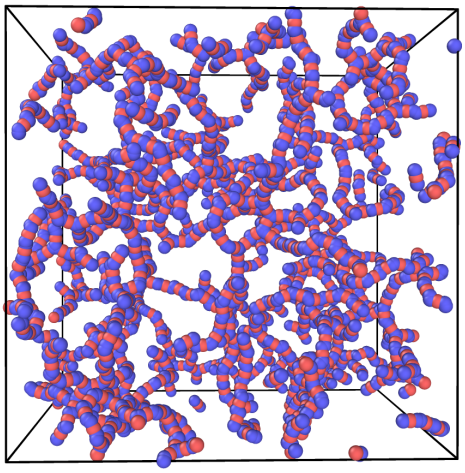
MTEK0033 Multiscale Modelling, University of Turku, January 2026

Brownian Dynamics Simulation

Project- II



Created by: Vikki Anand Varma
Supervised by: Prof. Alberto Scacchi

If you come across any problems, please email at vavarm@utu.fi

Table of Contents

1 Polymer Translocation in Non-Additive Binary Mixtures

In the non additive binary mxiture we define the total value of the givne system which could

This project focuses on the study of **polymer translocation through a nanopore** using **Brownian Dynamics** simulations in a two-dimensional geometry. Students will investigate how **non-additive interactions**, **temperature gradients**, and **pore geometry** influence the translocation dynamics of polymers across a separating wall.

Such translocation processes are central to many physical and biological phenomena, including DNA sequencing, protein transport through membrane channels, drug delivery, and selective filtration in synthetic membranes.

1.1 Introduction

Polymer translocation refers to the passage of a polymer chain through a narrow pore separating two compartments. This process is inherently stochastic and governed by thermal fluctuations, polymer entropy, confinement effects, and interactions with the surrounding medium.

In biological systems, translocation often occurs in heterogeneous environments where the properties of the solvent or surrounding molecules differ on either side of a membrane. These differences can generate effective driving forces even in the absence of external fields.

In this project, students will explore polymer translocation in a **binary mixture** where particles on the two sides of a separating wall interact via **non-additive potentials**. The wall contains a nanopore whose geometry can be systematically varied.

By tuning non-additivity, temperature, and pore geometry, students will study how asymmetric environments induce directional transport and alter the translocation time.

1.2 Model and Brownian Dynamics Description

The overdamped Langevin equation governing particle motion in two dimensions is

$$\gamma \frac{d\mathbf{r}_i}{dt} = \mathbf{F}_i + \boldsymbol{\xi}_i(t), \tag{1}$$

where γ is the friction coefficient, $\mathbf{F}_i$ is the total deterministic force, and $\boldsymbol{\xi}_i(t)$ is Gaussian noise satisfying

$$\langle \xi_{i\alpha}(t)\xi_{j\beta}(t')\rangle = 2k_B T(\mathbf{r})\gamma\delta_{ij}\delta_{\alpha\beta}\delta(t-t'). \tag{2}$$

The temperature $T(\mathbf{r})$ may vary spatially, allowing the introduction of temperature gradients across the wall.

1.3 Non-Additive Interactions

Particles belong to two species, A and B, located predominantly on opposite sides of the wall. Interactions are modeled using a non-additive Lennard–Jones (or WCA) potential:

$$\sigma_{AB} = \frac{1}{2}(\sigma_{AA} + \sigma_{BB})(1 + \Delta), \tag{3}$$

where Δ is the non-additivity parameter.

Positive non-additivity ($\Delta > 0$) enhances repulsion between species, leading to effective osmotic pressure differences that influence polymer translocation.

1.4 System Geometry

The simulation box is two-dimensional and divided into two compartments by a wall placed along the y-axis. A nanopore of width w is introduced at the center of the wall. The polymer is initially placed entirely on one side of the wall.

Wall geometry parameters such as thickness, pore width, and corner rounding can be varied.

1.5 Symbols

Symbol	Meaning
τ	translocation time
w	pore width
L_w	wall thickness
T_L, T_R	temperatures
ΔT	temperature difference
Δ	non-additivity parameter
s_p	polymer length
N_A, N_B	bath particles

Table 1: List of symbols used in the project.

1.6 Project Tasks

- Construct a 2D simulation box with a separating wall and nanopore
- Implement overdamped Brownian dynamics
- Introduce non-additive interactions between species
- Assign spatially varying temperatures
- Measure polymer translocation time
- Perform ensemble averaging over multiple runs

1.7 Simulation Studies

Study 1: Polymer Translocation Driven by a Temperature Gradient

In this study, you will investigate polymer translocation through a wall (or pore) induced by a temperature gradient applied across the system. A temperature difference between the left and right sides of the simulation box generates a non-equilibrium driving force, which affects the polymer translocation dynamics. The primary quantity of interest in this study is the *polymer translocation time* as a function of the applied temperature gradient.

