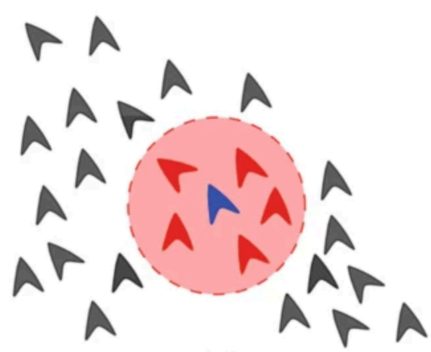
Take Home Assignment - Particle Interactions

Please accompany your solution with a succinct report (1-2 pages) detailing your approach, motivations, trade-offs, insights and any challenges you confronted.

Consider N particles in a 2D square box of side length L and periodic boundary conditions. Each particle is described by its position $\mathbf{r}_i(t)$ and orientation $\Theta_i(t)$ at time t.



At each discrete time step of size Δt, the system evolves according the following equations:

$$\Theta_i(t+\Delta t) = \arg\left(\frac{1}{|s_i(t)|}\sum_{j\in s_i(t)} v e^{i\Theta_j(t)} + \eta\, e^{i\xi_n(t)}\right) \tag{1}$$

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + v\Delta t \begin{pmatrix}\cos\Theta_i(t)\\ \sin\Theta_i(t)\end{pmatrix} \tag{2}$$

where $s_i(t) = \{j : |\,\mathbf{r}_i(t) - \mathbf{r}_j(t)\,| < R\}$ denotes the set of all neighboring particles within a distance R from the i-th particle, and v is the constant speed of all particles. Essentially, it means the orientation of the i-th particle at the next time step is determined as the average orientation of its neighborhoods, adjusted by the noise.

The noise term is parameterized by its intensity $0 \leq \eta \leq 1$ and phase $\xi_n(t)$, a random variable uniformly distributed over $[-\pi, \pi]$.

Problem 1

Assuming the following set of parameters

$$N = 125,\ L = 5,\ R = 1,\ v = 1,\ \Delta t = 0.25$$

and a random initial condition for the individual particles, simulate the evolution of the particles over a reasonable time period and discuss the dynamics for

- A small noise η value,
- A large noise η value.

Problem 2

The polarization of particles can serve as an instantaneous order parameter of the system.

$$P(t) = \frac{1}{Nv} \left| \sum_{i=1}^{N} v e^{i\Theta_i(t)} \right|$$

After a relaxation time, the transient behavior fades away, and the system reaches a stationary state. Compute the stationary order parameter, defined as the temporal average of $P(t)$,

$$\psi = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt\, P(t)$$

Plot the order parameter ψ as a function of η and confirm that the system exhibits a first-order phase transition.

Problem 3

Note that the order parameter ψ is implicitly dependent on the radius R of particle interaction and the speed v. Optimize R and v so that the critical value of the noise intensity η that the phase transition occurs is $\eta_c = 0.5$.