CHIMIE PARIS – PROJETS NUMÉRIQUES

Mouvements collectifs

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A différentes échelles de taille, on observe des mouvements collectifs dans les systèmes vivants : moteurs moléculaires, biofilms de bactéries, bancs de poissons, nuées d'oiseaux... Les ingrédients essentiels permettant l'émergence de tels mouvements coopératifs sont l'autopropulsion de chacun des agents constituant le système et les interactions entre les agents, qui les poussent à progressivement s'aligner les uns avec les autres. Le modèle de Vicsek, introduit en 1995, est un modèle central de la "matière active" – une branche de la physique hors-équilibre qui s'intéresse notamment aux mouvements collectifs. L'objectif de ce projet est, en partant du papier original de Vicsek et al. *[Phys. Rev. Lett. 75, 1226 (1995)], de simuler l'émergence de mouvements collectifs dans un système de spins en interaction, qui se déplacent avec une vitesse de propulsion fixée, et qui interagissent avec leurs voisins avec des paramètres variables.*

1 Modèle et implémentation

On réalisera les simulations telles que décrites dans l'article de Vicsek *et al*. On considère une boîte carrée à deux dimensions de taille L avec des conditions aux limites périodiques. A chacune des N particules on associe une position $\boldsymbol{x}_i$ et une vitesse $\mathbf{v}_i$, d'amplitude v et orientée dans une direction θ_i mesurée à partir d'un axe de référence. La condition initiale est la suivante : les N particules sont placées au hasard dans la boîte, et les orientations de leurs vitesses sont choisies aléatoirement dans l'intervalle $[0, 2\pi[$. A chaque pas de temps ($\Delta t = 1$), la position de chaque particule est mise à jour suivant :

$$\boldsymbol{x}_i(t+1) = \boldsymbol{x}_i(t) + \mathbf{v}_i(t)\Delta t. \tag{1}$$

La vitesse à l'instant $t+1$ a une amplitude v et un angle $\theta(t+1)$, déterminé grâce à la relation

$$\theta_i(t+1) = \langle\theta(t)\rangle_{i,r} + \Delta\theta, \tag{2}$$

où $\langle\theta(t)\rangle_{i,r}$ désigne la moyenne des directions des particules (i incluse) contenues dans un cercle de rayon r et centré sur i. La direction moyenne est donc donnée par l'angle $\arctan[\langle\sin\theta(t)\rangle_r / \langle\cos\theta(t)\rangle_r]$. $\Delta\theta$ est un nombre aléatoire choisi avec une distribution uniforme dans l'intervalle $[-\eta/2, \eta/2]$. Ce terme représente donc un bruit, c'est-à-dire l'effet de l'agitation thermique sur le système.

2 Observations

1. **Phénoménologie.** On pourra commencer par reproduire la phénoménologie du système. Générer quelques trajectoires pour des paramètres où le système reste désordonné, et pour des paramètres où on observe des mouvements collectifs. Ecrire un script python qui permet de visualiser des configurations du système.
2. **Paramètre d'ordre.** On définit le paramètre d'ordre $v_a(t) = \frac{1}{N}\left|\sum_{i=1}^{N} \frac{\mathbf{v}_i(t)}{v}\right|$. Mesurer $\lim_{t\to\infty} v_a(t)$ dans l'état stationnaire et tracer cette quantité en fonction de η pour une densité ρ fixée, et en fonction de ρ pour un bruit η fixé. Qu'observe-t-on ?

Novel Type of Phase Transition in a System of Self-Driven Particles

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A simple model with a novel type of dynamics is introduced in order to investigate the emergence of self-ordered motion in systems of particles with biologically motivated interaction. In our model particles are driven with a constant absolute velocity and at each time step assume the average direction of motion of the particles in their neighborhood with some random perturbation (η) added. We present numerical evidence that this model results in a kinetic phase transition from no transport (zero average velocity, $|\mathbf{v}_a| = 0$) to finite net transport through spontaneous symmetry breaking of the rotational symmetry. The transition is continuous, since $|\mathbf{v}_a|$ is found to scale as $(\eta_c - \eta)^\beta$ with $\beta \simeq 0.45$.

