

# Molecular Dynamics: Dissipative Particle Dynamics

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## Introduction

In this report the goal was to implement and analysis of Dissipative Particle Dynamics (DPD) simulations in 2D. DPD is a mesoscopic simulation method that bridges the gap between microscopic methods like Molecular Dynamics and macroscopic methods like Computational Fluid Dynamics. In DPD, particles represent clusters of molecules rather than individual atoms, allowing for simulation of larger systems and longer time scales. The simulation implements three types of forces between particles:

1. Conservative forces (soft repulsion)
2. Dissipative forces (friction-like)
3. Random forces (thermal fluctuations)

These forces combine to create a thermostat that maintains the system temperature while preserving hydrodynamic behavior. The simulation was implemented in Python, for further information regarding the key components of the implementation consult the README.md file.

## 1 Test Simulation

For the preliminary test, a system containing only fluid particles was simulated with conservative force coefficient  $a_{ij} = 25$  using various timestep over 1000 steps.

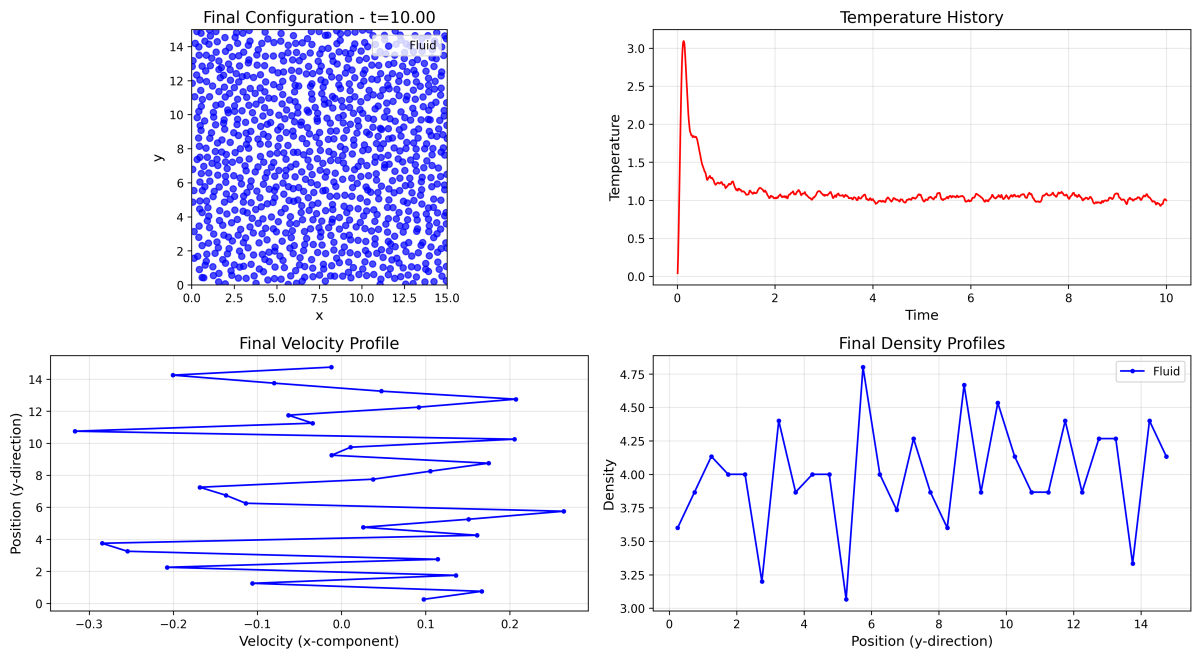


Figure 1: Test Scenario with  $dt = 0.01$  and 1000 steps

### 1.1 Temperature Stability

As shown in Figure 1, the temperature initially spiked but quickly stabilized around 1.0, which is the desired temperature set by the DPD thermostat parameters. This confirms proper implementation of the dissipative and random forces.

## 1.2 Conservation of Momentum

Total momentum was being tracked throughout the simulation and remained constant with only minor numerical fluctuations, confirming the correct implementation of the forces.

