Tutorial: BD Exercises

February 06, 2026

Note: Read the entire question paper carefully, before attempting to solve the problems to avoid any mistakes, and possible marks reduction.

Maximum marks: 70

Answer the following questions:

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

$$D = \frac{k_B T}{\gamma},$$

where D is the translational diffusion coefficient, k_B is the Boltzmann constant, T is the temperature, and γ is the friction coefficient. Using the folder `Exercise_1` and following the corresponding manual, perform the following tasks:

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

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

at a fixed mass $m = 1$ and $k_B T = 1.0$. Compute the diffusion coefficient D for each case and plot the relation between D and γ. Paste the generated PNG figure in your answer sheet. **[2.5 marks]**

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

$$k_B T = 1,\ 2,\ 3,\ 7,$$

at a fixed $\gamma^{-1} = 0.1$ and $m = 1$. Compute the diffusion coefficient for each temperature and plot the relation between D and T. Paste the PNG plot in your answer sheet. **[2.5 marks]**

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

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

at a fixed $k_B T = 1.0$ and $\gamma^{-1} = 0.1$. Compute the corresponding diffusivity and plot D as a function of mass m. Append the PNG image in your answer sheet.
- **[2.5 marks]**

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

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

are linear. Clearly describe your observation. **[2.5 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 `Exercise_2`)to compute the viscosity of a Lennard-Jones fluid at density**

$$\rho = 0.5$$

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

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

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 $\rho = 0.5$. Paste the relevent section in your answer sheet. 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. Paste the relevent section in your answer sheet. **[5 marks]**
- **Step 3:** Compute and report the final value of viscosity obtained from your simulation for different densities $\rho = 0.05, 0.1, 0.3, 0.4, 0.5$ make a plot for density vs viscosity. Discuss whether the result is physically reasonable.
  — **[5 marks]**
- **Step 4:**
  The shear viscosity obtained from the Green–Kubo calculation in LAMMPS is reported in reduced Lennard–Jones (LJ) units.
  In Lennard–Jones (LJ) reduced units, viscosity is expressed in terms of the fundamental LJ units of mass m, energy ϵ, and length σ. The dimensional form of viscosity is

$$[\eta] = \frac{\text{mass}}{\text{length}\,\text{time}}.$$

  In LJ units, the characteristic time scale is defined as

$$\tau = \sigma\sqrt{\frac{m}{\epsilon}}.$$

  and energy is defined as,

$$\epsilon = k_B T.$$

  Assume the following mappings between reduced LJ units and physical units: Length scale: $\sigma = 1$ Å $= 1 \times 10^{-10}$ m. Energy scale: $\epsilon = k_B T$, with $T = 300$ K, where the Boltzmann constant is $k_B = 1.380649 \times 10^{-23}$ J K^{-1}. Mass scale: corresponding to a single carbon atom, $m = 12$ amu, and 1 amu $= 1.660539 \times 10^{-27}$ kg

  (a) Derive the conversion factor that must be multiplied with the viscosity expressed in LJ units to obtain viscosity in SI units (Pa·s). **[2.5 marks]**
  (b) Clearly state the final numerical value of the conversion factor in SI units.
  - **[2.5 marks]**

Note: 10%, error in density is allowed, in case if parameters adjustment is not leading to an accurate particle number generation to get the target number density, for the given box size.

Hint: Use the appropriate time integration step size.

3. **Modify the provided LAMMPS molecular input template (folder `Exercise_3`) to construct a dumbbell-shaped patchy particle system. Each molecule consists of a central hard-core particle and a two patch particle located on opposite ends (poles of the spheres), with the intramolecular bond distance between the core and the patch fixed at 0.5 in reduced units.**

   Update the LAMMPS input script to change the existing Langevin thermostat temperature to an appropriate value, and study the phase behavior of the system over a range of temperatures. Now, perform the following tasks:

   - **Step 1:** Construct a correct molecular template file (with the `.mol` extension) defining a dumbbell-shaped molecule. The molecule should consist of three atoms (core and patch) connected by a rigid bond with a fixed bond length of 0.5 LJ Unit. Paste the complete contents of the `.mol` file in your answer sheet and clearly label all sections of the file. **[5 marks]**
   - **Step 2:** Perform simulations at appropriate temperatures and simulation time to identify, at least one temperature at which the system displays liquid-like, chain-forming behavior. Visualize the corresponding simulation using OVITO and capture a high-quality image of the final configuration. Ensure that core and patch particles are clearly distinguishable by size and color. Paste the image in your answer sheet and report the corresponding temperature at which the chain-forming phase is observed. **[5 marks]**
   - **Step 3:** Observing your system, write a maximum 200 words description about the stability of the chain structure? Are they stable or not in compare to to other structures (e.g, globular structures obtained at $k_{\mathrm{B}}T = 1.0$), specify some possible reasons?

