

Density Induced Milling in Two-Dimensional Self-Propelled Particles

Chengyi Long

Department of Civil and Environmental Engineering, MIT
77 Massachusetts Av., Cambridge, MA 02139, USA

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In this project, we use agent-based simulations to study the collective milling behavior of self-propelled particles in two dimensions. The milling behavior is measured using an order parameter from local angular moment and observed in a Vicsek-like model with confined circular boundary and non-additive velocity alignment. By tuning the mean particle density ρ , we observe qualitatively different behaviors in the time series of the milling order parameter, which suggests such emergence of milling might be tightly related to the density level of the system.

I. VICSEK MODEL, NON-EQUILIBRIUM PHASE TRANSITION

There has been a long history of understanding the functioning of living objects through lens of physics and mechanics. This type of work in biophysics and biomechanics can be seen as *induction* toward specific biological systems. Conversely, *deduction* through bio-inspired physics expects to capture universality across different systems, and this is naturally done by the mind-set of statistical physics.

The study of self-propelled particles (SPPs) in physics is of the second type. It is motivated by the study of motion in bacteria, swarming of insects, flocking of birds and schooling of fishes. Among numerous biotic categories, these systems can be seen as formed by *active* particles that are alive, acquire power themselves, interact through individual cognition or information pathways.

The seminal Vicsek model [1] consider a set of SPPs with constant velocity v and changing moving directions θ_i . Hence the velocity of particles is $\mathbf{v}_i = v\mathbf{e}_{\theta_i}$. The interactions of particles only influence their moving directions, which evolve in a velocity-velocity *aligning* mechanism

$$\theta(t+1) = \langle \theta(t) \rangle_r + \Delta\theta \quad (1)$$

Regarding the similarity of this mechanism and the spin-spin alignment, it is natural to think if the system can attain an ordered state. Specifically, as a two dimensional system, Mermin-Wagner Theorem would predict no spontaneous symmetry breaking in $d = 2$ equilibrium system with continuous symmetry [2]. However, the Vicsek model can have a kinetic phase transition that break the rotational symmetry, leading to a polarized flocking direction. The order parameter here is the average velocity

$$v_a = \frac{1}{Nv} \left| \sum_{i=1}^N \mathbf{v}_i \right| \quad (2)$$

which is also referred to as P in other literature. In practice, the updating rules in Vicsek model are easy to implement numerically and they have reported the anticipated phase transition.

Aside from the agent-based Vicsek model, it is also possible to coarse-grain the system which, in a continuum limit, gives hydrodynamic field theory. In a closely related work by Toner and Tu [3], it chooses the velocity and density field for macro-scale description that satisfies

$$\begin{aligned} \partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = & \alpha \mathbf{v} - \beta |\mathbf{v}|^2 \mathbf{v} - \nabla p + D_L \nabla (\nabla \cdot \mathbf{v}) \\ & + D_1 \nabla^2 \mathbf{v} + D_2 (\mathbf{v} \cdot \nabla)^2 \mathbf{v} + \mathbf{f} \\ \frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{v} \rho) = & 0 \end{aligned} \quad (3)$$

where pressure $p = p(\rho)$ can be expanded, and \mathbf{f} is the noise term. It can be derived from this equation that fluctuations perpendicular to the spontaneously chosen direction $\langle |\mathbf{v}_\perp(\mathbf{r}, t)|^2 \rangle = \text{const.} - L_\perp^{2\chi} g(\frac{L_\parallel}{L_\perp^\xi})$, where $\chi = -\frac{1}{5}$ and $\xi = \frac{3}{5}$ are the scaling exponent of \mathbf{v}_\perp and \mathbf{x}_\perp in $d = 2$, respectively. Therefore, fluctuations will decay and stay finite as the perpendicular size L_\perp grows.

II. MILLING BEHAVIORS

Here we have presented two classical types of methodology that established a whole research agenda on collective behaviors of SPPs. In fact, by allowing velocity to change, coupling to other fields, adjusting interaction rules or applying confined geometry and boundary conditions, it is possible to generate new phenomena that are qualitatively different from the universality class which Vicsek model represents. For example, there could be the so-called *milling* behaviors when altering the interaction potential to be distance dependent, speed-dependent or incorporating blind-cognitive regions, confined geometry [4–6].