## 1.3 Timestep Dependency

Multiple test runs were performed using different timestep values. For  $dt = 0.01$ , the system showed good stability while having reasonable computational efficiency. Larger timesteps led to instabilities, while smaller timesteps significantly increased computation time without relevant accuracy improvements.

## 2 Couette flow with chain molecules

The next task was to simulate a Couette flow system with two walls moving in opposite directions at velocity  $v_{wall} = 5$ . Furthermore the system contained 42 chain molecules, which are structured as  $A - A - B - B - B - B - B$ , and fluid particles. Bond parameters were given as  $K_S = 100$  and  $r_S = 0.1$ , in addition conservative force coefficients were set according to the matrix given in the assignment.

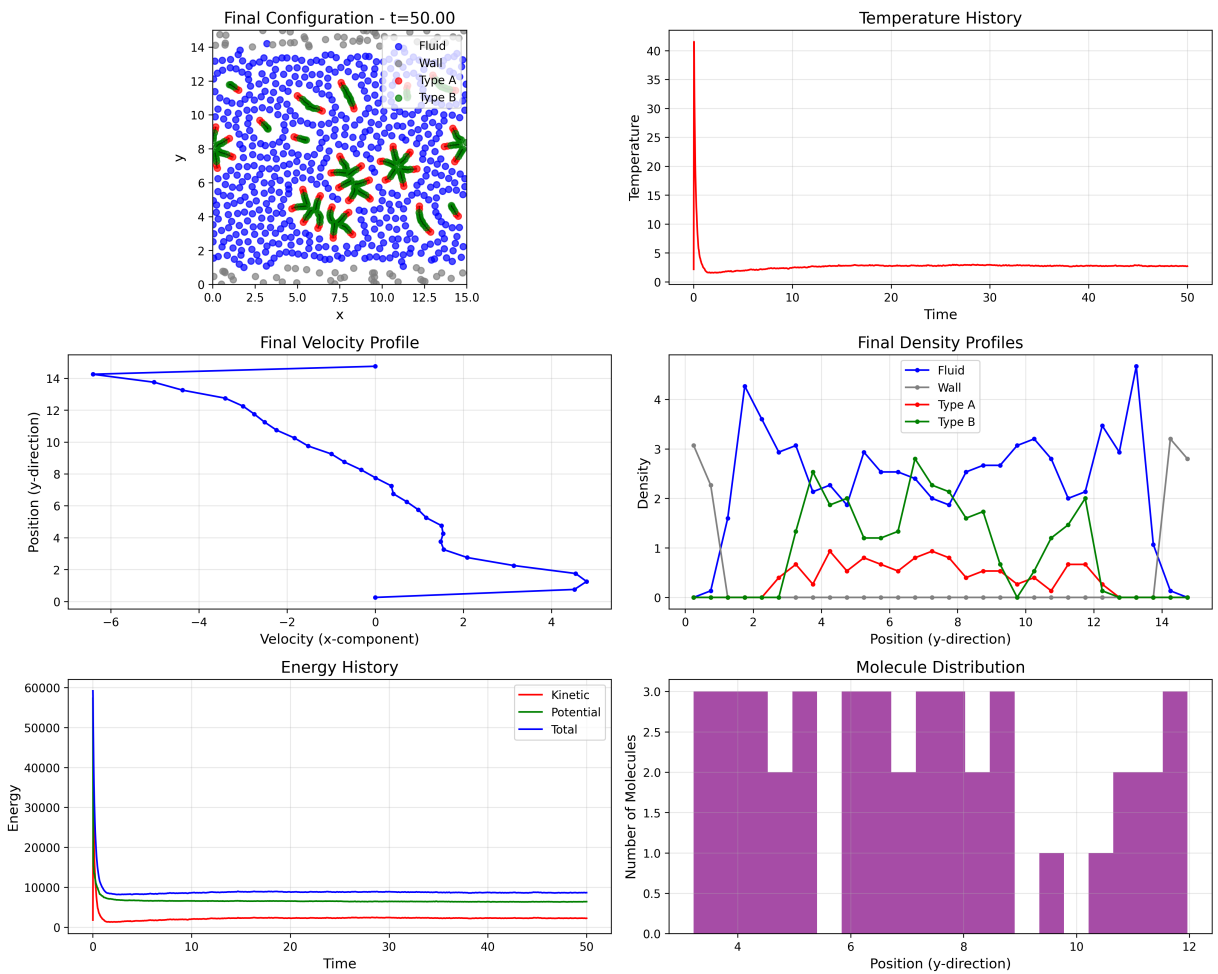


Figure 2: Couette flow with  $dt = 0.01$  and 5000 steps.

