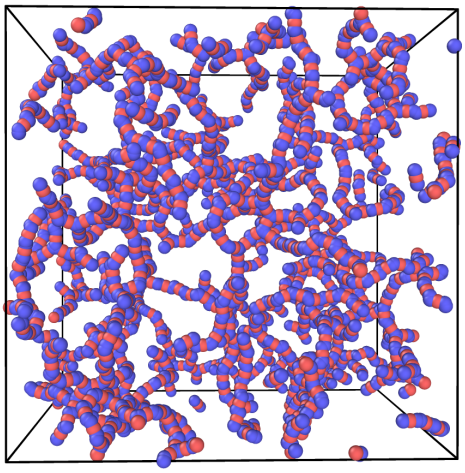
MTEK0033 Multiscale Modelling, University of Turku, January 2026

Brownian Dynamics Simulation

Project- V



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1 Thermostating Strategy, Relaxation Dynamics, and Tracer Motion

This project focuses on understanding **thermalization**, **momentum relaxation**, and the role of **thermostats** in molecular simulations. Students will compute the **velocity autocorrelation function (VACF)** in microcanonical (NVE) simulations, estimate the characteristic **relaxation time**, and extract the corresponding **friction coefficient**. These parameters will then be validated using **tracer particles** of varying sizes.

By systematically comparing bath particles, large tracers, and ideal tracer particles, students will assess the consistency of coarse-grained Langevin descriptions with underlying molecular dynamics.

1.1 Introduction

Thermostats are commonly used in molecular simulations to maintain a target temperature. However, improper thermostatting can distort dynamical properties such as diffusion, viscosity, and velocity correlations. To understand these effects, it is essential to analyze relaxation dynamics in the absence of external thermal control.

In an NVE ensemble, energy is conserved and thermalization emerges from particle interactions alone. The decay of velocity correlations in such systems provides direct information about momentum relaxation and effective friction.

Tracer particles offer a powerful probe of the surrounding medium. If the bath dynamics are well captured by a Langevin description, tracer motion should exhibit consistent relaxation behavior governed by the same friction coefficient.

1.2 Model and Simulation Details

Particles interact via the Lennard–Jones potential:

$$U_{\mathrm{LJ}}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]. \tag{1}$$

All simulations are first equilibrated using a thermostat and then switched to the **NVE ensemble** for production runs. Velocity data are recorded for correlation analysis.

1.3 Velocity Autocorrelation Function

The velocity autocorrelation function (VACF) is defined as

$$C_v(t) = \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle, \tag{2}$$

where the angular brackets denote an ensemble and time-origin average.

For simple fluids, the VACF exhibits an exponential decay at intermediate times:

$$C_v(t) \sim e^{-t/\tau}, \tag{3}$$

where τ is the characteristic relaxation time.

1.4 Relaxation Time and Friction Coefficient

The relaxation time τ is extracted by fitting the decay of the VACF obtained from NVE simulations. Assuming an effective Langevin description, the friction coefficient γ is related to τ by

$$\gamma = \frac{m}{\tau}, \tag{4}$$

where m is the particle mass.

This friction coefficient serves as an effective parameter characterizing momentum dissipation due to the surrounding fluid.

1.5 Tracer Particle Dynamics

To test the robustness of the extracted friction coefficient, tracer particles are introduced into the system.

1.5.1 Large Tracer Particles

A small number of tracer particles with increased size and mass are added to the equilibrated bath. These tracers interact with bath particles via scaled Lennard–Jones parameters.

The VACF of the tracer particles is computed and compared with that of the bath particles. Due to their larger inertia, tracers are expected to exhibit slower relaxation while remaining consistent with Langevin predictions.

1.5.2 Ideal Tracer (Passive Probe)

In the final step, purely tracer particles are simulated using a Langevin equation with the previously extracted friction coefficient γ. No explicit bath particles are present.

The VACF obtained from these Langevin tracer simulations is compared directly with that of the large tracers embedded in the bath. Agreement between the two confirms the validity of the coarse-grained description.

1.6 Symbols

Symbol	Meaning
$C_v(t)$	velocity autocorrelation function
τ	relaxation time
γ	friction coefficient
m	particle mass
N	number of bath particles
N_t	number of tracer particles

Table 1: List of symbols used in the project.

