Langevin Dynamic Simulation of self-propelled particles in two-dimensional systems

L. Amallah a, *, A. Hader a,c, R. Bakir a, H. Sbiaai a, I. Tarras a and Y. Bougahle b

a LBGIM, Ecole Normale Supérieure, University Hassan II, Casablanca, Morocco
b LPMC, University Chouaib Doukkali, El Jadida, Morocco
c Centre régional des métiers d’éducation et de formation Casablanca-Settat/établissement Settat, Morocco

* Corresponding author: layla.amallah-etu@etu.univh2c.ma
ORCID ID: 0000-0002-4536-9253

Abstract: Collective motion of self-propelled particles is one of basic phenomenon observed in large spectra of biological system behavior due to the correlated process evolution in space and time. In this manuscript, we study numerically the kinetic properties and the correlation process in complex systems evolves out equilibrium phase by employing the Langevin dynamics. In this model, we have adopted one zone of orientation where the system evolves spontaneously in presence of quenched stochastic noise. The results show that the system evolves to its equilibrium phase by reaching one orientation. Hence, this evolution is characterized by a correlation process increasing in time but with decelerate profile. However the obtained profile of the correlation function per time unity shows that the collective motion in complex system, can be characterized by a characteristic time when the system change the acceleration of the correlation process. Our result shows that this characteristic time decreases exponentially with the quenched noise. In the additional crossover time at when the system reaches its equilibrium phase, scales with quenched noise as power law. This result is more consisting with the one of Vicsek model

Keywords: Collective motion; Flocks; Self-propelled particles; Noise; Orientation zone; Langevin dynamics; Correlation process.

1. Introduction

Collective phenomena are ubiquitous in nature on many different scales, at any time and space such as: mammal herds [1], fish schools [2], bird flocks [3], insect swarms [4], bacterial colonies [5] and even motion of molecular [6], these biological systems have many similarities with the behaviors observed in the crowds of pedestrians [7]. The captivating characteristics of these organisms are their ability to align and move together in the same direction, in order to avoid collision with nearest neighbours or predators [8]. The omnipresence of these phenomena has attracted attention of biologists and physicists, for understanding the collective movements of these groups of animals [9]. Enormous studies [10-13] have been consecrated to study and analyze the dynamic properties of complex living systems [14], by using computational or simulation approaches, the aim of this study to explain how these groups of animals move together, align their motion with their neighbours, find food or escape
and disperse predators [15]. Therefore, the notion of self-propelled particles was used to pattern the collective motion of these biological phenomena [16]. Moreover, a major aspect in the study of these collective behaviors is that an individual’s behavior is influenced by the behavior of other members of the group [17]. This distinguishing between each individual and the group of individuals leads to important phenomena; like self-organization and emergence of the collective motion [9]. These complexes self-propelled systems have wide applications in our lives for example: the control of human interactions in crowded situations [17], or an artificial swarm of autonomous vehicles [18].

The several collective models have been developed for self-propelled particles, which depend on interactions between particles. Reynolds it was the first model proposed to describe the collective behavior of groups of animals; especially flocks, herds and schools [19]. A decade later, Vicsek et al introduced a minimalist model which describes the collective motion of self-propelled particles in tow-dimensional space, under the effect of noise [20]. In the Vicsek model or flock model the individuals (particles) move with constant velocity and at each time step the individuals align with the average orientation of their neighbours. The results showed that the dynamics of these systems in the presence of noise; is governed by a second-order phase transition from disordered to an ordered state [20]. Couzin et al model, also called three-zones model [21]. In this model all individuals have a specific area of motion direction, each zone has a specific rule: the first structural rule is that each individual must have a minimum distance in order to avoid collision with other neighbours, the second rule requires that individuals attract and orient themselves to avoid isolation, when all individuals were greater than the minimum separation, the third structural rule each individual moves with his neighbours in the same direction in order to maintain group cohesion [21]. These behavioral rules are used to reproduce the collective movement observed in nature of fish schools and bird flocks [2-3].

In this study, we propose a new pattern to study the collective behavior of these living systems, by using the Langevin dynamics; it is a computational approach to model the dynamics of complex systems. In our work we investigated the dynamic properties and correlation process of interacting self-propelled particle in two-dimensional systems; through the Langevin dynamic simulations, as a stochastic differential equation. Also, this dynamic has been used to simulate Brownian motion [22-23]. Our investigation involves noise \( \eta \), density of system \( \rho \) and orientation zone of radius \( R \) as control parameter, and velocity as order parameter to discuss the different kinetic properties and correlation process of the system studied. In order to confirm the validity of our pattern, the results show that the system velocity increases with time and reaches to finite value at the equilibrium phase, which describe the real behavior of these living systems in nature.

