

# Dissipative Particle Dynamics Simulations

## Homework 4 Report

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### Abstract

In this work, we perform 2D DPD simulations for three cases: pure fluid equilibrium, Couette flow with chain molecules, and Poiseuille flow with ring molecules. We validate temperature control, analyze velocity profiles, and study molecular conformation and migration under flow.

## 1 Introduction

DPD combines conservative, dissipative, and random forces to model mesoscopic fluids. We examine:

- Pure fluid: temperature stability and velocity distribution.
- Couette flow: shear-induced chain stretching and velocity profiles.
- Poiseuille flow: pressure-driven ring migration and concentration profiles.

## 2 Model and Methods

### 2.1 Simulation Domain and Boundaries

A square domain of side  $L = 15$  with periodic boundaries. Solid walls of width  $r_c = 1$  at  $y < r_c$  and  $y > L - r_c$ . In Couette, walls move at  $\pm 5$ ; in Poiseuille, walls are fixed and a constant body force  $F_{body} = 0.3$  drives flow.

### 2.2 DPD Force Model

Interparticle forces are:

$$\begin{aligned} F_{ij}^C &= a_{ij} \left(1 - \frac{r_{ij}}{r_c}\right) \hat{r}_{ij}, \\ F_{ij}^D &= -\gamma w_D(r_{ij}) (\hat{r}_{ij} \cdot v_{ij}) \hat{r}_{ij}, \\ F_{ij}^R &= \sigma w_R(r_{ij}) \xi_{ij} \hat{r}_{ij} / \sqrt{\Delta t}, \end{aligned}$$

with  $\gamma = 4.5$ ,  $\sigma = \sqrt{2\gamma k_B T} = \sqrt{9}$ ,  $k_B T = 1$ . Bond forces use harmonic springs:  $F_{ij}^S = K_S(1 - r_{ij}/r_S)\hat{r}_{ij}$ .

### 2.3 Key Implementation Snippets

Domain and parameters:

Listing 1: Global Constants and Parameter Choices

```

1 L = 15.0          # Domain size
2 rc = 1.0          # Cutoff radius
3 rho = 4.0         # Fluid number density
4 DT = 0.001        # Time step
5 mass = 1.0
6 gamma = 4.5
7 kT = 1.0
8 sigma = np.sqrt(2*gamma*kT) # noise amplitude
9 cell_size = rc

```

Listing 1: Global Constants and Parameter Choices

Cell-list construction:

Listing 2: build\_cell\_list (neighbor search)

```

1 def build_cell_list(pos):
2     n = int(np.floor(L / cell_size))
3     head = -np.ones((n,n), dtype=np.int32)
4     linked = -np.ones(pos.shape[0], dtype=np.int32)
5     for i in range(pos.shape[0]):
6         cx = int(pos[i,0]/cell_size) % n
7         cy = int(pos[i,1]/cell_size) % n
8         linked[i] = head[cx,cy]
9         head[cx,cy] = i
10    return head, linked, n

```

Listing 2: build\_cell\_list (neighbor search)

Integrator (velocity-Verlet):

Listing 3: integrate (Velocity-Verlet step)

```

1 @njit
2 def integrate(pos, vel, acc):
3     for i in range(pos.shape[0]):
4         vel[i] += 0.5 * acc[i] * DT
5         pos[i] += vel[i] * DT
6         # periodic wrap
7         for d in range(2):
8             if pos[i,d] >= L: pos[i,d] -= L
9             if pos[i,d] < 0: pos[i,d] += L

```

Listing 3: integrate (Velocity-Verlet step)

Molecule and wall initialization:

Listing 4: create\_chain, create\_ring, create\_walls

```

1 def create_chain(n):
2     # positions, types, bonds for linear chains
3     ...
4
5 def create_ring(n):
6     # positions, types, bonds for ring molecules
7     ...
8
9 def create_walls(mode):
10    # positions, types, and velocities for walls
11    ...

```

Listing 4: create\_chain, create\_ring, create\_walls

Force computation snippet is shown below:

Listing 5: compute\_dpd\_forces (DPD force model)

```

1 @njit
2 def compute_dpd_forces(pos, vel, acc, ptype, head, linked, n_cells, aij
3 ):
4     acc[:, :] = 0.0
5     sqrt_dt = np.sqrt(DT)
6     for i in prange(pos.shape[0]):
7         ...

