

BE/Aph 161: Physical Biology of the Cell, Winter 2025

Homework #8

Due at the start of lecture, 2:30 PM, March 5, 2025.

Problem 8.1 (The Vicsek model, 100 pts).

As we have discussed in lecture, the Vicsek model (Vicsek, et al., *PRL*, **75**, 1226–1229, 1995) was in many ways the start of the theory of active matter. The model consists of a collection of individual agents called “boids,” sometimes referred to as self-propelled particles (SPPs). Like Vicsek, we will consider boids on a two-dimensional plane. Consider a single boid i . At time point t , the boid moves with a velocity v_0 along a unit vector $\mathbf{u}_i(t + \tau) = (\cos \theta_i(t + \tau), \sin \theta_i(t + \tau))^T$. The vector $\mathbf{u}_i(t + \tau)$ is uniquely defined by the angle $\theta_i(t + \tau) \in (-\pi, \pi]$. The angle $\theta_i(t + \tau)$ is determined by averaging the value of $\theta_i(t)$ for every boid (including boid i itself) that is within a distance r from boid i , plus some added noise. This happens every time interval τ . Stated mathematically, the position \mathbf{x}_i of boid k evolves according to

$$\theta_i(t + \tau) = \arctan \left(\frac{\langle \sin \theta(t) \rangle_{r_i}}{\langle \cos \theta(t) \rangle_{r_i}} \right) + \eta \zeta_{i,t}, \quad (8.1)$$

$$\mathbf{u}_i(t + \tau) = \begin{pmatrix} \cos \theta_i(t + \tau) \\ \sin \theta_i(t + \tau) \end{pmatrix}, \quad (8.2)$$

$$\mathbf{x}_i(t + \tau) = \mathbf{x}_i(t) + v_0 \tau \mathbf{u}_i(t + \tau). \quad (8.3)$$

The $\eta \zeta_{i,t}$ term give the noise. Here, $\zeta_{i,t}$ is a random number drawn from a uniform distribution on the interval $[-\pi, \pi]$. As such, maximal noise is achieved when $\eta = 1$. The notation $\langle \cdot \rangle_{r_i}$ denotes an average over all boids within a distance r of boid i , including boid i .

The parameters for this system are the velocity v_0 , the interaction radius r , the noise strength η , the time between reorientations τ , the total size of the system L (we assume an $L \times L$ 2D surface), and the density of boids, $\rho = N/L^2$, where N is the number of boids. We can choose our spatial units to be such that $r = 1$ and our time units such that $\tau = 1$. We are then left with parameters v_0 , η , ρ , and L . Note that if we are trying to avoid finite size effects, we take L to be large, leaving only v_0 , η , and ρ as parameters.

Throughout this problem, we will consider $r = 1$ and $\tau = 1$. Like Vicsek, we will set $v_0 = 0.03$, but you are welcome to play with that parameter if you want to explore further. We will primarily be considering different values of the noise η and of the density ρ of boids. We use **periodic boundary conditions**. This means that if a boid moves rightward from position $x = L$, it will move to a position near $x = 0$, and similarly in the y -direction. It also means that a boid at position $x = L$ can have neighbors near position $x = 0$. Periodic boundary conditions are employed in an effort to mitigate boundary effects.

We will leave N fixed and vary L to adjust the density. You should use a minimum value of $N = 100$, but you should use larger N if your code is fast enough to handle it. I found that $N = 4000$ worked well, and I could do all calculations of this homework in several hours.

You may use AI tools to complete parts (b) and (c) under the following conditions.

- You clearly indicate which AI tool(s) you use.
- You clearly delineate what is your own, what comes directly from AI, and what came from AI but was then edited by you.
- You include all prompts you gave.

a) The expression

$$\arctan \left(\frac{\langle \sin \theta(t) \rangle_{r_i}}{\langle \cos \theta(t) \rangle_{r_i}} \right) \quad (8.4)$$

in equation (8.1) is meant to compute the average of the orientations of the neighboring boids. Why are we computing it this way instead of simply averaging all of the neighboring θ values directly?

- b) Write code to simulate the Viscek model. You should have a function that takes as input N , η , v_0 , and L , as well as any other inputs you see fit (e.g., obviously the number of steps you want to run the simulation should be an input), and returns the x , y , and θ values over time for all of the boids.
- c) Run a few simulations for various interesting values of ρ and η and make graphical displays (either plots, movies, or interactive plots) of the dynamics.
- d) We can define a vectorial **order parameter**

$$\varphi(t) = \frac{1}{N} \sum_{i=1}^N \mathbf{u}_i(t). \quad (8.5)$$

This is the average orientation of the boids at time t . We often consider its magnitude, $\varphi(t) = |\varphi(t)|$. Finally, we define ϕ as the long-time average of $\varphi(t)$. That is, we compute ϕ by averaging $\varphi(t)$ over all time points beyond some time point after which the dynamics do not qualitatively change. Plot $\varphi(t)$ for the simulations you visualized in part (d). Looking at these plots should help you know roughly at what time point you should start averaging for calculation of ϕ .

- e) For a density of $\rho = 4$, compute and plot ϕ for values of η ranging from zero to one. Do you see a transition from disorder to order as the noise decreases? *Hint:* So you do not have to redo calculations, read part (g) before doing the calculations of parts (e) and (f). That is, be sure to store your trajectories!

- f) For $\eta = 1/3$, compute and plot ϕ for ρ values ranging from 0.1 to 10. Do you see a transition from disorder to order as the density increases?
- g) Thermodynamic phase transitions occur when the variance of an order parameter (related to a susceptibility) diverges. Plot the variance of the order parameter ϕ versus η using your results from part (e) and versus ρ using your results from part (f). Do you see transitions? (Note that the variance will not formally diverge due to finite size effects.) Is this a thermodynamic transition? Why or why not?