This paper is organized as follows. After, this introduction in the first part to the second section, in which we discuss our model based in the use of Langevin Dynamics. In the third section, we present and we discuss the results of our numerical simulations. In the last section, we summarize the main conclusion.

2. The Model

To better understand the collective behavior of complex systems, we investigate the dynamic proprieties and correlation process of interacting self-propelled particle in two-dimensional systems, by employing the Langevin dynamic simulations.

In our pattern, we consider a group of indiscernible particles distribute randomly in a two-dimensional space, with periodic boundary conditions. In which the density of system is given by \( \rho = \frac{N}{L^2} \). Let \( m_i \), \( \mathbf{x}_i \) and \( \mathbf{v}_i \) be respectively the mass, position and velocity of each particle \( i \). The collective motion of self-driven particles is described by the stochastic equation below, which is the Langevin dynamics:

\[
    m_i \frac{d\mathbf{v}_i}{dt} = -m_i \eta \mathbf{v}_i + \mathbf{F}_i(t) \tag{1}
\]

Where \( \eta \) represents the quenched noise is related to the random force \( \mathbf{F}_i(t) \) by the fluctuation-dissipation theorem according to:
\[
\langle F_i(t) \rangle = 0 \quad \text{and} \quad \langle F_i(t) F_i(t') \rangle = 2m\eta K_B T \delta(t-t') \tag{2}
\]

Where \( K_B \) is Boltzmann’s constant.

Initially, each particle (individual) move with some random perturbation \( \eta \) added in the motion of particles. The particle \( i \) seek to maintain a minimum distance from its local neighbors, in order to avoid collisions with the other individuals. However, the number of particles in orientation zone is given by \( N_R \) with \( i = 1, \ldots, N_R \) and \( j = \# \). At each time step \( t \), the particles adopt the average direction \( \theta_i(t) \), as is the mean of the \( N_R \) individual’s orientation in the orientation zone of radius \( R \):

\[
\theta_i(t) = \frac{1}{N_R} \sum_{j=1}^{N_R} \theta_j(t) \tag{3}
\]

With noise \( \eta \) affect the individual orientation \( \theta_i(t+1) \) at time \( t+1 \) as: \( \theta_i(t+1) = \theta_i(t) + \theta \) and \( \theta \) is chosen randomly from the interval \([\eta/2, \eta/2]\). Thus, to study the time evolution of the collective behavior of self-propelled particles in twodimensional system, in order to determine the kinetic proprieties and correlation process of the studied system, under effect of orientation zone for radius \( R \). We calculate the order parameter which is the normalized average velocity \( v_t \), giving by:

\[
v_t = \frac{1}{N_R} \left[ \sum_{j=1}^{N_R} v_j \right] \tag{4}
\]

The time evolution depending on the variation of control parameters namely: the density of system \( \rho \), the quenched noise \( \eta \) and the orientation zone for radius \( R \), we remark that the particle density \( \rho \) and the quenched noise \( \eta \) play an important role and their variations can affect significantly the collective behavior of the system.

## 3. Results and Discussions

In order to investigate the collective motion of \( N \) self-propelled particles in two-dimensional system, we consider square lattice of size \( L \times L \), on which we distribute randomly the above particles. Each particle \( i \) move with the same initial velocity \( v_0 \), with a random orientation \( \theta_0 \). The system evolves dynamically according to the above model. In our investigation, we adopted a cyclic boundary condition. At each time \( t \), we calculate the time evolution of the both velocity and direction \( \theta_i(t) \) by using the Langevin equation 1. However, the direction \( \theta_i(t) \) of the particle \( i \) is calculated by the mean of the orientation of all its neighboring ones within orientation zone of radius \( R \). In the additional, the system evolves in presence of different of quenched noise \( \eta \). The physical parameter, which describes the self-propelled dynamic of the used system, is the mean velocity system defined as \( v = \frac{1}{N_R} \sum_{j=1}^{N_R} v_j \).