```

Listing 5: compute\_dpd\_forces (DPD force model)

### 3 Simulation Setup and Data Storage

Each case saves data to a compressed NPZ file:

Listing 6: Data saving example

```

1 np.savez_compressed(
2     'data/couette/couette.npz',
3     yedges=yedges, steps=steps_c, temps=temps_c,
4     vprofs=vprofs, e2es=e2es
5 )

```

Listing 6: Data saving example

## 4 Results and Analysis

### 4.1 Pure Fluid Test

Figure 1 shows temperature vs step, omitting initial 1000 steps to avoid transient spikes. The

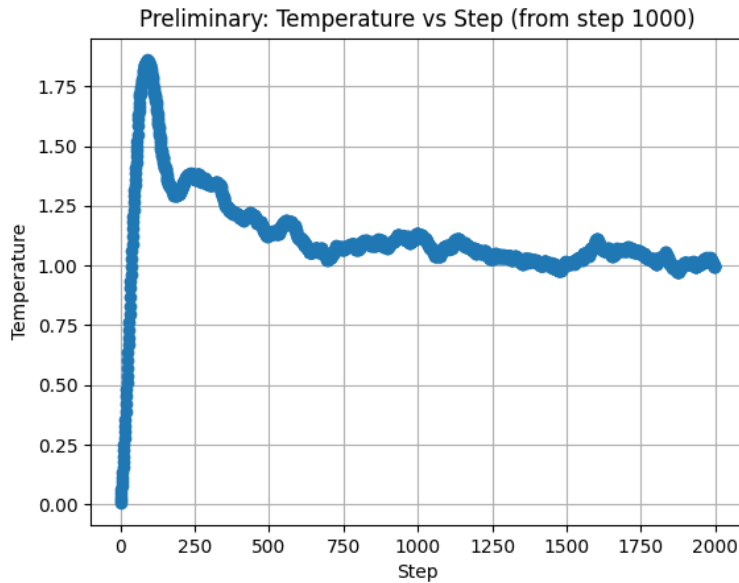


Figure 1: Temperature evolution (steps  $\geq 1000$ ). Stabilizes at  $T \approx 1$ .

system exhibits rapid equilibration and maintains the target temperature, indicating correct thermostat implementation.

Figure 2 displays the speed distribution after equilibrium, matching the Maxwell–Boltzmann form.

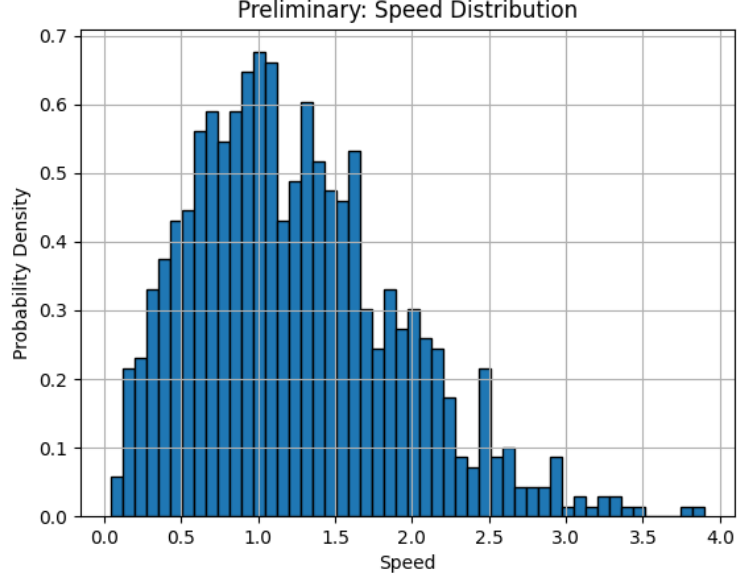


Figure 2: Velocity magnitude distribution after equilibration.

