HW 1

Homework Assignment 1
for the course FFR120/FIM750 in HT24

Instructions
HW1 consists of four exercises. For each exercise, the corresponding chapter is indicated.
Each exercise has a score of 2.5 points.
The maximum number of points for HW1 is 10.
The assessment of your solution of HW1 happens during the HW1 correction session on Wednesday, 13 November.

Remember to:
1. Register to the HW1 correction by Monday 11 November 23:59 *at the latest*. After that time, it won't be possible to get a slot for the HW1 correction.
2. Submit your solution for the HW1 to Canvas by Tuesday 12 November 23:59 *at the latest*. The solution must be in pdf format and should contain figures and code.

On correction day:
1. Arrive to the correction room about 10-20 minutes before your registered time slot.
2. Prepare the solution report ready on your computer, so the assessment can start without further delays.
3. Bring along a valid ID.

Chapter 01: Molecular Dynamics

Exercise 1. [Score: **2.5** pt] **Brownian disk with Lennard Jones potential**

Simulate a Brownian disk (see Fig. 1.8 in the book). Start with a single disk (radius R_{disk}, mass m_{disk}) and N_{part}^2 particles (point-like, mass m). The particles *do not mutually interact*. The interaction happens only among the disk and the particles through a Lennard-Jones potential (parameters: $\sigma = 1$, $\epsilon = 1$).
The system is enclosed in a squared box with reflecting boundaries. The size of the box is $L \times L$. Initially, the particles are positioned on a squared lattice. They have a velocity with random orientation and magnitude v. The disk start from the center of the box from rest (i.e., its velocity is 0). In the simulation, use the following parameters:

$$\begin{array}{ll} \text{Particles:} & m = 1, \quad v = 10, \quad N_{\text{part}} = 25, \\ \text{Disk:} & m_{\text{disk}} = 10, \quad R_{\text{disk}} = 10, \\ \text{Box:} & L = 260. \end{array}$$

Express the interaction force between disk (center position in $(X_{\text{disk}}, Y_{\text{disk}})$) and one of the particles (with position (x, y)) as follows:

$$F(r) = 24\frac{\epsilon}{r}\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \quad \text{with } r = \sqrt{(X_{\text{disk}} - x)^2 + (Y_{\text{disk}} - y)^2} - R_{\text{disk}}$$

Simulate for a duration of $T_{\text{tot}} = 400$ (expressed as dimensionless units of time for the Lennard-Jones system). Use a time step of $\Delta t = 0.005$.
Important! Before the simulation starts, remove the particles that are located inside the disk. Also, remove every particle that is closer that a distance of 3σ from the disk rim.

Provide a plot for:
P1 - the trajectory of the disk in the Cartesian plane.
P2 - the mean square displacement of the disk MSD as a function of time $t = n\Delta t$, calculated as:

$$\text{MSD}(n\Delta t) = \left\langle (X_{i+n} - X_i)^2 + (Y_{i+n} - Y_i)^2 \right\rangle = \frac{1}{N-n}\sum_{i=1}^{N-n}(Y_{i+n} - Y_i)^2 + (Y_{i+n} - Y_i)^2$$

where N is the number of time steps in the trajectory.

Calculate an estimate for:
Q1 - an estimate for the diffusion coefficient D, given that $\text{MSD}(\tau) = 4D\tau$. *[Hint: perform a fit of MSD versus τ]*

Chapter 02: Ising Model

Exercise 2. [Score: 2.5 pt] **Magnetic susceptibility of the 2-d Ising model**

Simulate the Ising model on an $N \times N$ squared lattice, as shown in class. Initialize the spins randomly with equal probability for being $+1$ or -1. At each step, pick randomly $5\% \sim 10\%$ of the spins in the lattice and update their state following the Monte Carlo method (see Chapter 2 of the book, page 2-4).
Simulate the system setting $N = 100$ (or larger if you can), $J = 1$, $k_\mathrm{B} = 1$. The magnetic field H and the temperature T are parameters that we will vary in the following exercises.
Moreover, remember that the magnetization, in the Ising model, is defined as:

$$m = \frac{1}{N^2} \sum_{i,j} \sigma_{i,j}.$$

Task 1. In this task we show that the 2D Ising model behaves like a paramagnetic material at temperatures T higher than its critical temperature (e.g., $T > T_\mathrm{c} \approx 2.269$).