In figure 1, we represent the time evolution of the mean velocity system for system density \( \rho = 0.3 \) and radius value \( \kappa = \frac{1}{2} \). The obtained profile shows that the system evolves with two different regimes separated by characteristic time \( t_c \). In the first regime where \( t < t_c \), the particles evolves with correlated and self-criticality process until reaching its equilibrium phase in the second regime when \( t > t_c \). Hence the obtained profile of the mean velocity system is well fitted by \( v_d(t) = v_f(1 - e^{-t/t_c}) \), where \( v_f \) is the phase equilibrium velocity. This result is more consisting with the Vicsek model [24]. Figure 2, represents an image system calculated for noise value \( \eta = 0.2 \) and at time \( t = 0.1 t_c \) where \( t_c \) is the time when the system reaches its phase equilibrium. This image proves that system evolves with clusters of different sizes separated by characteristic length \( \xi \), which exhibits a maximal value at crossover time, which scales with one of the equilibrium phase [25-26]. One of the characteristic parameter of the kinetic system, is the scale time \( t_c \). So, in order to determinate the effect of the quenched noise \( \eta \) on dynamic system, we plot in figure 3, the characteristic time \( t_c \) versus quenched noise. The results on log-log plot, shows that \( t_c \) scales with
quenched noise as power law: $v(t) = \eta^\beta$, where the exponent value is $\beta = 0.9$. Hence, the quenched noise has an effect to accelerate the phase equilibrium phase system. These results are more consisting with the ones obtained by the Vicsek model [24].

![Figure 1: Time evolution of the mean velocity system for fixed values of density and noise.](image1.png)

![Figure 2: Image system calculated at time $t/t_f = 0.14$ for fixed values of density and noise.](image2.png)
Figure 3: Log-Log plot of the characteristic time $t_c$ versus quenched noise $\eta$.

In reality the systems increases its mean velocity in the out equilibrium phase but with decreasing its mean acceleration $a = \frac{dy}{dt}$. In the figure 4, we represent the time evolution of the mean acceleration system for different values of quenched noise. So, for higher quenched noise value, the system reaches very wickedly its equilibrium phase. In the out equilibrium, phase the mean acceleration system decreases exponentially with the quenched noise $\eta$. 

```
$\rho=0.5$
$R=5$
```
Correlation motion is the basic phenomenon in all biological system [27-30] as an alternative for selection. The idea is to represent available objects by motion in the system, have users identify a target by mimicking its specific motion. The resulting interaction has compelling properties, as users are guided by oriented motion. To quantify the correlation process in the collective motion, we investigated the correlation function of the mean velocity system $v_x$ defined as:

$$G(t) = \langle v_x(t)v_x(t+\tau) \rangle_t$$

Corresponding results calculated for system density $\rho = 0.5$ and for two different values of quenched noise are presented in the figure 5. The results show that particles evolve to its equilibrium phase with increasing correlation process due by reaching homogenate orientation. However, in the earlier time, the correlation process is more accelerated, but after crosser over time $t_e$ corresponding to inflexion point, the acceleration of the correlation process decreases until reaching zero value in the phase equilibrium. To highly this result, we plotted in figure 6 the derivate of the correlation function $\frac{dG}{dt}$ versus time. In reality, the obtained profile of $\frac{dG}{dt}$ is well fitted by Gaussian function, which is characterized by point inflexion at cross over time according to results of figure 5. Hence, at the phase equilibrium system $\frac{dG}{dt} = 0$. 

![Figure 4: the time evolution of the acceleration system for different values of quenched noise.](image_url)
Figure 5: The time correlation function system for fixed noise value.

Figure 6: The correlation functions per time unity versus time for different quenched values.
To check the effect of the quenched noise on the cross over time $t_c$, we plot in figure 7, $t_c$ versus noise $\eta$. As, we observe, the characteristic time of the correlation function $G$ decreases exponentially with quenched noise. So, for higher quenched noise value, the correlated motion time of system decreases and the system reach very quickly its phase equilibrium. This result is more consisting with the one of [25].