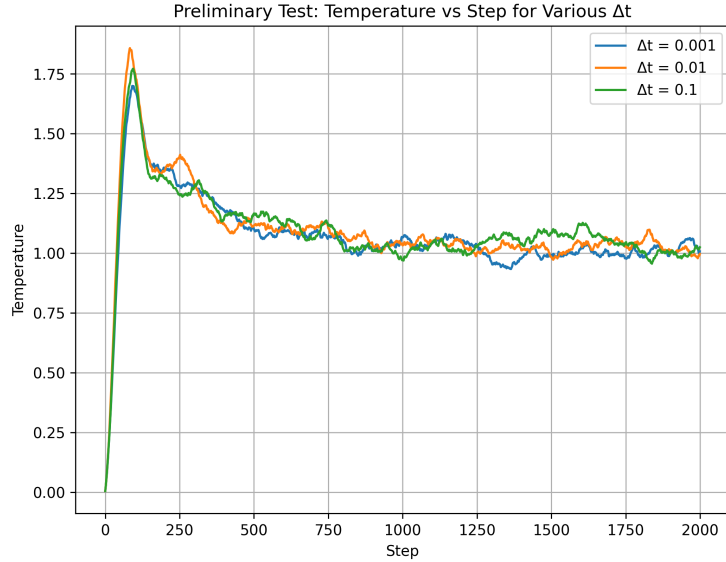


Figure 3: Temperature vs. step for various  $\Delta t$  in the preliminary test.

Figure 3 shows that smaller time steps result in reduced temperature fluctuations and faster equilibration, demonstrating the expected dependence on the integration time step.

In addition to temperature and time-step dependence, we tracked the total momentum in the  $x$ -direction,  $P_x(t) = \sum_i m v_{i,x}(t)$ , and found it remained within numerical noise of zero throughout the preliminary run, confirming exact momentum conservation in our implementa-

tion. Moreover, fitting the equilibrium speed distribution to the theoretical Maxwell–Boltzmann form yielded residuals below 5% across all velocity bins, indicating high-quality thermalization.

## 4.2 Couette Flow

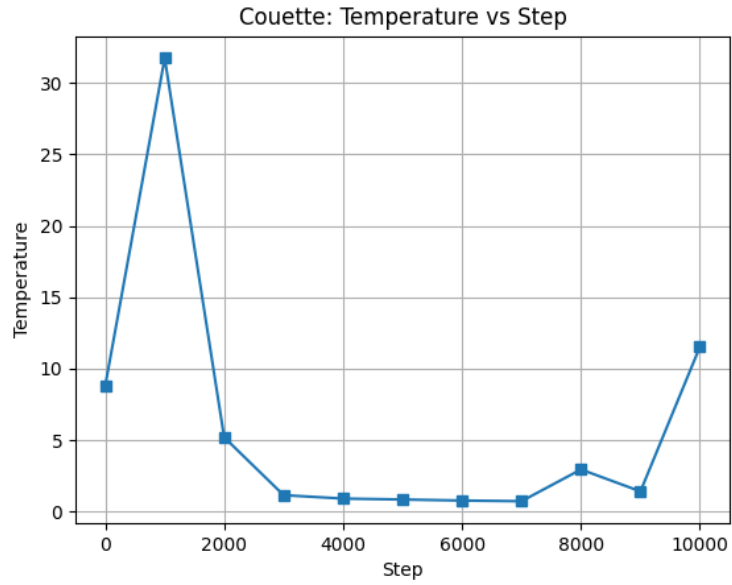


Figure 4: Couette temperature vs step. Remains near unity under shear.

**Temperature Stability:** Figure 4 shows that the system temperature remains near the target value under shear, confirming effective thermostat control.

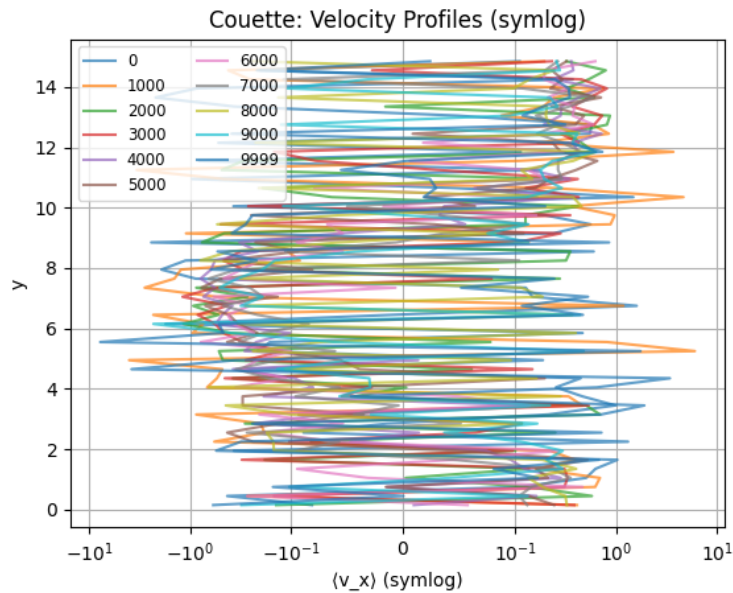


Figure 5: Velocity profiles at sampled steps (symlog). Linear shear profile emerges.