The milling behavior can be qualitatively defined as the overall revolution of particles around a single reference point. It is the angular version of flocking in terms of its direction of symmetry breaking. Quantitatively, the order parameter for milling is often defined as

$$M = \frac{1}{N} \sum_{i=1}^N \frac{\mathbf{r}_i \times \mathbf{v}_i}{|\mathbf{r}_i \times \mathbf{v}_i|} \quad (4)$$

which can be seen as an angular counterpart of P from (2). Let $m = \sin(\theta_i - \alpha_i)$ denotes the local milling, where $\alpha_i = \arctan \frac{y_i}{x_i}$ is the direction of location for particle i . Considering $M = \frac{1}{N} \sum_{i=1}^N m$, this ensemble average $\langle M \rangle$ should change from zero to nonzero if there is any corresponding phase transition, signaling a phase transition.

In this project, we are focused on the simplest model that explicitly implements velocity alignment (1) through *non-additive* interactions

$$\dot{\theta}_i = \frac{1}{n_i} \sum_{j \in \Omega_i} \sin(\theta_j - \theta_i) + \sqrt{2D} \xi_i(t) \quad (5)$$

The alignment interaction is valid only for nearby particles Ω_i , which is usually defined as inside a sphere of radius R . However, the interaction is not additive from pair-wise interactions, since there is a term $n_i = \sum_{j \in \Omega_i} 1$ that takes the average effect of the $\sin(\cdot)$ alignment. The $\frac{1}{n_i}$ form makes a huge difference, as *without* such term,

$$\left\langle \sum_i \dot{\theta}_i \right\rangle = \left\langle \sum_i \sum_{j \in \Omega_i} \sin(\theta_j - \theta_i) + \sum_i \sqrt{2D} \xi_i(t) \right\rangle = 0 \quad (6)$$

and an effective momenta is conserved. On the other hand, adding $\frac{1}{n_i}$ loses such symmetric interactions and are called non-momenta-conserving (NMC). In Chepizhko et al. It is shown that with reflection boundary conditions and NMC interactions, milling can be induced for appropriate noise level [6].

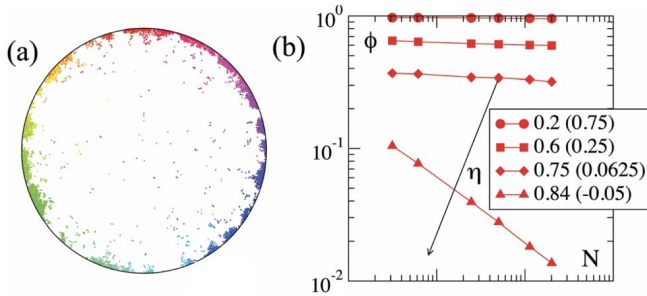


FIG. 1. Milling is induced from reflection B.C. and NMC interactions; Changing the size of the system, milling behaves at least a QLRO. Originally from Fig.4 of [6],

It is worthy noting that aside from agent-based simulations, there are also data-driven approach in researches like [7, 8] that analyze the experimental data directly and translate it into physical results as distribution of order parameter or phase diagram of different collective behaviors.

III. DENSITY EFFECT ON MILLING

In the study of milling behaviors (and other similar research of collective behaviors), much of the focus is

on the systematic parameters such as moving velocity v , coupling constant J and thermal fluctuation strength D . Since it is a nice picture in general that coupling constant J tends to align particles while noise proportional to $\sqrt{2D}$ leads to misalignment, all in contrast to the background moving mode characterized by v (when v goes to zero, the system is just a XY model; when v goes to infinity, the system is well mixed.)

However, less focus is on the parameter $\rho = N/A$, where N is the particle numbers and A the size confined or effective moving area. It is more natural to consider growing N alone, since the specific behavior of order parameter (P or M) on changing N is a manifestation of true or quasi long range order. Meanwhile, the are of particles are often circumvented by periodic boundary conditions. Though [6] made it clear that such geometric conditions are crucial to the emergence of milling.

Here we use simple simulations to demonstrate that the emergence of milling can be directly affected and controlled by the parameter $\rho = N/A$. The agent-based simulation is largely inspired by the Vicsek model, while using the NMC interaction and reflection boundary conditions in the form of (4).

The parameters of the model are set as follows. The Ω_i to be a 2D sphere with cutoff radius $r_{\text{off}} = 0.1$, giving a relatively small region of interaction compared to the total allowed region that has radius from $R = 1$ to $R = 4$. The velocity $v = 1$ that ensures a quick moving.

First of all, while keeping all the other parameters unchanged, we set 6 different parameter combinations for (N, R) in order to investigate the density effect. These 6 parameter combinations are chosen such that they have significant difference but their average densities are in 3 groups, allowing for possible comparisons. Each configuration is replicated for 6 trails, and each trail takes a period of $T_{\text{real}} = 100$ at an updating rate of $dt = 0.01$ per step.