![Figure7: The characteristic time $t_c$ versus quenched noise $\eta$.](image)

4. Conclusion

In summary, we simulate the dynamical properties and the correlation process of self-propelled particles in two-dimensional systems, by employing the Langevin model. However, we have considered $N$ particles evolving from out equilibrium phase to its equilibrium one by reaching a homogenate orientation according to a specific correlation process. In the additional, we have adopted a single orientation zone in which the particles assume a mean orientation direction and we have modeling the interaction process by quenched noise. Our results show the mean velocity system increases exponentially with time until reaching a static velocity in the equilibrium phase after characteristic time, which scales as a power law with quenched noise. Moreover, the collection motion of the considered system is characterized by correlation process, which changes the acceleration at crossover time decreasing exponentially with quenched noise. Moreover, obtained results with Langevin model are more consisting with the ones obtained by Vicsek model.
References

[1] J. K. Parrish, W. M. Hamner, Animal Groups in Three Dimensions. Cambridge University Press (1997).
[2] Katz Y et al. Inferring the structure and dynamics of interactions in schooling fish. Proc. Natl Acad. Sci. USA . (2011).
[3] Attanasi A et al. Information Transfer and Behavioural Inertia in Starling Flocks. Nat. Phys. (2014).
[4] A. C. Mailleux, J.-L. Deneubourg, C. Detrain, Animal behaviour 59 (2000).
[5] M.P. Brenner, L.S. Levitov, E.O. Budrene. Physical mechanisms for chemotactic pattern formation by bacteria. Biophysical Journal 74 (1998).
[6] M. Badoual, F. Julicher, J. Prost. Bidirectional cooperative motion of molecular motors. Proceedings of the National Academy of Sciences of the United States of America 99 (2002) 6696.
[7] D. Helbing, I. Farkas, T. Vicsek. Simulating dynamical features of escape panic. Nature (2000).
[8] C. K. Hemelrijk, H. Kunz, Behavioral Ecology 16 (2005).
[9] Vicsek T and Zafeiris A. Phys. Rep. 517 71 (2012).
[10] I. Tarras, N. Moussa, M. Mazroui, Y. Bouhahleb, A. Hajjaji. Modern Physics Letters B (2013).
[11] T. Iliass, D. Cambui, International Journal of Modern Physics B 30 (2016) 1650002.
[12] I. Tarras, N. Moussa, M. Mazroui, Y. Bouhahleb, International Journal of Computer Applications 46 (2012).
[13] R. Bakir, I. Tarras, L. Amallah, H. Sbiaa, A. Hader, M. Mazroui, Y. Bouhahleb, Chin. J. Phys. (2017).
[14] E. Ben-Jacob, I. Cohen, H. Levine. Cooperative self-organization of microorganisms. Advances in Physics 49 (2000).
[15] L.L. Bajec and F.H. Heppner. Organized flight in birds. Animal Behaviour (2009).
[16] Couzin I. D. Collective cognition in animal groups, Trends in Cognitive Sciences (2009).
[17] T. Vicsek and A. Zafeiris. Collective motion. Physics Reports (2012).
[18] Martinez S, Cortes J and Bullo F. IEEE Contr. Syst. Mag. (2007).
[19] C. W. Reynolds. Flocks, herds and schools: A distributed behavioural model. Computer Graphics (1987).
[20] Vicsek. T. A. Czirok, E. Ben-Jacob, I. Cohen, and O. Shochet, Novel type of phase transition in a system of self-driven particles, Phy.Rev. Let (1995).
[21] Iain D Couzin, Jens Krause, Richard James, Graeme D Ruxton, and Nigel R Franks. Collective memory and spatial sorting in animal groups. Journal of theoretical biology (2002).
[22] M. Mazroui, A. Asakli, Y. Bouhahleb. Conductivity of two-dimensional systems of interacting Brownian particles within the effective potential description. Surface Science (1998).
[23] M. Mazroui, Y. Bouhahleb. Surface Diffusion in Systems of Interacting Brownian Particles. International Journal of Modern Physics B (2001).
[24] A. Czirok, H. E. Stanley and T. Vicsek, J. Phys. A: Gen. (1997).
[25] L. Amallah, A. Hader, R. Bakir, I. Achik, H. Sbiaa, I. Tarras, and Y. Bouhaleb, Sensor Letters. (2018).
[26] L. Amallah, A. Hader, M. Tanasehte, Y. Hariti, H. Sbiaa, Y. Bouhaleb. Kinetic and scaling behavior of collective motion in biomaterials. Materials Today: Proceedings (2020).
[27] I. D. Couzin, J. Krause, N. R. Franks and A. S. Levin, Nature (2005).
[28] H. Chate, F. Ginelli, G. Gregoire, F. Peruani and F. Raynaud, Eur. Phys. J. B (2008).
[29] J. Krause and G. D. Ruxton, Living in Groups. Oxford University Press (2002).
[30] I. D. Couzin and J. Krause, Adv. Stud. Behav. (2003).