     - **[5 marks]**

4. **You have generated a carbon nanotube (CNT) structure for molecular dynamics simulations in LAMMPS and written a Python code to construct its molecular topology (bonds, bond angles, dihedral angles, and improper dihedrals). To verify that your generated topology is correct, you must compute the expected number of each topological element analytically.**

   Consider a CNT consisting of **288 carbon atoms**, of which:

   - **264 atoms are bulk atoms**, each bonded to exactly three nearest neighbors, and
   - **24 atoms are edge atoms**, each bonded to exactly two nearest neighbors.

   Assume an sp^2-bonded hexagonal carbon network with no dangling bonds.

   Answer the following:

   - Calculate the total number of **unique bonds** in the CNT, ensuring that each bond is counted only once. Write the value in the answer sheet along with the logic involved in your calculation. **[5 marks]**

- Calculate the total number of **bond angles**, where a bond angle is defined as two bonds sharing a common central atom. Write the value in the answer sheet along with the logic involved in your calculation. **[5 marks]**
- Calculate the total number of **dihedral angles**, where a dihedral angle is defined by four atoms bonded sequentially $A-B-C-D$, with the bond $B-C$ acting as the central bond. Write the value in the answer sheet along with the logic involved in your calculation. **[5 marks]**
- Calculate the total number of **improper dihedral angles**, assuming that each atom bonded to exactly three neighbors defines one improper dihedral centered on that atom. Write the value in the answer sheet along with the logic involved in your calculation. **[5 marks]**

5. **Suppose you are using the Martini force-field, which employs a coarse-grained carbon-carbon interaction potential, where each particle represents four carbon atoms. Now, answer the following questions?**

   - Determine the appropriate bond length in a chain configuration between two martiny coarse-grained carbon particles, assuming the real carbon-carbon bond length is 1.2 Å in an sp^3 configuration.
     - **[2.5 marks]**
   - On the provided lattice (Fig. 1), indicate the positions of single Martini carbon particles by drawing circles. The circles should form a lattice that aligns perfectly with the real carbon lattice without leaving any voids or defects. **[2.5 marks]**

   Hint: Assume that each Martini carbon particle represents four real carbon atoms.

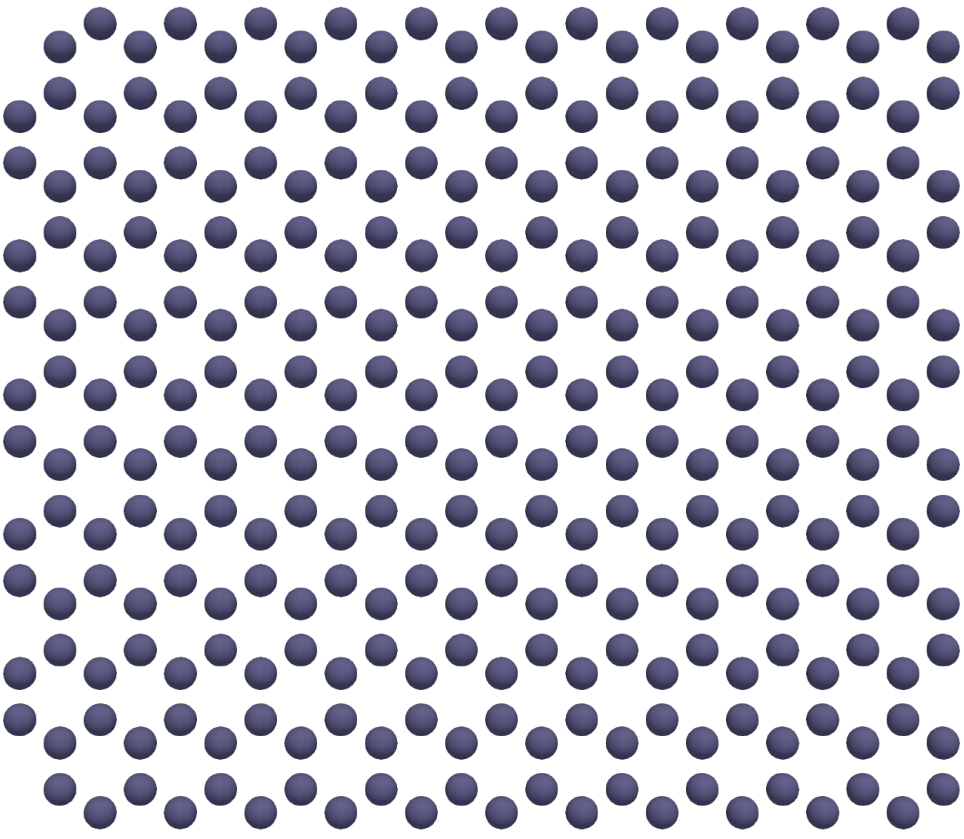

Figure 1: Graphene sheet.