Unlike previous studies, only **one type of polymer** is used here. The polymer properties remain fixed, and the study is performed by systematically varying the temperature difference across the wall.

#	T_L	T_R
1	0.50	1.00
2	0.60	1.00
3	0.70	1.00
4	0.80	1.00
5	0.90	1.00
6	1.00	1.00

Table 2: Temperature values applied on the left (T_L) and right (T_R) sides of the wall to generate different temperature gradients.

Step 1: Folder structure and setup

1. Navigate to the main directory:

   `Project_2/Polymer_Translocation/Temperature_Gradient/`

2. Inside this directory, you will find six subfolders corresponding to the temperature pairs listed in Table 1. The folder names follow the format:

   `TL_0.50_TR_1.00`, `TL_0.60_TR_1.00`, ..., `TL_1.00_TR_1.00`

3. Each folder contains:

   - the LAMMPS input script,
   - configuration input file,
   - the polymer template file,
   - and the analysis scripts required for post-processing.

Step 2: Polymer and simulation parameters

1. The polymer length and interaction parameters are fixed for all simulations.
2. Only a single polymer chain is present in the system.

3. The temperature on the left side of the wall is maintained at T_L, while the right side is maintained at T_R using separate thermostats.

4. Change the temperature specified in your system.

5. Ensure that the temperature gradient is applied along the translocation direction, which must be from the left side of the box to the right side.

Step 3: Running the simulations

1. For each temperature pair (T_L, T_R), run the simulation until the polymer fully translocate through the wall.

2. The translocation time is defined as the time required for the polymer's center of mass (or last bead) to cross the wall completely.

3. After running the data, you will get `bin_position.lammpstrj`.

4. Run the python file `translocation_time_calculator.py`.

5. To improve statistical reliability, repeat each simulation multiple times (with different random seeds) and compute the average translocation time.

Step 4: Data collection

1. For each temperature gradient, store the averaged translocation time in a text file named:

   `translocation_time.txt`

   inside the corresponding folder.

2. Also record the temperature difference:

   $$\Delta T = T_R - T_L$$

   for each case.

Step 5: Plotting and analysis

1. Plot the polymer translocation time as a function of the temperature difference ΔT.

2. Use the provided Python plotting scripts (if available) or your own plotting tools.

3. Analyze how increasing the temperature gradient affects the translocation dynamics.

4. Comment on whether the translocation time decreases monotonically with increasing ΔT and discuss possible physical mechanisms.

Study 2: Non-Additivity vs. Translocation Time

In this study, you will investigate how *non-additive interactions* influence the polymer translocation dynamics. The degree of non-additivity is controlled by the parameter Δ, which modifies the interaction strength between different species in the system. All other system parameters, including polymer length and temperature, are kept fixed. The primary quantity of interest is the polymer translocation time as a function of the non-additivity parameter Δ.

#	Δ
1	0.0
2	0.1
3	0.2
4	0.3
5	0.4

Table 3: Effect of non-additive interactions on polymer translocation time.

Step 1: Folder structure and setup

1. Navigate to the main directory:

   `Project_2/Polymer_Translocation/Non_Additivity/`

2. Inside this directory, you will find five subfolders corresponding to the values of Δ listed in Table 2. The folder names follow the format:

   `Delta_0.0`, `Delta_0.1`, `Delta_0.2`, `Delta_0.3`, `Delta_0.4`

3. Each folder contains:

   - the LAMMPS input script,
   - configuration input file,
   - the polymer template file,
   - and the analysis scripts required for post-processing.

Step 2: Polymer and simulation parameters

1. The polymer length and all interaction parameters are fixed, except for the non-additivity parameter Δ.
2. Only a single polymer chain is present in the system.
3. The system temperature is kept constant for all simulations.
4. Modify the value of Δ in the input script according to the folder name.
5. Ensure that all other parameters remain unchanged when varying Δ.

Step 3: Running the simulations

1. For each value of Δ, run the simulation until the polymer fully translocates through the wall.
2. The translocation time is defined as the time required for the polymer's center of mass (or the last bead) to completely cross the wall.
3. After completing the simulation, you will obtain the trajectory file:

   `bin_position.lammpstrj`

4. Run the Python script:

   `translocation_time_calculator.py`

   to compute the translocation time.
5. To improve statistical reliability, repeat each simulation multiple times using different random seeds and compute the average translocation time.