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One of the most interesting aspects of many particle systems is that they exhibit a complex cooperative behavior during phase transition [1]. This remarkable feature of equilibrium systems has been studied in great detail for the last couple of decades leading to a deeper understanding of processes which may take place in an assembly of interacting particles. Concepts like scaling, universality, and renormalization have resulted in a systematic picture of a wide range of systems in physics [1,2].

Recently, there has been an increasing interest in the rich behavior of systems which are far from equilibrium. Processes such as aggregation, viscous flows, or biological pattern formation have been shown to involve scaling of the related geometrical and dynamic quantities characterizing these phenomena [3,4]. As a further similarity with equilibrium systems, the existence of phase transition type behavior has also been demonstrated in several investigations of growth processes [5–8]. These analogies with the basic features of equilibrium systems have represented a particularly important contribution to the understanding of the complex behavior of nonequilibrium processes.

In this work we introduce a model with a novel type of dynamics in order to investigate clustering, transport, and phase transition in nonequilibrium systems where the *velocity* of the particles is determined by a simple rule and random fluctuations. The only rule of the model is *at each time step a given particle driven with a constant absolute velocity assumes the average direction of motion of the particles in its neighborhood of radius r with some random perturbation added.* We show using simulations that, in spite of its simplicity, this model results in a rich, realistic dynamics, including a kinetic phase transition from no transport to finite net transport through spontaneous symmetry breaking of the rotational symmetry.

In this sense our model is a transport related, nonequilibrium analog of the ferromagnetic type of models, with the important difference that it is inherently dynamic: The elementary event is the motion of a particle between two time steps. Thus the analogy can be formulated as follows: The rule corresponding to the ferromagnetic interaction tending to align the spins in the same direction, in the case of equilibrium models, is replaced by the rule of aligning the *direction of motion* of particles in our model of cooperative motion. The level of random perturbations we apply are in analogy with the temperature.

Beyond the above aspects, the proposed model is interesting because of possible applications in a wide range of biological systems involving clustering and migration. Biological subjects have the tendency to move as other subjects do in their neighborhood [9]. In addition to such trivial examples as schools of fish, herds of quadrupeds, or flocks of flying birds, our model can be applied to the less known phenomena during bacterial colony growth [10]. There are bacteria (e.g., a strain of *Bacillus Subtilis*) which exhibit cooperative motion in order to survive under unfavorable conditions. The present model, with some modifications, is already capable of reproducing the main observed features of the motion (collective rotation and flocking) of bacteria [10]. Other biologically motivated, recent theoretical investigations of clustering, aggregation, and orientational order in systems with diffusing directed objects have concentrated on the possible spatial patterns arising from an integro-differential equation approach and from cellular automata type models [11].

Furthermore, we expect that our model can be used to interpret the results of experiments on clustering and convection in a system of disks floating on air table [12]. These experiments represent a physically motivated possible application of the present model, since they are being carried out in order to understand the flow of granular materials under specific conditions. We are aware that two groups are working on developing models similar to ours in order to interpret these air table experiments [13].

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The actual simulations were carried out in a square shaped cell of linear size L with periodic boundary conditions. The particles were represented by points moving continuously (off lattice) on the plane. We used the interaction radius r as the unit to measure distances ($r = 1$), while the time unit $\Delta t = 1$ was the time interval between two updatings of the directions and positions. In most of our simulations we used the simplest initial conditions: (i) at time $t = 0$, N particles were randomly distributed in the cell and (ii) had the same absolute velocity v and (iii) randomly distributed directions θ. the velocities $\{\mathbf{v}_i\}$ of the particles were determined simultaneously at each time step, and the position of the ith particle updated according to

$$\mathbf{x}_i(t + 1) = \mathbf{x}_i(t) + \mathbf{v}_i(t)\Delta t . \quad (1)$$

Here the velocity of a particle $\mathbf{v}_i(t + 1)$ was constructed to have an absolute value v and a direction given by the angle $\theta(t + 1)$. This angle was obtained from the expression

