# Tutorial II: BD Exercises

February 06, 2026

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**Caution: Read the entire question paper carefully before attempting to solve the problems to avoid any mistakes.**

## Exercise II

1. **Verify the validity of the Einstein diffusion equation for Brownian motion, given by**

$$D = \frac{k_{\mathrm{B}}T}{\gamma},$$

**where $D$ is the translational diffusion coefficient, $k_{\mathrm{B}}$ is the Boltzmann constant, $T$ is the temperature, and $\gamma$ is the friction coefficient. Using the folder `e2_brownian_dynamics` and following the corresponding manual, perform the following tasks:**

- **Step 1:** Run the system for the values

$$\gamma^{-1} = 0.1,\ 0.3,\ 0.6,\ 1.0.$$

  Compute the diffusion coefficient $D$ for each case and plot the relation between $D$ and $\gamma$. Paste the generated PNG figure in your answer sheet. **[5 marks]**

- **Step 2:** Run the system for the values

$$k_{\mathrm{B}}T = 1,\ 2,\ 3,\ 4,\ 5.$$

  Compute the diffusion coefficient for each temperature and plot the relation between $D$ and $T$. Paste the PNG plot in your answer sheet. **[5 marks]**

- **Step 3:** Run the system for particle masses

$$m = 1,\ 2,\ 3,\ 4,\ 6.$$

  Compute the corresponding diffusivities and plot $D$ as a function of mass $m$. Append the PNG image in your answer sheet. **[5 marks]**

- **Step 4:** Based on your plots, discuss whether the relations

$$D \text{ vs. } \gamma^{-1}, \qquad D \text{ vs. } m^{-1}, \qquad D \text{ vs. } k_{\mathrm{B}}T$$

are linear. Clearly describe your observation. **[5 marks]**

**Note:** All plots must be saved as separate PNG files and pasted into your answer sheet.

2. **Modify the given LAMMPS input template (use the folder `e2_lj_viscosity`)to compute the viscosity of a Lennard-Jones fluid at density**

$$\rho = 0.6$$

**using the Green-Kubo relation. The shear viscosity is defined by**

$$\eta = \frac{V}{k_{\mathrm{B}}T} \int_0^\infty \langle P_{\alpha\beta}(0)\, P_{\alpha\beta}(t) \rangle \, dt,$$

**where $P_{\alpha\beta}$ are the off-diagonal components of the pressure tensor, $V$ is the system volume, and $T$ is the temperature. Perform the following tasks:**

- **Step 1:** Modify the simulation box and generate particles corresponding to the target density $\rho = 0.6$. Describe and justify all changes made to the LAMMPS input script. **[5 marks]**
- **Step 2:** Apply an appropriate timestep, thermostat and integrator to equilibrate the Lennard-Jones fluid at the desired thermodynamic state. **[5 marks]**
- **Step 3:** Compute and report the final value of viscosity obtained from your simulation. Compute the viscosity for different densities $\rho = 0.3, 0.4, 0.5$ make a plot for density vs viscosity. Discuss whether the result is physically reasonable. — **[5 marks]**

**Hint:** Use the off-diagonal components of the pressure tensor ($P_{xy}, P_{xz}, P_{yz}$), which describe momentum transport and are necessary for the Green–Kubo viscosity calculation.

3. **Modify the provided LAMMPS molecular template (folder `e2_mole_template`)in order to construct a dumbbell-shaped patch arrangement with an intramolecular bond distance between patch and the central hard core fixed at** 0.5**. Update the corresponding LAMMPS input script to perform constant-pressure, temperature (NPT) simulations and investigate the phase behavior of the system at different pressures. Identify any at least one values of temperature and pressure where the system exhibits liquid-like (chain-forming)**

- **Step 1:** Construct the correct molecular template (the file with the `.mol` extension) defining a dumbbell-shaped molecule with bond length fixed at 1.0. Paste the complete contents of the `.mol` file in your answer sheet. **[5 marks]**
- **Step 2:** Open the LAMMPS manual, search for the npt thermostat in the fixes section and modify the LAMMPS input script to perform simulations under constant pressure and temperature using an appropriate barostat (e.g., `fix npt`). Clearly specify the thermostat-barostat parameters. **[5 marks]**

- **Step 3:** Visualize a simulation in which the system exhibits a **liquid-like (chain-forming)** phase using OVITO. Capture a high-quality screenshot of the final configuration, ensuring that the core particles and patch particles are clearly distinguishable by size and color. Paste the image in your answer sheet and report the corresponding pressure and temperature value. **[5 marks]**

4. **Assume that you have created a carbon nanotube to simulate in LAMMPS. You wrote a Python code that generates the total number of bonds, bond angles, dihedral angles, and improper dihedral angles. You now want to check whether the generated topology is correct. Answer the following questions for the CNT made of 286 Carbon atoms:**

   - How many pairs of bonds are possible if the nanotube contains 260 bulk atoms and 26 edge atoms, where edge atoms have only two bonds each? **[5 marks]**
   - How many bond angles are possible in the system? **[5 marks]**
   - How many dihedral angles are possible, considering each plane formed by any four atoms bonded sequentially? **[5 marks]**
   - How many improper dihedral angles are possible if each atom with exactly three bonded neighbors represents a center for an improper dihedral? **[5 marks]**

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