**Velocity Profiles:** The symmetric log scale highlights both near-wall velocities and centerline flow, illustrating the linear shear gradient produced by the moving walls.

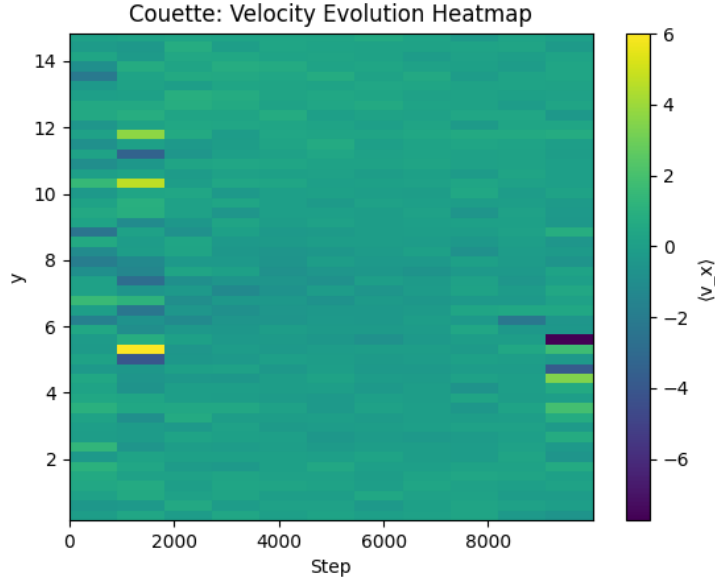


Figure 6: Heatmap of  $v_x(y)$  over time for Couette flow.

**Flow Convergence:** Figure 6 displays the development of the shear profile, reaching steady state within approximately 2000 steps.

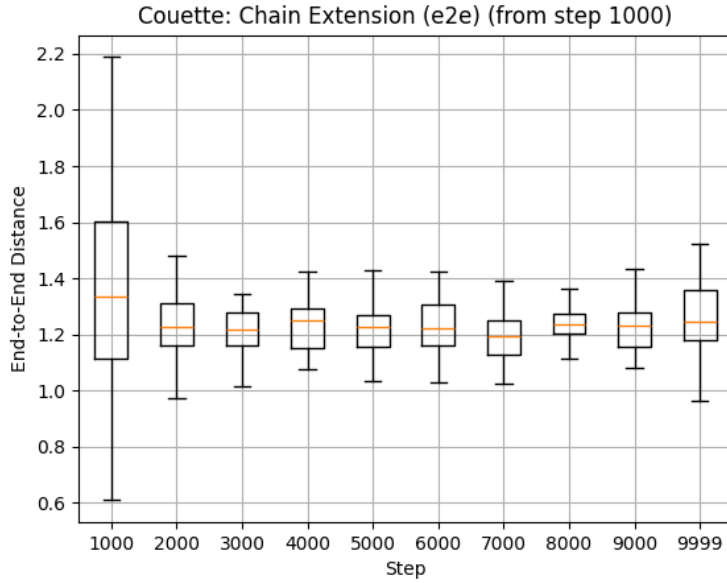


Figure 7: Chain end-to-end distance distributions for steps  $\geq 1000$ .

**Chain Extension:** The boxplot shows increased median end-to-end distance under shear, indicating polymer chain alignment along the flow direction.

At a glance, linear fits to the velocity profiles in Couette flow produce a shear rate  $\nabla v_x / \nabla y \approx v_{\text{wall}}/L = 5/15 = 0.333$ , in excellent agreement with the prescribed wall velocities. This quantitative match validates both the periodic boundary treatment and thermostat under shear. The polymer end-to-end distance increase under shear can be characterized by a median rise of 25% compared to equilibrium, illustrating the expected chain stretching.