$$\theta(t + 1) = \langle\theta(t)\rangle_r + \Delta\theta , \quad (2)$$

where $\langle\theta(t)\rangle_r$ denotes the average direction of the velocities of particles (including particle i) being within a circle of radius r surrounding the given particle. The average direction was given by the angle $\arctan[\langle\sin(\theta(t))\rangle_r/\langle\cos(\theta(t))\rangle_r]$. In Eq. (2) $\Delta\theta$ is a random number chosen with a uniform probability from the interval $[-\eta/2, \eta/2]$. Thus the term $\Delta\theta$ represents noise, which we shall use as a temperaturelike variable. Correspondingly, there are three free parameters for a given system size: η, ρ, and v, where v is the distance a particle makes between two updatings.

We have chosen this realization because of its simplicity, however, there may be several more interesting alternatives of implementing the main rules of the model. In particular, the absolute value of the velocities does not have to be fixed, one can introduce further kinds of particle interactions and or consider lattice alternatives of the model. In the rest of this paper we shall concentrate on the simplest version, described above, and investigate the nontrivial behavior of the transport properties as the two basic parameters of the model, the noise η and the density $\rho = N/L^2$, are varied. We used $v = 0.03$ in the simulations we report on for the following reasons. In the limit $v \to 0$ the particles do not move and the model becomes an analog of the well-known XY model. For $v \to \infty$ the particles become completely mixed between two updates, and this limit corresponds to the so-called mean-field behavior of a ferromagnet. We use $v = 0.03$ for which the particles always interact with their actual neighbors and move fast enough to change the configuration after a few updates of the directions. According to our simulations, in a wide range of the velocities ($0.003 < v < 0.3$), the actual value of v does not affect the results.

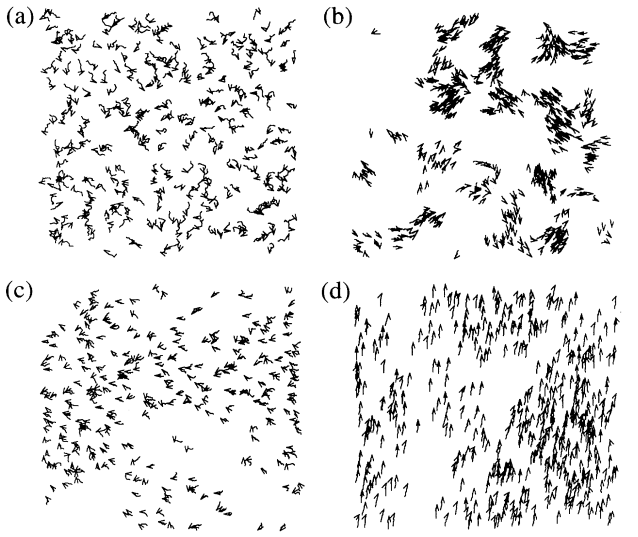

FIG. 1. In this figure the velocities of the particles are displayed for varying values of the density and the noise. The actual velocity of a particle is indicated by a small arrow, while their trajectory for the last 20 time steps is shown by a short continuous curve. The number of particles is $N = 300$ in each case. (a) $t = 0$, $L = 7$, $\eta = 2.0$. (b) For small densities and noise the particles tend to form groups moving coherently in random directions, here $L = 25$, $\eta = 0.1$. (c) After some time at higher densities and noise ($L = 7$, $\eta = 2.0$) the particles move randomly with some correlation. (d) For higher density and *small noise* ($L = 5$, $\eta = 0.1$) the motion becomes ordered. All of our results shown in Figs. 1–3 were obtained from simulations in which v was set to be equal to 0.03.