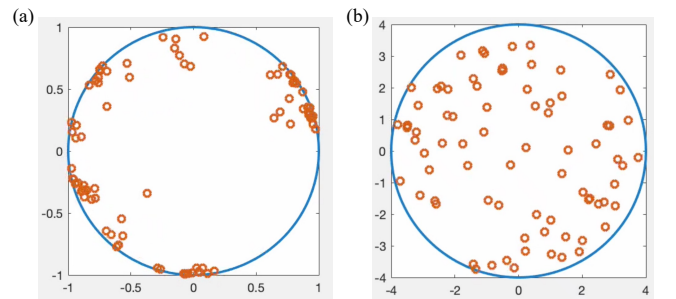


FIG. 2. Two snapshots when simulating $N = 80$. In panel (a), $R = 1$. The particles are already gathered around the geometric boundaries and start milling clock-wise at $T = 32$; In panel (b), $R = 4$. The particles fail to gather and there is no milling at $T = 74$.

For certain parameters chosen, we reproduced what has been shown in [6]. Two typical snapshots are shown in Fig.2. Importantly different from Fig.1(b), the emergence of milling is seen at the same N and the same η ,

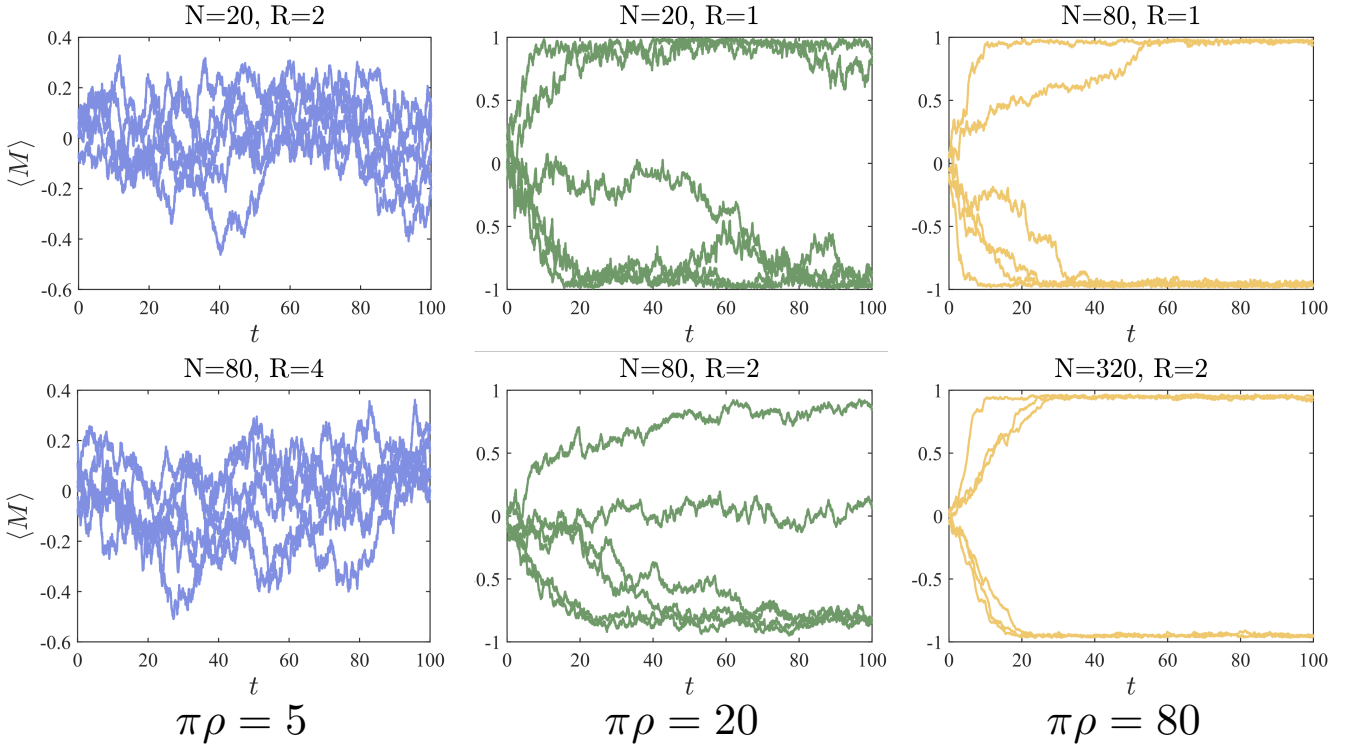


FIG. 3. Simulating the system with different particle size and radius and fixing other parameters. There is a clear trend of the system from disordered (first column in purple), then intermediate (second column in dark green) to milling/ordered (third column in yellow) demonstrated by $\langle M(t) \rangle$. Notice that the trend is highly related to the density level $\rho = \frac{N}{\pi R^2}$ instead of N or R alone.

while destroyed by decreasing density ρ .