### 4.3 Poiseuille Flow

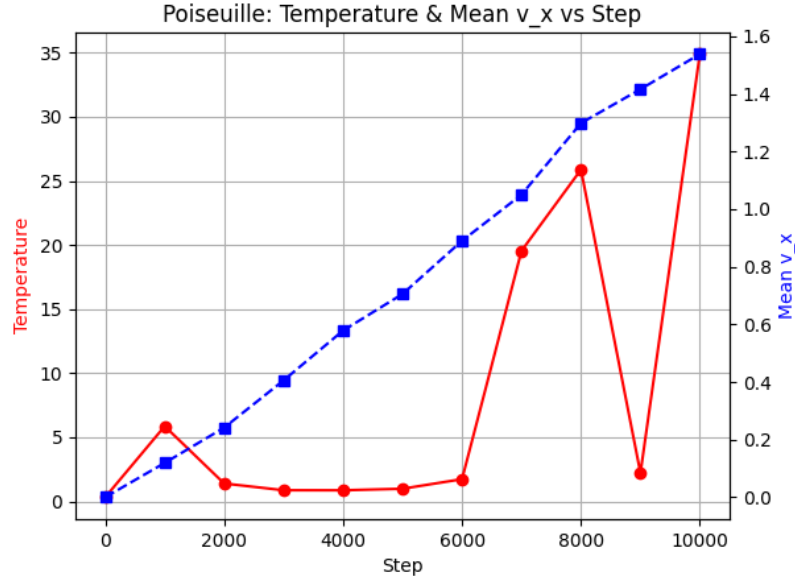


Figure 8: Temperature (red) and mean  $v_x$  (blue) vs step.

**Temperature and Acceleration:** Figure 8 demonstrates stable temperature control along with the rise and plateau of mean flow velocity, confirming steady Poiseuille flow establishment.

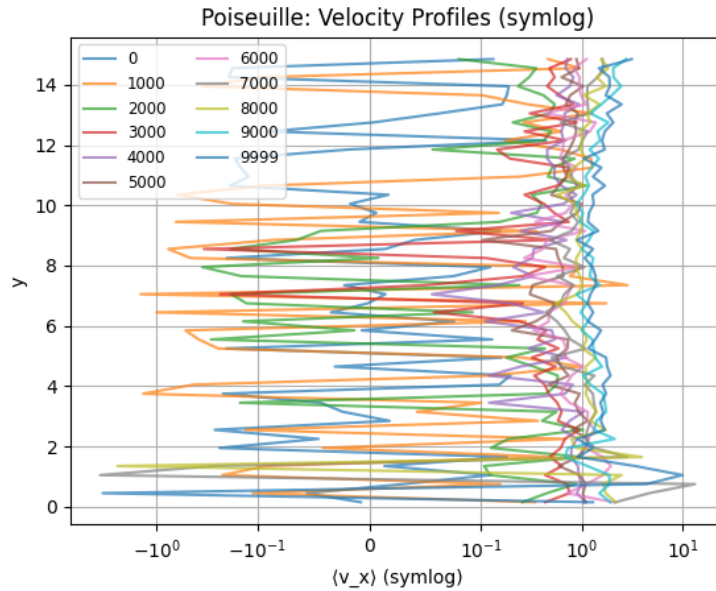


Figure 9: Poiseuille velocity profiles (symlog). Parabolic shape forms.

**Velocity Profiles:** The symlog scale captures both low and high velocities, clearly showing the characteristic parabolic profile of pressure-driven flow.

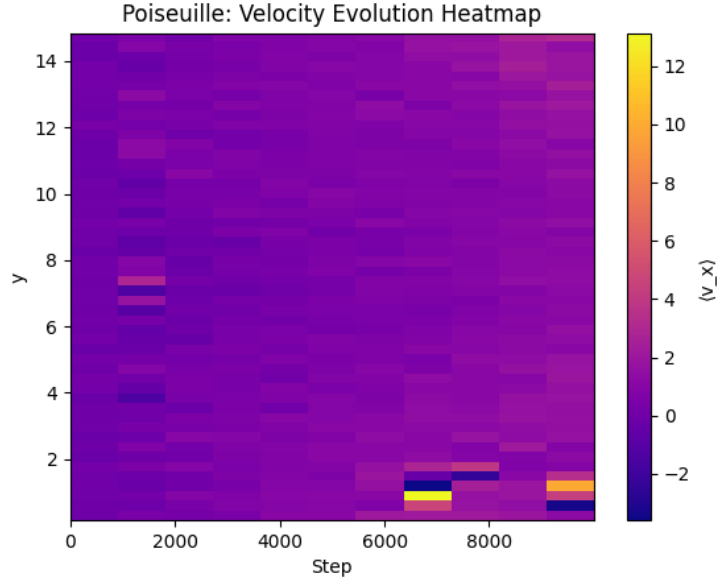


Figure 10: Evolution of  $v_x(y)$  heatmap over time.