1.7 Project Tasks

- Equilibrate an LJ fluid using a thermostat
- Switch to NVE ensemble and record velocity trajectories
- Compute the velocity autocorrelation function
- Extract the relaxation time from VACF decay
- Compute the effective friction coefficient
- Introduce large tracer particles and compute their VACF
- Simulate ideal tracer particles using Langevin dynamics
- Compare correlation functions across all cases

1.8 Simulation Studies

Study 1: Effect of Density on Velocity Relaxation (NVE Ensemble)
In this study, you will investigate how particle density affects microscopic dynamical relaxation in a many-particle system. The dynamics are analyzed using the *velocity auto-correlation function (VACF)*, which quantifies how long a particle retains memory of its initial velocity. By varying the number of particles N at fixed volume, you will control the system density and examine its influence on the relaxation (response) time.

#	Number of particles N
1	256
2	500
3	1000
4	2000

Table 2: Effect of particle number (density) on relaxation dynamics.

Step 1: Folder structure and setup

1. Navigate to the directory:

   `Project_5/VACF/Density_Study/`

2. Inside this directory, you will find four subfolders corresponding to the particle numbers listed in Table 1:

   `N_256`, `N_500`, `N_1000`, `N_2000`

3. Each folder contains:

   - the LAMMPS input script,
   - initial configuration and data files,
   - and Python scripts for VACF and relaxation-time analysis.

Step 2: Simulation protocol

1. The system volume is kept fixed for all simulations; changing N therefore changes the particle density.
2. Inter-particle interactions and particle mass are identical across all runs.
3. The system is first equilibrated using a thermostat to reach the desired temperature.
4. After equilibration, switch to the **microcanonical (NVE) ensemble** to study intrinsic dynamics without external damping.

Step 3: Velocity auto-correlation function (VACF)

1. During the NVE run, record particle velocities as a function of time.
2. Compute the velocity auto-correlation function:

$$C_v(t) = \frac{\langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle}{\langle \mathbf{v}(0) \cdot \mathbf{v}(0) \rangle}$$

   where the average is taken over particles and time origins.

3. Use the provided Python script to generate the VACF curve for each value of N.

Step 4: Relaxation (response) time

1. Define the relaxation time τ as:

   - the integral of the VACF over time, or
   - the time at which the VACF decays to $1/e$ of its initial value.

2. Compute the relaxation time τ for each density.

3. Store the results in a file named:

   `relaxation_time.txt`

   using the format:

   $$\rho \quad \tau$$

Step 5: Density vs. relaxation time

1. Plot relaxation time τ as a function of particle density ρ.
2. Analyze how increasing density affects velocity memory and momentum transport.

Step 6: Physical interpretation

1. Explain why the NVE ensemble is essential for studying time-correlation functions.
2. Discuss how increased collision frequency at higher density influences the decay of the VACF.
3. Relate the relaxation time to transport properties such as diffusion and viscosity.
4. Comment on the connection between microscopic dynamics and macroscopic response.

Study 2: Tracer Size Dependence of Velocity Relaxation

In this study, you will investigate how the *size and mass of tracer particles* affect microscopic velocity relaxation in a dense bath of larger particles. Tracer particles do **not interact with one another**, but interact with the surrounding bath particles. This setup mimics dilute tracer diffusion in a complex medium and allows direct access to memory effects via the velocity auto-correlation function (VACF).

The tracer size is controlled by the Lennard–Jones diameter σ_t. The tracer mass is chosen to scale with size as:

$$m_t \propto \sigma_t^3,$$

corresponding to particles of constant material density.

#	Tracer diameter σ_t
1	1.0
2	1.5
3	2.0
4	2.5

Table 3: Effect of tracer size (and mass) on VACF decay.

Step 1: Folder structure and setup

1. Navigate to the directory:

   `Project_5/VACF/Tracer_Study/`

2. Inside this directory, you will find four subfolders corresponding to the tracer sizes listed in Table 2:

   `Tracer_sigma_1.0`, `Tracer_sigma_1.5`, `Tracer_sigma_2.0`, `Tracer_sigma_2.5`

3. Each folder contains:

   - the LAMMPS input script,
   - system configuration files,
   - tracer definition files,
   - and VACF analysis scripts.

Step 2: System composition and interactions

1. The system consists of:

   - a dense bath of interacting particles, and
   - a small number of tracer particles (dilute limit).