Set $T = 5$. Calculate the total magnetization of the system as a function of H. We suggest you to use the following values for H:

$$H = -5,\ -2,\ -1,\ -0.5,\ -0.2,\ -0.1,\ 0,\ 0.1,\ 0.2,\ 0.5,\ 1,\ 2,\ 5.$$

Moreover, as the magnetization fluctuates in time around an average value due to T, we suggest to calculate the magnetization m as an average on the last $\approx$ 100-300 iterations.

Show that, for small values of H, the magnetization density of the system scales like $m = \chi H$, where χ is the *magnetic susceptibility*. To do this:
P1 - Plot $m(H)$.
Q1 - Calculate χ. *[Hint: perform a linear fit of m around $H = 0$]*

Task 2. In this exercise we aim at finding the critical temperature of the Ising model by monitoring the behavior of the absolute magnetization $|m|$ at $H = 0$ as a function of the temperature T. See reference figure in the book Fig. 2.5. *[Note: To obtain a figure like Fig. 2.5, you have to simulate for at least 10^5 steps for each value of the temperature, as explained in the book. In this task, we will use an alternative method that provides a good first estimate of the critical temperature with significantly less iterations.]*
Set the temperature T. We suggest you to use the following values for T:

$$T = 0.1,\ 0.2,\ 0.5,\ 1,\ 2,\ 2.1,\ 2.2,\ 2.3,\ 2.4,\ 2.5,\ 2.6,\ 2.7,\ 2.8,\ 2.9,\ 3,\ 5.$$

For each value of the temperature, start from a random state and perform 5000 iterations.
For the first 300 iterations, set $H = 0.1$.
For the remaining iterations, set $H = 0$.
After reaching the last iteration for a given T, calculate the total magnetization of the system $m(T)$.
P2 - Plot $m(T)$.
Q2 - Estimate T_c from your graph. Explain your reasoning. Compare with the theoretical value $T = 2.269...$ predicted by Onsager.

Chapter 03: Forest Fires

Exercise 3. [Score: 2.5 pt] **Exponent α for a forest fire model and extrapolation to $N = \infty$**

In this exercise, we will try to extrapolate the exponent α in the case of very large N, even beyond what we can simulate with our computational resources. Choose $p = 0.01$, $f = 0.2$. Make sure to simulate long enough to collect at least 300 fire events.

Set N equal to 16, 32, 64, 128, 256, 512, 1024. For each case, run a simulation and find the value of the exponent α. In order to reduce noise, repeat each case 10 times and take the average α. *[Note: if the case $N = 1024$ is too slow, do less repetitions]*.
Let us call these different numbers by α_{16}, α_{32}, and so on.
P1 - Plot the exponents α_N as a function of N^{-1}, as shown in Fig. 3.6 of the book.
Q1 - Extrapolate your results to $N^{-1} \to 0$ (i.e., $N \to \infty$). Explain the reason for your choice of the fitting function and provide your extrapolation for α_∞. Compare your plot and your fitting procedure with Figs. 3.6.
Q2 - How does the value estimated in the previous point relate to the estimate $\alpha = 1.15$ given in Ref. [15] in Chapter 3?

Chapter 04: The Game of Life

Exercise 4. [Score: **2.5** pt] **The Game of Life**

Simulate the game of life on a lattice $N \times N$, as shown in class. Start from a random configuration. Use periodic boundary conditions. Set $N = 100$ or larger. In each run, let the system evolve for at least $T = 300$ time steps. Perform at least 5 runs starting from different random configurations.

Task 1: For each run, record the number of live cells A as a function of the time step t.
P1 - Plot $A(t)$ for the different runs.
Q1 - What is the average density of alive cell per unit area for the game of life?
Q2 - After *approximately* how many iterations a *steady state* with average density is reached, from the initial random configuration?

Task 2: For each run, monitor the changes in the configuration of the game of life. After the initial transient has passed and the configuration is settle down around its average density, record, for each time step t, how many cells C change their state in the following time step (i.e., how many cells that were alive die and how many empty cells generate a new live cell.)
P2 - Plot $C(t)$ for the different runs.