

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 $R = 1 \times 10^{-6}$ m) self-propelling with a speed $v = 5 \times 10^{-6}$ m/s in a fluid with viscosity $\eta = 1 \times 10^{-3}$ Pa.s.

Consider a squared arena with side $L = 100 R$ and periodic boundary conditions.

The particles interact via a phoretic interaction with $v_0 = 20 \times 10^{-6}$ m/s. Use a cut-off radius for the interaction of $r_c = 10 R$. 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 $t = 0$ s, 5 s, 10 s, 20 s, 50 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 $t = 0$ s, 5 s, 10 s, 20 s, 50 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:

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

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:

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

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

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

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.