Figures 1(a)–1(d) demonstrate the velocity fields during runs with various selections for the value of the parameters ρ and η. The actual velocity of a particle is indicated by a small arrow, while their trajectory for the last 20 time steps is shown by a short continuous curve. (a) At $t = 0$ the positions and the direction of velocities are distributed randomly. (b) For small densities and noise the particles tend to form groups moving coherently in random directions. (c) At higher densities and noise the particles move randomly with some correlation. (d) Perhaps the most interesting case is when the density is large and the noise is small; in this case the motion becomes ordered on a macroscopic scale and all of the particles tend to *move in the same spontaneously selected direction.*

This kinetic phase transition is due to the fact that the particles are driven with a constant absolute velocity; thus, unlike standard physical systems in our case, the *net momentum of the interacting particles is not conserved* during collision. We have studied in detail the nature of this transition by determining the absolute value of the average normalized velocity

$$v_a = \frac{1}{Nv}\left|\sum_{i=1}^{N}\mathbf{v}_i\right| \quad (3)$$

of the entire system of particles as the noise and the density were changed. This velocity is approximately zero if the direction of the motion of the individual particles is distributed randomly, while for the coherently moving phase (with ordered direction of velocities) $v_a \simeq 1$ so that we can consider the average velocity as an *order parameter*.

First we gradually decreased the amount of noise η in cells of various sizes for a fixed density ρ and observed a transition from a disorderly moving phase to a phase with a coherent motion of the particles [Fig. 2(a)]. The uncertainty of the data points is within the range of the symbols except for runs carried out with 4000 and 10 000 particles close to the transition. For these η values the statistical errors estimated from five runs with different initial conditions are in the range of 5% (resulting in an overlap of the results for a limited number of η values) due to the slow convergence and large fluctuations. In Fig. 2(b) we show how v_a changes if the noise is kept constant and the density is increased.

Quite remarkably, the behavior of the kinetic order parameter v_a is very similar to that of the order parameter of some equilibrium systems close to their critical point. The strongest indication of a transition in our nonequilibrium model is the fact that as we go to larger system sizes the region over which the data show scaling is increasing [see Fig. 3(a)]. Only an extremely unusual crossover could change this *tendency*. A plausible physical picture behind our finding is the following: Since the particles are diffusing, there is mixing in the system resulting in an effective (long range) interaction radius.

Thus we can assume that in the thermodynamic limit our model exhibits a kinetic phase transition analogous to the continuous phase transition in equilibrium systems, i.e.,

$$v_a \sim [\eta_c(\rho) - \eta]^{\beta} \qquad \text{and} \qquad v_a \sim [\rho - \rho_c(\eta)]^{\delta}, \tag{4}$$

where β and δ are critical exponents and $\eta_c(\rho)$ and $\rho_c(\eta)$ are the critical noise and density (for $L \to \infty$), respectively. We can determine β and δ corresponding to the rate of vanishing of the order parameter from plotting $\ln v_a$ as a function of $\ln([\eta_c(L) - \eta]/\eta_c(L))$ and $\ln([\rho - \rho_c(L)]/\rho_c(L))$ for some fixed values of ρ and η, respectively (Fig. 3). For finite sizes $\eta_c(L)$ and $\rho_c(L)$ are L dependent; thus we used such values of quantities for which the plots in Fig. 3 were the straightest in the relevant region of noise or density values. The slope of the lines fitted to the data can be associated with the critical exponents for which we obtained $\beta = 0.45 \pm 0.07$ and $\delta = 0.35 \pm 0.06$. The errors in determining β and δ are due to the uncertainties in the (i) v_a and the (ii) $\eta_c(L)$ and $\rho_c(L)$ values. Since

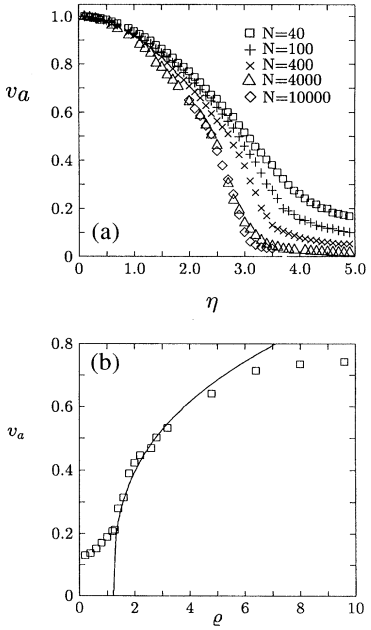

FIG. 2. (a) The absolute value of the average velocity (v_a) versus the noise η in cells of various sizes for a fixed density ρ. The symbols correspond to □ : $N = 40$, $L = 3.1$; + : $N = 100$, $L = 5$; × : $N = 400$, $L = 10$; △ : $N = 4000$, $L = 31.6$; ◇ : $N = 10\,000$, $L = 50$. In (b) (for $L = 20$) we show how v_a changes if the noise is kept constant and the density is increased.