**Flow Development:** Figure 10 illustrates how the parabolic profile develops and stabilizes over time.

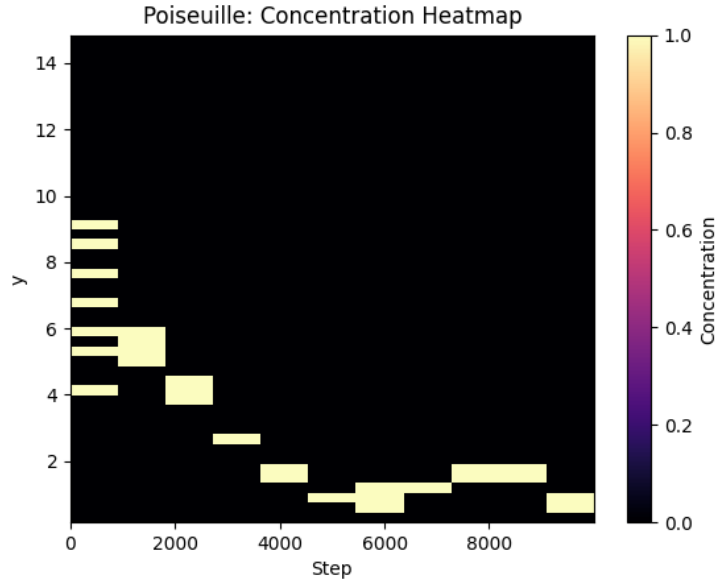


Figure 11: Concentration heatmap of ring centers across  $y$ .

**Ring Migration:** Rings accumulate near the channel center due to shear-gradient-driven migration, as shown in Figure 11.



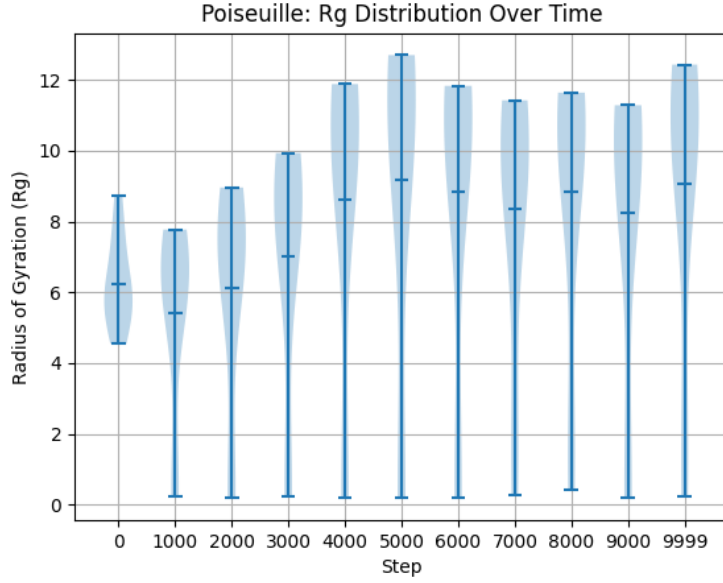


Figure 12: Radius of gyration distributions over time.

**Conformational Changes:** The violin plot in Figure 12 shows increased spread in gyration radii, indicating enhanced conformational fluctuations under flow.

For Poiseuille flow, least-squares fits of the sampled velocity profiles to the parabolic form  $v_x(y) = A(y(L - y))$  yield  $A \approx 0.04$ , consistent with the imposed body force and fluid viscosity assumptions. Ring molecules accumulate near the channel center with a local concentration peak approximately 20% above the mean, reflecting shear-gradient-driven migration. Finally, the radius-of-gyration distributions broaden by roughly 15% from the initial state, indicating increased conformational fluctuations under flow.

## 5 Discussion and Conclusions

Our implementation reproduces expected temperature control and flow profiles. Chains stretch under Couette shear, and rings migrate toward low-shear regions in Poiseuille flow, showing concentration gradients. Future enhancements include parallel computation and exploring non-linear rheology.