HW 3

Homework Assignment 3
for the course FFR120/FIM750 in HT24

Instructions
HW3 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 HW3 is 10.
The assessment of your solution of HW3 happens during the HW3 correction session on Wednesday, 27 November 8-11:45 and Thursday, 28 November 8-11:45.

Remember to:
1. Register to the HW3 correction by Monday 25 November 23:59 *at the latest*. After that time, it won't be possible to get a slot for the HW3 correction.
2. Submit your solution for the HW3 to Canvas by Tuesday 26 November 23:59 *at the latest*. The solution must be in pdf format and should contain figures and code.

On correction day:
1. Arrive in front of the assessment 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 09: Living Crystals

Exercise 1. [Score: 2.5 pt] **Particles with phoretic interaction.**

In this exercise we have $N = 200$ active particles (radius $R = 1 \times 10^{-6}\,\mathrm{m}$) self-propelling with a speed $v = 5 \times 10^{-6}\,\mathrm{m/s}$ in a fluid with viscosity $\eta = 1 \times 10^{-3}\,\mathrm{Pa\,s}$.
Consider a squared arena with side $L = 100\,R$ and periodic boundary conditions.
The particles interact via a phoretic interaction with $v_0 = 20 \times 10^{-6}\,\mathrm{m/s}$. Use a cut-off radius for the interaction of $r_\mathrm{c} = 10\,R$. Avoid overlap between the particles with the volume exclusion method.

Address the following points:

Q1 - Decide the time step Δt for your simulation. When you choose it, what elements you have to consider? Does the value of the speed v, the radius R, or other parameters play a role in your decision? Write down your Δt.

P1 - Initialize the position of the particles at random. Set their initial direction at random. Plot the configuration at $t = 0\,\mathrm{s}$, $5\,\mathrm{s}$, $10\,\mathrm{s}$, $20\,\mathrm{s}$, $50\,\mathrm{s}$. You have to indicate the orientation of each particle in the plot.

Q2 - Describe the behavior of the system in **P1**.

P2 - Now set $L = 50\,R$ and re-run the simulation. Initialize the position of the particles at random. Set their initial direction at random. Plot the configuration at $t = 0\,\mathrm{s}$, $5\,\mathrm{s}$, $10\,\mathrm{s}$, $20\,\mathrm{s}$, $50\,\mathrm{s}$.

Q2 - Describe the behavior of the system in **P2**. Compare it with the system in **P1**.

Chapter 10: Sensory Delay

Exercise 2. [Score: 2.5 pt] **Ensemble of light-sensitive robots: clustering**

Simulate a system of $N = 50$ light-sensitive robots with $\tau = 1$, generating a Gaussian light-intensity profile zone of the form:

$$I(x, y) = I_0 \exp\left(-\frac{x^2 + y^2}{r_0^2}\right),$$

centered around the robot position. Take $I_0 = 1$ and $r_0 = 0.3$ for this exercise.
A robot senses the sum of the contributions of *all the other robots* but is not affected by the light intensity it generates. When a robot senses a light intensity I, it adjusts its speed to:

$$v(I) = v_\infty + (v_0 - v_\infty) \exp\left(-\frac{I}{I_\mathrm{c}}\right),$$

where $I_c = 0.1$, $v_\infty = 0.01$, $v_0 = 0.1$.
Take a squared arena with side $L = 30\,r_0$. Use periodic boundary conditions as shown in class.
When calculating the interaction between robots, set a cut-off radius $r_c = 4\,r_0$ to speed up the calculations.

P1 - Starting from a random initial configuration simulate the system with a *positive* delay of $\delta = 5\tau$. Let the system evolve for enough time (check that your simulation works as expected by looking at the animation). Suggested time step: $\Delta t = 0.05$. Plot the simulation at the following elapsed times:

$$t = 0\,\tau,\ 10\,\tau,\ 100\,\tau,\ 500\,\tau, 1000\,\tau$$

P2 - Repeat the simulation with a *negative* delay of $\delta = -5\tau$ starting from a random initial configuration. Plot the simulation at the following elapsed times:

$$t = 0\,\tau,\ 10\,\tau,\ 100\,\tau,\ 500\,\tau,$$

P3 - Write a function that, given a configuration of particles, returns the clusters of particles present in the configuration. Two particles are considered in the same cluster if they are either mutually closer than r_0 or closer than r_0 to a third particle that belongs to the same cluster of each of the particles separately. Mark the clusters in **P1** and **P2** for $t = 100\tau$ and $t = 500\tau$.

Q1 - Do you notice any difference for the two clustering in **P3**? Comment.

Chapter 11: Disease Spreading

Exercise 3. [Score: 2.5 pt] **SIR model with temporary immunity**

In this exercise, we will simulate the agent-based SIR model adding a probability α to become again susceptible for recovered agents. Use a total of $N = 1000$ agents. The arena is a square with side $L = 200$. Use periodic boundary conditions.
Simulate the system for $d = 0.95$, $\beta = 0.05$, $\gamma = 0.001$, $\alpha = 0.05$.

P1 - Starts with $I_0 = 30$ infected agents. Let the system evolve until either there are no more infected agents or for at least 50000 steps *(ideally, run the simulation over 100 thousands or more steps, if your computer allows it)*. Perform at least five different independent runs with the same I_0.
Plot the number of susceptible $S(t)$, infected $I(t)$, recovered $R(t)$ agents as a function of the time step t for each run.

Q1 - Comment on your plots: with the parameters as in **P1**, is the disease endemic or does it die out?

P2 - Starts with $I_0 = 10$ infected agents and $\alpha = 0.005$ this time. Proceed as in **P1**.

Q2 - Comment on your plots. In what the situation in **P2** differs from the situation in **P1**?

Chapter 12: Network models

Exercise 4. [Score: 2.5 pt] **Average path length and clustering coefficients of graphs.**

Consider an Erdős-Rényi random graph with n nodes and probability p. Consider the following values for the probability p:

$$p = 0.02,\ 0.03,\ 0.04,\ 0.05,\ 0.06,\ 0.07,\ 0.08,\ 0.09,\ 0.1,\ 0.2,\ 0.4,\ 0.5,\ 0.6,\ 0.7,\ 0.8,\ 0.9,\ 1$$

Task 1: For this task set $n = 100$. For each n and p, generate at least 3 different Erdős-Rényi random graphs. For each of them, calculate the average path length and clustering coefficients, as done in class.

P1 - Plot the average length (include error bars) as a function of p. Compare with the plot in Fig. 12.5a in the book. Plot on the same figure also the theoretical dependences:

$$L_{\mathrm{av},0} = \frac{\log(n) - \gamma}{\log[p(n-1)]} + \frac{1}{2}, \qquad \text{for small } p\ (p \ll 1)$$

where $\gamma = 0.57722$ is the Euler-Mascheroni constant; and

$$L_{\mathrm{av},1} = 2 - p, \qquad \text{for } p \text{ close to } 1\ (p \to 1)\ .$$

P2 - Plot the clustering coefficient (include error bars) as a function of p. Compare with the plot in Fig. 12.5b in the book.

Task 2: For this task set $n = 200$. Like in **Task 1**, for each n and p, generate at least 3 different Erdős-Rényi random graphs. For each of them, calculate the average path length and clustering coefficients.

P3 - Plot the average length (include error bars) as a function of p. Plot on the same figure also the theoretical dependences (see **P1**). Comment on your plots.

P4 - Plot the clustering coefficient (include error bars) as a function of p.

Q1 - Why is the clustering coefficient for Erdős-Rényi random graphs with parameter p simply equal to p? Explain.