of the box edges same:

#	Δx
1	10
2	15
3	20
4	25
5	30

Table 6: Simulation parameters for different systems corresponding to the plot 5. Where independent variable which are constants, are fixed in the following way , $\rho_t = 3.0$, $\rho_p = 0.16$, $a_r = 0.32$, $s_p = 16$. Students are supposed to displace the pseudo wall to get the desired value of δx, while keeping the wall with opening at a constant distance $5, 0, 0$.

Study 6 (Γ vs τ)

To study the effect of surface to volume ratio one need to change the box edges in such a way that the total volume of the system remains the same, however the box edges change:

#	Γ
1	0.1
2	0.15
3	0.2
4	0.25
5	0.3

Table 7: Simulation parameters for different systems corresponding to the plot 5. Where independent variable which are constants, are fixed in the following way , $\rho_t = 3.0$, $\rho_p = 0.16$, $s_p = 16$.

Project Reports

Students are required to submit a report on their projects, which should include:

- **Introduction to the Problem**
  This section should be approximately one page long (or slightly more) and must include around five scientific references. Students must discuss the significance of the project, particularly in the context of role of DNA translocation in the functioning the of the cell and DNA sequencing etc.

- **Technical Description**
  This section should provide a clear description of the theory and model, where in model part student should discuss about the DPD simulation method, where it can be mentioned about the pros and cons of the method along with basic equations and conservation laws being followed in the simulation box e.g, momentum, angular momentum, energy etc. It must also include at least one reference and be approximately half a page to one page in length.

- **Main Findings**
  This section, forming the core of the report, should provide a thorough explanation of the results and how they were obtained. It should be between 5 to 10 pages long.

- **Conclusion**
  Summarize the key findings and their implications. This section should be about half a page to one page in length.

Although students are encouraged to collaborate and divide tasks as needed, each student must submit a complete, individual report for evaluation. Data can be shared among students, but writing and other technical components must be completed independently.

Future aspects

The primary objective of this project is to introduce students to transport phenomena in a complex system. Through simulations of polymer transport across membranes driven by enthalpic interactions, students can explore how spatial constraints affect polymer dynamics.
The foundational study regarding the subject can be expanded to investigate several critical aspects of the system in greater detail, such as,
Effect of Charge: The electrical charge of polymers can significantly impact their behavior in confined spaces. By studying the interactions between charged polymers and the surrounding medium, students can gain insights into how charge affects transport dynamics.
Effect of polymer morphology: The polymers with segments having different chemical properties can enhance the dynamics and play and important role during the translocation process.
Effect of Chemical Stream: Introducing a chemical gradient allows students to explore how it modifies polymer escape dynamics. This aspect is crucial for understanding applications in drug delivery and filtration systems, where controlled transport is essential.
By investigating these factors, students will enhance their understanding of transport processes in confined geometries and develop analytical skills relevant to real-world applications.