Chapter 1

Analysis of Structure and Dynamics

Simulations of ABPs ensembles offer an interesting possibility: they make it possible to investigate the physical systems without the limitations that an experimental setup would have. In simulations it is possible to work in a case with the same number of agents every time, keeping the physical conditions fixed, without all non-idealities, having computational power and time as the only limitation. This is crucial to study statistical properties of a system that displays fascinating behaviors.

1.1 Methods

Our investigation in structure and dynamics is based upon a small, but hopefully complete, set of tools that help unveiling how particles place themselves with respect to one another and how do they move insert citation about 1994 Nobel, "where atoms are, what atoms do".

1.1.1 Pair Correlation Function

Pair correlation function, *radial distribution function*, or simply $g(r)$ is a statistical mechanic property of a system, which is a function only of the separation $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ between any pair of particles. It quantifies how particle in an ensemble position one with respect to each other, giving information about the *structure* of the system. This function plays a key role in physics of matter since it is possible to measure it in radiation-scattering experiments and it is often used in cases where, differently from our problem, particles' positions are not directly accessible.

It is possible to derive definitions for $g(r)$ starting from first principles, like phase-space distribution functions, as it is done in [**hansen90a**]. Here we will use the Dirac's δ-based expression, since it the most useful in cases where particle's positions are known,

$$\left\langle \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N}{}' \delta(\mathbf{r} - \mathbf{r}_j + \mathbf{r}_i) \right\rangle = \rho g(r) \tag{1.1}$$

where the prime on the summation sign means not counting terms with $i = j$. It is possible to show that the left hand side approaches the value of the overall number density ρ at large distance.

In order to compute $g(r)$ in our simulations, we first need to take distances between all pairs of particles (counting twice the same couple) accounting for periodic boundary conditions as any particle became the center of the system, similarly to the periodic interaction method in section **??**. Then, to simulate the behavior of a sum of deltas, we divide simulation space in bins by radius, where the area of each bin is computed as the intersection between a circular crown and a square, to respect the geometry of our simulation box without introducing biases. Now we just normalize by the number of particles and the density to make $g(r) \to 1$ at long distance.

1.1.2 Polarization

Whenever the agents of a system have a preferred axis, as is the case for ABPs, it becomes worthwhile to analyze their nematic order, i.e. the order in the orientation degree of freedom of agents. This is useful especially when particles have non symmetric (in some axis) shape. Our particles are assumed to be perfectly symmetrical circles (spheres in 3D), but still, the presence of a well defined swimming direction introduces a relevant anisotropy in the system.

For global polarization, we use the following definition

$$P = \frac{1}{N}\left|\sum_{k=1}^{N} e^{i\theta_k(t)}\right| \tag{1.2}$$

where θ_k is the orientation of k-th particle. This parameter is 1 when all particles directions are aligned and 0 when all particles are pointing in different directions.

1.1.3 Local Polarization

1.1.4 Cluster Size Distribution