2. Tracer–tracer interactions are turned **off**.

3. Tracer–bath interactions are identical in functional form to bath–bath interactions, but use the tracer diameter σ_t.

4. The tracer mass m_t is set proportional to σ_t^3.

5. Bath particle properties and overall density are kept fixed.

Step 3: Simulation protocol

1. Equilibrate the full system at the desired temperature using a thermostat.

2. After equilibration, switch to the **NVE ensemble** to study intrinsic tracer dynamics.

3. During the NVE run, record velocities of tracer particles only.

Step 4: Velocity auto-correlation function (VACF)

1. Compute the tracer velocity auto-correlation function:

$$C_v^{(t)}(t) = \frac{\langle \mathbf{v}_t(0) \cdot \mathbf{v}_t(t) \rangle}{\langle \mathbf{v}_t(0) \cdot \mathbf{v}_t(0) \rangle},$$

   where the average is taken over tracer particles and time origins.

2. Use the provided Python script to generate VACF curves for each tracer size.

Step 5: Relaxation (response) time

1. Define the tracer relaxation time τ_t as:

- the integral of the tracer VACF, or
- the time at which $C_v^{(t)}(t)$ decays to $1/e$.

2. Compute τ_t for each tracer size.

3. Store the results in:

   `tracer_relaxation_time.txt`

   using the format:

   $$\sigma_t \quad m_t \quad \tau_t$$

Step 6: Tracer size vs. relaxation time

1. Plot the tracer relaxation time τ_t as a function of tracer size σ_t.

2. Alternatively, analyze τ_t as a function of tracer mass m_t.

Step 7: Physical interpretation

1. Explain why tracer–tracer interactions are neglected in this study.

2. Discuss how increasing tracer size and mass affects momentum exchange with the bath.

3. Relate the observed trends to Brownian motion and hydrodynamic drag.

4. Comment on the crossover from ballistic to diffusive motion as tracer size increases.

Study 3: Effect of Langevin Thermostat Strength on Relaxation Dynamics

In this study, you will investigate how the Langevin thermostat damping parameter γ affects dynamical properties of the system. While thermostats are commonly used to control temperature, they can modify the intrinsic dynamics of particles. Your goal is to determine the appropriate value of γ that maintains temperature control without distorting the natural relaxation behavior.
The analysis will again be based on the velocity auto-correlation function (VACF) and the extracted relaxation time.

#	γ (ps^{-1})
1	0.01
2	0.1
3	0.5
4	1.0

Table 4: Langevin damping parameters used to study thermostat influence on dynamics.

Step 1: Folder structure and setup

1. Navigate to:

   `Project_5/VACF/Langevin_Study/`

2. Inside this directory, you will find subfolders corresponding to each damping parameter:

   `gamma_0.01`, `gamma_0.1`, `gamma_0.5`, `gamma_1.0`

3. Each folder contains:

   - the LAMMPS input script using the Langevin thermostat,
   - system configuration files,
   - and VACF analysis scripts.

Step 2: Simulation protocol

1. The particle number N, density, and interaction parameters are kept fixed.
2. The system is equilibrated and evolved using the Langevin thermostat with damping parameter γ.
3. Record particle velocities during the production run.

Step 3: Velocity auto-correlation function

1. Compute the normalized VACF:

$$C_v(t) = \frac{\langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle}{\langle \mathbf{v}(0) \cdot \mathbf{v}(0) \rangle}.$$

2. Generate VACF curves for each value of γ.

Step 4: Relaxation time extraction

1. Define the relaxation time $\tau(\gamma)$ as:

   - the $1/e$ decay time, or
   - the integral of the VACF.

2. Store the results in:

   `gamma_vs_relaxation.txt`

   using the format:

   $\gamma \quad \tau$

Step 5: Determination of optimal γ

1. Plot relaxation time τ as a function of γ.
2. Compare the Langevin results with the NVE relaxation time obtained in Study 1.
3. Identify the range of γ values that:

   - maintain stable temperature control,

- reproduce relaxation times closest to the NVE result.

4. Report the optimal γ and justify your choice physically.

Step 6: System-size dependence

1. Repeat the above procedure for different particle numbers N (from Study 1).
2. For each N, determine the optimal γ.
3. Plot:

$$\gamma_{\text{optimal}} \quad \text{vs.} \quad N$$

and analyze the trend.

Step 7: Physical interpretation

1. Explain how the Langevin thermostat modifies the equations of motion:

$$m\dot{\mathbf{v}} = \mathbf{F} - \gamma m\mathbf{v} + \mathbf{R}(t).$$

2. Discuss how increasing γ increases friction and suppresses velocity correlations.
3. Distinguish between:
   - underdamped regime (small γ),
   - critically damped regime,
   - overdamped regime (large γ).
4. Explain why too large a γ destroys true dynamical information.

