Project BD II: Dynamics

Transport phenomena in biologically inspired system

This project is designed to provide students with an understanding of transport phenomenon derived by thermal energy. Students will use LAMMPS codes and Python scripts to generate and analyze data. In this phase, they will explore the dynamics of the polymer blobs, learn various computational methods to characterize them, and find their relevance within the context of experimental data.

Introduction

Transport phenomena in biological systems refer to the movement of mass, energy, and momentum within living organisms. These processes are essential for maintaining homeostasis and include diffusion, osmosis, active transport, and bulk flow. Examples include gas exchange in the lungs, nutrient absorption in the intestines, and blood circulation. These mechanisms are governed by principles of fluid dynamics, thermodynamics, and molecular transport, ensuring the efficient distribution of essential substances like oxygen, nutrients, and waste products throughout the body.

In biological systems, the transport of large protein molecules across membranes plays a crucial role in gene regulation. Several factors, such as electron transport, molecular crowding, and solvent activity, influence the system's dynamic behavior.

This project aims to model such a system in a simplified manner. A shell filled with polymers of varying sizes is placed at the center of the studied region. Through passive diffusion, the polymers escape from the shell, with the escape rate depending on the width of its opening. By introducing a difference in noise levels inside and outside the shell, students will explore how this variation affects polymer transport.

The objective is to study how noise differences influence the escape rate of polymers under different geometric configurations of both the confinement and the polymers themselves.
In this project, students will simulate the diffusivity of the polymer blobs through the narrow channel, while controlling the process through the systematic introduction of noise. Initially, polymers are confined to one region and can escape into the other, where the confinement is done by connecting spherical shells, where students will also introduce the shell walls with thermal undulation.

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 a few of the following problems,

- How does the confinement opening affect the dynamics of polymer blobs?
- What is the effect of container volume on the dynamics of the polymer blobs?
- Can we control the dynamics of polymers using thermal gradient?
- What is the effect of noise on the escape rate of the polymers through a narrow compartment?
- What is the role of container wall in the escapement of the polymers?

There are a number of studies done in the past. For example, study of escape rate of polymers. In the given project students are performing the similar calculation but in a more complex and detailed way.

Project tasks

In the given project, students will be provided all the templates including LAMMPS code, polymer molecule template and the relevant python codes. Where students are supposed to customize all the templates according to their need. Following are the lists of tasks.

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

- Create a spherical shells with opening one sided or two sided.
- Place the shells in simulation box in such a way that it remains connected.
- Compute the binned particle distribution data and observe its time evolution.
- Measure the MSD of the system if required.

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
r_g	radius of gyration for polymers	
r_s	radius of the spherical shell	
V_s	spherical container volume	$\frac{4}{3} \cdot \pi \cdot r_s^3$
v	polymer volume	$\frac{4}{3} \cdot \pi \cdot r_g^3$
V_p	volume ratio	$\frac{v}{V_s}$
r_o	radius of confinement opening	
r_p	length ratio	$\frac{r_o}{r_g}$
N	number of polymers	
n_p	total number of polymer beads	
n_c	total number of escaped beads	
ρ_p	polymer density	total number of polymer beads/total volume
s_p	total polymer length	total number of beads in a single polymer
k	spring constant	deciding the fluctuation of membrane wall
C	number of thermal segments	number of regions with different temperature

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 (Scaling laws, V_o vs D_t)

To study the effect of system size scaling students are supposed to consider a large spherical container with opening on both the sides and then add them to form a channel periodically connected along one of the axes (let us say z-axis) randomly generate the polymer blobs and measure the MSD of the beads. Now, they are going to change the beads size of the polymers which will change the radius of gyration of the polymres and therefore the polymer blob size. To reduce the effect and fit with the scaling, they are supposed to increase the container size so that the quantity V_p and the r_p remains the same. Now, calculate the MSD and the corresponding diffusivity. In container does not fit within the simulation box then students can increase the total simulation box length.

#	r_g
1	0.5
2	1.0
3	1.5
4	2.0
5	2.5

Table 2: Simulation parameters for different systems corresponding to the plot 1. Where independent variable, which are constants, are fixed in the following way, $N = 30$, $s_p = 16$.

Study 2 (s_p vs τ)

To study the effect polymer length students are supposed to change the number of beads within the polymer template and simulate the system at the same temperature and confinment geometry,

#	s_P
1	11
2	12
3	13
4	14
5	15
6	16

Table 3: Simulation parameters for different systems corresponding to the plot 1. Where independent variable, which are constants, are fixed in the following way $N = 30$, $s_p = 16$.

Study 3 (C vs τ)

To study the effect of thermal gradient, we segment the whole confinement region by assigning a different temperature:

#	C	ΔT
1	2	0.5
2	4	0.5

Table 4: Simulation parameters for different systems corresponding to the plot 2. Where independent variable, which are constants, are fixed in the following way , $N = 30$, $s_p = 16$.

Study 4 (ΔT vs τ)

To study the effect of thermal gradient, students are supposed to simulate the system at different temperature gradient and calculate the escape rate of polymers:

#	T_b
1	1.0
2	0.5
3	0.25

Table 5: Simulation parameters for different systems corresponding to the plot 4. Where independent variable which are constants, are fixed in the following way , $N = 30$, $s_p = 16$.

Study 5 (k vs τ)

To study the effect of the fluctuation of the container wall students are supposed to change the force constant of the container spring and check its effect on the escape time of the polymers:

#	k
1	500
2	600
3	700
4	800
5	900
6	1000

Table 6: Simulation parameters for different systems corresponding to the plot 5. Where independent variable which are constants, are fixed in the following way , $N = 30$, $s_p = 16$.

Study 6 (V_s vs τ)

To study the effect of V_S on the escape time of polymers one need to increase the volume of shells without changing the radius of the opening:

#	r_s
1	5
2	6
3	7
4	8
5	9

Table 7: Simulation parameters for different systems corresponding to the plot 6. Where independent variable which are constants, are fixed in the following way, $N = 30$, $s_p = 16$.

Presentation

Project Reports

Students are required to submit a detailed 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 should discuss transport phenomena within biological shells, such as protein polymer diffusion, ion transport, or chemical signal transmission in confined environments. The discussion should highlight the relevance of these processes in biological and synthetic systems.

- **Technical Description**
  This section should provide a clear description of the theory and model, where in model part student should discuss about the BD 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 present a comprehensive analysis of the results and the methodology used to obtain them. The section should be between 5 to 10 pages long.

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

While 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 of the Study

The study of transport through a narrow opening provides insights into complex biological systems, such as molecular transport across membranes and ion channel regulation. While this project offers a simplified model, several aspects remain unexplored.

One key extension is the introduction of charge at the opening, which could influence transport dynamics through electrostatic interactions, mimicking ion channels in biological membranes.

Polymer-polymer and polymer-solvent interactions could also be studied to examine the role of attractive or repulsive forces in selective transport.

The effect of confinement geometry is another important factor. Asymmetric openings or funnel-like structures may lead to directed motion, resembling natural biological pores. Additionally, noise-induced transport mechanisms can be explored by varying noise levels inside and outside the shell, providing insights into stochastic directionality effects in biological systems.