Step 4: Data collection

1. For each value of Δ, store the averaged translocation time in a file named:

   `translocation_time.txt`

   inside the corresponding folder.
2. Clearly label each value of Δ alongside the recorded translocation time.

Step 5: Plotting and analysis

1. Plot the polymer translocation time as a function of the non-additivity parameter Δ.
2. Use the provided Python plotting scripts (if available) or your own plotting tools.
3. Analyze how increasing non-additivity affects the translocation dynamics.
4. Discuss whether the translocation time increases or decreases with Δ, and provide possible physical explanations based on changes in effective interactions.

2 Project Report Guidelines

1. Introduction to the Problem

This section should be approximately one page long (or slightly more) and should include five (minimum three) scientific references from peer-reviewed literature.
The introduction should present an overview of polymer translocation as a fundamental process in soft matter and biological physics. In particular, students should:

- Define polymer translocation and explain its physical meaning.
- Distinguish between unbiased and driven translocation.
- Briefly describe entropic barriers associated with nanopore confinement.
- Introduce nonequilibrium driving mechanisms in nanoscale transport.

Students should also motivate the relevance of polymer translocation by discussing applications such as:

- DNA and RNA transport through biological nanopores,
- nanopore sequencing technologies,
- controlled drug delivery and filtration,
- nonequilibrium statistical mechanics.

The goal of the project should be clearly stated:

To investigate how different nonequilibrium driving mechanisms influence polymer translocation dynamics and translocation time.

2. Technical Description of the Simulations

This section should describe the molecular dynamics framework used to model polymer translocation.
Students must describe:

- The polymer model used (e.g., bead–spring chain).
- Bonded and non-bonded interaction potentials.
- The construction of the membrane and nanopore.
- The ensemble employed (e.g., Langevin dynamics).

The definition of the translocation coordinate and the method used to measure translocation time must be clearly explained. All relevant simulation parameters (polymer length, friction coefficient, timestep, system size) should be explicitly stated.

3. Study 1: Temperature Gradient Driven Translocation

In this study, students will examine polymer translocation driven by a temperature difference across the membrane.

Procedure

- Impose different temperatures on the two sides of the membrane ($T_L \neq T_R$).
- Perform simulations for multiple temperature gradients.
- Keep polymer length and interaction parameters fixed.

Analysis

Students should:

- Plot the translocation time τ as a function of temperature difference $\Delta T = T_R - T_L$.
- Analyze how increasing the temperature gradient affects translocation speed.
- Discuss the role of thermophoresis and entropy-driven motion.

Students should comment on fluctuations in the translocation coordinate and possible nonlinear behavior at large temperature gradients.

4. Study 2: Non-Additivity Driven Translocation

In this study, students will investigate how non-additive interactions across the membrane influence polymer translocation.

Procedure

- Introduce a non-additivity parameter in cross-interactions across the membrane.
- Perform simulations for different values of the non-additivity parameter.
- Keep temperature uniform throughout the system.

Analysis

Students should:

- Plot translocation time τ as a function of the non-additivity parameter.
- Compare the effects of attractive and repulsive non-additive interactions.
- Discuss how non-additivity modifies the effective free-energy barrier.

Physical interpretations should focus on interaction asymmetry and nonequilibrium driving.

5. Main Findings and Discussion

This section should form the core of the report and be approximately 5–10 pages long (or 3–6 pages for a shorter report).
Students should integrate results from both studies and discuss:

- Differences between temperature-gradient-driven and interaction-driven translocation.
- The dominant physical mechanisms in each case.
- The role of fluctuations and stochastic forces.
- Limitations of the simulation model.

Connections to nonequilibrium statistical mechanics and entropic barrier crossing should be made wherever appropriate.

6. Conclusion

This section should be approximately half a page to one page long.
The conclusion should:

- Summarize how temperature gradients and non-additivity influence translocation time.
- Highlight key physical insights gained from the simulations.
- Reflect on the usefulness of molecular dynamics in studying nanoscale transport.
- Suggest possible extensions, such as varying polymer length, pore size, or solvent properties.

References

[1] Sarabadani, Jalal, Sahin Buyukdagli, and Tapio Ala-Nissila. **"Pulling a DNA molecule through a nanopore embedded in an anionic membrane: tension propagation coupled to electrostatics."** Journal of Physics: Condensed Matter 32.38 (2020): 385101.

[2] **Computer Simulation of Liquids** by Allen and Tildesley.

[3] **Theory of Simple liquids** by Hansen and McDonald.

[4] **Nonequilibrium Statistical Mechanics** by Robert Zwanzig