### 2.1 Flow Profile Analysis

Figure 2 shows that after 5000 timesteps, the velocity profile demonstrates a nearly linear relationship between position and velocity in the central region, which is an expected characteristic of Couette flow. Near the walls, there are some deviations from linearity due to the discrete nature of the walls and molecular interactions.

### 2.2 Molecule Distribution and Motion

We can observe several interesting behaviors of the chain molecules during the simulation:

1. The molecules tend to align with the flow direction due to shear forces.
2. There is a noticeable depletion of chain molecules near the walls and some concentration in the center region.
3. The distribution of molecules is not completely uniform across the channel.

This behavior can be explained by the interactions. The repulsion between type B and fluid particles ( $a_{BF} = 300$ ) leads to the ends which have B particles to avoid fluid-dense regions. Additionally, the weak interaction between B-B particles ( $a_{BB} = 1$ ) leads to them approaching each other rather closely, leading to aggregation of the chains. The walls on the other hand repel all particle types ( $a_{iW} = 200$ ), creating a "depletion layer" near the boundaries. The molecules are rotating as they move through the flow, with the shear forces causing them to tumble. This rotation is more noticeable in the center of the channel where the velocity gradient is the highest.

### 3 Poiseuille flow with ring-molecules

For the final task the goal was to perform Poiseuille flow simulation, where two stationary walls were placed on opposite sides of the domain. In addition a constant body force  $F_{body} = 0.3$  was applied to all non-wall particles. The system contained 10 ring molecules, each with 9 particles of type A, alongside fluid particles. The bond parameters were given as  $K_S = 100$  and  $r_S = 0.3$ .

#### 3.1 Temperature and Energy Analysis

The temperature history plot in Figure 3 shows a rapid initial equilibration followed by a steady increase, reaching approximately 40 units by the end of the simulation. This temperature rise is to be expected in a Poiseuille flow setup where kinetic energy is continuously added to the system by the body force.

#### 3.2 Flow Profile Analysis

The velocity profile shows the characteristic parabolic shape expected for Poiseuille flow, with maximum velocity in the center of the channel and zero velocity at the walls. On top over the duration of the simulation this velocity stays constant. This confirms the correct implementation of the body force and wall boundary conditions.

#### 3.3 Molecule Distribution and Evolution

The ring molecules show a distribution pattern across the channel:

1. Initially randomly distributed, the rings form and then afterwards gradually migrate toward the center of the channel over time.
2. The molecule distribution histogram shows higher concentrations near the center and decreased presence near the walls.
3. The rings appear to maintain their circular structure throughout the simulation, showing the effectiveness of the bond implementation.

The migration of ring molecules toward the center is a known effect as "cross-stream migration" or "tubular pinch effect." The primary reason for this migration is the balance between:

1. Wall-induced migration: The interaction with walls creates an effective repulsive force pushing particles away from the walls.
2. Shear-induced migration: The non-uniform shear rate across the channel, where it is the highest near walls and lowest at center in Poiseuille flow, creates a driving force that moves particles from high-shear to low-shear regions.

This effect is especially visible for structures like our ring molecules, as they experience different shear forces across their structure. The resulting hydrodynamic lift pushes them toward the center of the channel where the shear rate is minimal.