1.9 Presentation and Project Report

- **Introduction (1 page)**: Diffusivity and Brownian dynamics.
- **Model and Theory (1 page)**: Basics of Langevin dynamics, major characteristics of the dynamics.
- **Results and Discussion (6-10 pages)**: Velocity autocorrelation function, characteristic time for the smaller molecules and large tracer paticles.
- **Conclusion (1 page)**: Physical interpretation, limitations and future aspects.

1.10 Future Aspects

The present study can be extended in several directions to explore more complex and realistic dynamical behaviour in soft-matter and fluid systems. One important extension is the inclusion of **hydrodynamic interactions**, which are neglected in simple Langevin descriptions but play a crucial role in collective relaxation and long-time correlations.

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 introduce tracer dynamics as a fundamental tool for probing transport properties in many-body systems. In particular, students should:

- Explain the concept of a tracer particle and its role in statistical mechanics.
- Introduce the velocity autocorrelation function (VACF):

$$C_v(t) = \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle$$

- Discuss the connection between VACF decay and microscopic relaxation processes.
- Briefly mention Green–Kubo relations and their relevance to transport coefficients.

Students should motivate the relevance of tracer studies by discussing applications such as:

- Diffusion in crowded environments,
- Microrheology and probe-based measurements,
- Transport in biological and soft-matter systems.

The goal of the project should be clearly stated:

To investigate how density, tracer size, and thermostatting affect velocity relaxation and transport dynamics.

2. Technical Description of the Simulations

This section should describe the molecular dynamics framework used to study tracer dynamics. Students must describe:

- The interaction potential used for the background particles.
- The tracer particle interactions:
  - Tracers interact with background particles,
  - Tracer–tracer interactions are disabled.
- The relationship between tracer size σ_t and tracer mass m_t.
- The simulation ensemble used:
  - NVE for microcanonical dynamics,
  - Langevin dynamics where applicable.

Students should also describe how velocities and correlation functions are computed.

3. Study 1: Effect of Density on Relaxation Dynamics

In this study, students will examine how system density affects tracer relaxation.

Procedure

- Perform simulations with different numbers of background particles N.
- Keep the tracer properties fixed.
- Compute the VACF for the tracer particle.

Analysis

Students should:

- Plot the VACF as a function of time for different densities.
- Extract a characteristic relaxation time τ from the VACF decay.
- Plot relaxation time τ as a function of number density.

4. Study 2: Tracer Size and Mass Dependence

In this study, students will explore how tracer size and mass influence relaxation dynamics.

Procedure

- Perform simulations for different tracer diameters σ_t.
- Scale tracer mass according to:
$$m_t \propto \sigma_t^3$$
- Ensure that tracer–tracer interactions remain disabled.

Analysis

Students should:

- Plot VACF for different tracer sizes.
- Extract and compare relaxation times.
- Discuss inertial versus collisional contributions to relaxation.

5. Study 3: Effect of Thermostatting (Langevin Dynamics)

In this study, students will analyze how Langevin thermostat parameters affect tracer dynamics.

Procedure

- Perform simulations using a Langevin thermostat.
- Vary the friction coefficient γ over a suitable range.
- Repeat simulations for different system sizes.

Analysis

Students should:

- Plot relaxation time τ as a function of γ.
- Identify the regime where dynamics is overdamped or underdamped.
- Determine an optimal range of γ that minimally perturbs natural dynamics.
- Plot γ versus system size and discuss scaling behavior.

6. 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 all three studies and discuss:

- How microscopic interactions control relaxation.
- The role of inertia, collisions, and thermal noise.
- Differences between microcanonical and Langevin dynamics.

Connections to kinetic theory and Brownian motion should be made wherever appropriate.

7. Conclusion

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

- Summarize how density, tracer size, and thermostatting influence relaxation.
- Identify conditions for physically meaningful tracer dynamics.
- Reflect on the usefulness of tracer-based methods in transport studies.
- Suggest extensions such as multiple tracers or confined geometries.

References

[1] Sevilla, Francisco J., Adriano Valdés-Gómez, and Alexis Torres-Carbajal. **"Anomalous diffusion of scaled Brownian tracers."** Physical Review E 110.1 (2024): 014113. DOI: 10.1103/PhysRevE.110.014113.

[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