We further confirm this density effect on the collective behaviors by looking at all time series of $\langle M \rangle$. The results, along with the parameters and density levels are shown in Fig.3.

The pattern that same particle numbers N (and other system parameters) can lead to different milling results in Fig.2 is again demonstrated here. Taking $N = 80$ as an example, when the radius of the sphere ranges from 1, 2 to 4, the time series shows a clear symmetry breaking of $\langle M \rangle$ tends to ± 1 quickly, gradual evolution toward ordered phase, to mixed $\langle M \rangle$ through out the simulation.

However, the variety of milling behaviors seem to be determined, at least in our range of simulation parameters, by the density level of particles. One can instantly recognize that the three qualitative categorizations of milling are repeated in different setup of particle numbers and geometric sizes, as long as they share the same density level.

One may concern that simulation in a short time range cannot reveal the whole dynamical behaviors of $\langle M \rangle$. Since phase transition could still happen if wait sufficiently long. We argue that the behaviors shown for $\pi\rho = 5$ is most likely disordered, with a much longer simulation of $T_{\text{real}} = 5000$ at $N = 20, R = 2$. We analyze the time series by its histogram shown in Fig.4. The red line here is the fitted Gaussian distribution with a

mean value of 0.01. Hence we claim the order parameter distributed here is a single peak Gaussian variable with mean zero, which is standard in the sense of a disordered state. Ideally, the Gaussian curve would sharpen with larger particle number N .

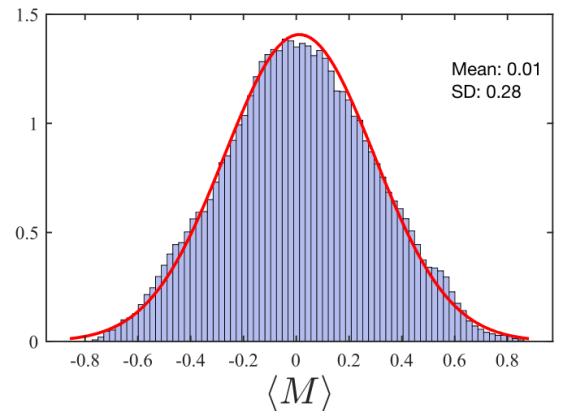


FIG. 4. Histogram of $\langle M(t) \rangle$ whose length $T_{\text{real}} = 5000$ is 50 times longer than that in shorter simulations. The histogram shows a clear Gaussian shape, and it fits well with a Normal distribution of $\mu = 0.01, \sigma = 0.28$.

At the same time, the simulation for $\pi\rho = 80$ is also

valid, since when the system reaches a milling state, it is actually a stable state that is hard to alter, so the yellow curves is expected to describe the behaviors of the system even in longer time. It is only the green curves that are hard to attribute whether ordered or disordered. Though it still shows a trend of being intermediate in terms of its mediate level of local fluctuations and unclear trends of $\langle M(t) \rangle$. But we cannot relate this to criticality without further evidence. After all, the precise estimation of the critical point and its critical exponent remains an open question that can be answered with proper theories or finer numerical simulations.

IV. CONCLUSIONS

In this project, we study the collective milling behavior of Self-propelled particles using agent-based numerical simulations. It is demonstrated that density level $\rho = \frac{N}{\pi R^2}$ above some critical value may induce the milling behavior. Thus more attention should be paid on the important parameter of ρ aside from the more often concerned ones such as η , v in order to fully understand the intriguing milling phenomena.

In our current simulation, the requirement of reflection boundary conditions is quite crucial for the emergence of milling, but it is also quite unrealistic. In experiments, milling can be observed without the requirements of such

confined geometry. There might be other mechanisms that help particles to aggregate instead of moving away from the center. And we anticipate the density dependent motility [9] could be a potential way to address such discrepancy. If the velocity v is not a constant, but depends on the local density $\rho(\mathbf{r})$ in a negative way like $v(\rho) = v_0 e^{-\lambda \rho} + v_1$, then particles could slow down at a high density region, and at the same time milling if the average density is above some threshold. This conjecture is consistent with our findings here, since milling can happen when the average density is sufficient. Theoretically, one might derive some hydrodynamics equation similar to eq(5) in [9], and eq(1) in [3] with the coarse-graining field of $W = \rho M(\mathbf{r})$ that would explain the phase transition of milling behavior.

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