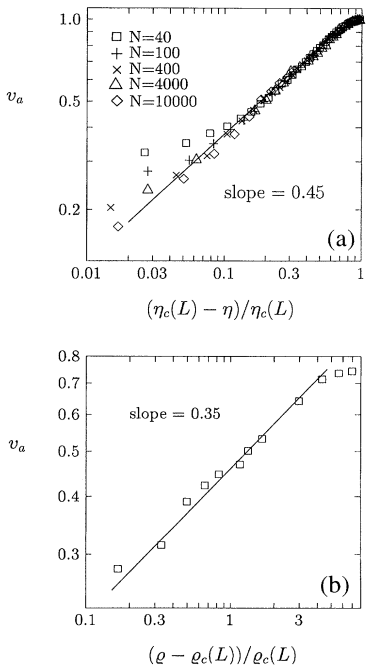

FIG. 3. Dependence of $\ln v_a$ on $\ln([\eta_c(L) - \eta]/\eta_c(L))$ and $\ln([\rho - \rho_c(L)]/\rho_c(L))$. The slope of the lines fitted to the data can be associated with the critical exponents β and δ. (a) is for $\rho = 0.4$, (b) is for $L = 20$ and $\eta = 2.0$.

the scaling plots in Fig. 3 depend sensitively on the choice of the critical noise and density and our method of determining their value is indirect (from the straightness of the data sets), we give rather conservative estimates for the errors of β and δ.

We have carried out a finite size scaling analysis of $\eta_c(L)$ and obtained $\eta_c(\infty) = 2.9 \pm 0.05$ for $\rho = 0.4$ (note that the "infinite temperature" limit of our model is $\eta_c = 2\pi$). As indicated, η_c depends on ρ, in fact, we expect a phase diagram (a line of critical temperatures) analogous to that of disordered ferromagnets, η_c playing the role of temperature, and ρ playing the role of the density of spins. In this case β and δ are expected to have the same value. On the other hand, strong crossover effects are likely to effect their actual values in a finite size simulation. Although our estimates for β and δ are different, on the basis of our simulations we cannot exclude the possibility (allowed by our error bars) that they become equal in the thermodynamic limit. However, the determination of the phase diagram and a more precise calculation of the exponents of our new model are outside of the scope of the present work, which concentrates on demonstrating the main features of a novel nonequilibrium system.

The emergence of cooperative motion in our model has analogies with the appearance of spatial order in equilibrium systems. This fact and the simplicity of our model suggests that, with appropriate modifications, the theoretical methods for describing critical phenomena may be applicable to the present kind of far-from-equilibrium phase transition. The kinetic phase transitions which have been observed in surface growth models [5–8] are both in analogy and different from the situation described here. The similarity is in the scaling behavior of an inherently nonequilibrium order parameter, while the two kinds of processes are distinct from the point of the driving force acting on the particles. Self-driven particles are uncommon in physics, but they are typical in biological systems, including live organisms and the so-called "molecular motors", having attracted great interest recently [14]. Transitions have been observed in traffic models [15] consisting of particles (cars) which can also be interpreted as self-driven particles.

There are interesting further variations of the model investigated in this work. It is expected that taking into account a hard core term in the interaction or using semiperiodic or open boundary conditions results in additional nontrivial effects. Our preliminary results [10] indicate that a model with hard core repulsion and specific boundary conditions can be successfully used to interpret recent observations of coherent motions in geometrically complex bacterial colonies growing on soft agar surfaces [10,16–18].

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