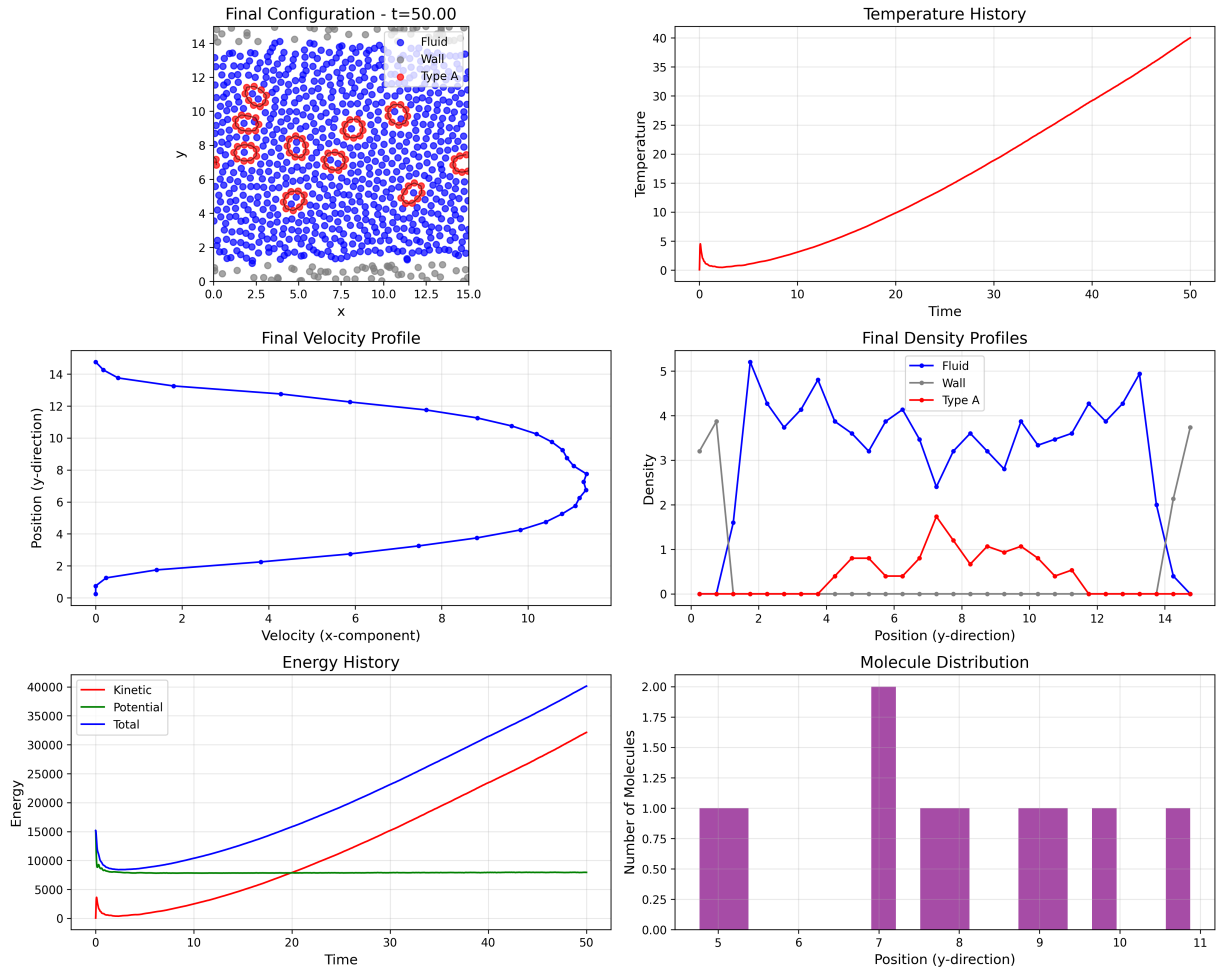


Figure 3: Poiseuille flow with  $dt = 0.01$  with 5000 steps

## Conclusion

The DPD simulations that were performed successfully captured the expected behaviors of the Test, Couette and Poiseuille behaviors and flows for the latter two. The implementation of different types of molecules (chain and ring) showed the capability of DPD to model complex fluids with structured components. Key findings include:

1. The DPD thermostat effectively maintained system temperature around the desired value.
2. Chain molecules in Couette flow aligned with the flow direction and showed a level of aggregation.
3. Ring molecules in Poiseuille flow exhibited cross-stream migration toward the center of the channel.

These simulations showed the validity and potential of DPD as a simulation method that can capture complex phenomena when molecular and continuum scales meet. The soft repulsive potentials and momentum-conserving thermostat make it particularly suitable for simulating soft matter and complex fluids.