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1995 J. Phys. A: Math. Gen. 28 4245

(http://iopscience.iop.org/0305-4470/28/15/005)

J. Phys. A: Math. Gen. 28 (1995) 4245–4250. Printed in the UK

Modellization of self-propelling particles with a coupled map lattice model

Jan Hemmingsson†
PMMH, ESPCI, 10 rue Vauquelin, 75231 Paris Cedex 05, France

Received 21 February 1995

Abstract. We make a simple coupled map lattice model for simulating self-propelling particles. The interaction consists of three parts: viscous 'smearing' where the momenta are averaged over some neighbourhood, the collision where the momenta are conserved and, finally, the acceleration. As in externally forced fluids we find three regions: diffusion, convection and intermittency.

1. Motivation

There are examples in nature where the participating organisms form spatial patterns considerably larger than the particles themselves [1]. Examples include birds flying in formation, schools of fish, and swimming micro-organisms. Here we consider such systems as special cases of granular media on an air table, where energy is dissipated in collisions. The energy input in granular media is often the result of a static field like gravitation, or by a less ordered input through shaking or stirring. Here, the acceleration of each particle is, for simplicity, taken to be in the direction of its velocity. Attempts to understand such systems include molecular dynamic models by Vicsek *et al* [2] and Duparcmeur [3], who also found vortex formation.

Instead of working with distinct particles, here we suggest a model similar to several lattice gas models where the particles—or, here, organisms—are represented by densities or probabilities on a triangular lattice. This has the advantage of allowing fast simulations of large systems resulting in good statistics. There are, of course, drawbacks. The velocities are discrete and along fixed directions; this makes it difficult to continuously change a movement in a direction between two lattice directions. The suggested model takes only particle–particle interactions into account, in contrast to, for instance, Childress' models (see [1] and references therein) where the particles interact through the medium. As we will see, however, it is not necessary to consider movements of the medium in order to obtain ordered behaviour.

2. The model

The model that we have used in the numerical simulations has three parameters; viscosity η, acceleration γ, and dispersion $1 - \nu$. We take a phenomenological approach without

† Permanent address: IFM, Linköping University, S–58183 Linköping, Sweden.

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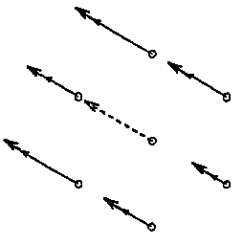

Figure 1. A fraction $\eta/6$ of the mass at the site in the centre of the picture is distributed to its six neighbours. This is done for all sites and repeated in all six directions.

considering a specific natural system. In the following, we will describe the model in detail.

On a triangular lattice, each site has six nearest neighbours. On each site we store real numbers representing densities of mass travelling in each of the six lattice directions, and an extra variable for storing the rest mass. This is a technique often used for simulating lattice gases [4].

Let us now introduce some notation. On each site i, there are six densities $N_{i,j}$ where $j \in [1, 6]$ represents the six lattice directions. The rest mass is written as $N_{i,0}$. At any instant the sum of these seven variables over all sites is, thus, a constant to ensure mass conservation.

The update of the system contains four steps, namely viscous 'smearing', collision, acceleration and propagation. Each of these steps are performed in parallel. In the propagation step, the densities are just transferred in the corresponding direction, i.e. the density $N_{i,j}$ is moved to site i's neighbour in direction j—let us call that site n—and stored as $N_{n,j}$. This means that all mass that is not resting moves with the unit velocity one lattice spacing per time step. Both energy and linear momentum are conserved, except at the walls where the particles are reflected and the linear momentum is locally changed. After this translation, mass is exchanged to simulate viscosity. A fraction η of the mass $N_{i,j}$ will be distributed to the site i's six neighbours, $n \in [1, 6]$, if $N_{i,j}$ is larger than $N_{n,j}$. Thus, 'smearing' only moves mass from denser to less dense regions.

For each of site i's six neighbours denoted by n, we can write

$$N'_{n,j} = N_{n,j} + \frac{\eta}{6} N_{i,j} \tag{1}$$

$$N'_{i,j} = N_{i,j} \left(1 - \frac{\eta}{6}\right) \tag{2}$$

if $N_{i,j} > N_{n,j}$, and

$$N'_{i,j} = N_{i,j} + \frac{\eta}{6} N_{n,j} \tag{3}$$

$$N'_{n,j} = N_{n,j} \left(1 - \frac{\eta}{6}\right) \tag{4}$$

otherwise.

The next part of the updating is the collision. This is simply a vector addition of the $N'_{i,j}$ over the directions j. We can write this as

$$p_i = \sum_{j=1}^{6} N'_{i,j}. \tag{5}$$

Here we have written $N'_{i,j}$ as a vector, to make clear that it is a vector sum. The direction of this vector is, thus, the jth lattice direction. The resulting vector $\boldsymbol{p}_i$ is nothing but the linear momentum at site i.

In general, the momentum $\boldsymbol{p}_i$ lies between two lattice directions $\hat{a}_i$ and $\hat{b}_i$, and we decompose $\boldsymbol{p}_i$ in these two directions. The $N''_{i,a}$ and $N''_{i,b}$ are chosen so that $N''_{i,a}+N''_{i,b} = \boldsymbol{p}_i$. Since the angle between $\hat{a}$ and $\hat{b}$ is always $\pi/3$, it is easy to do this in a unique way:

$$N''_{i,a} = r_i \sin(\pi/3 - \theta_i)/\sin(2\pi/3) \tag{6}$$

$$N''_{i,b} = r_i \sin\theta_i/\sin(2\pi/3) \tag{7}$$

where θ_i is the angle between $\boldsymbol{p}_i$ and $\hat{a}_i$.

Since the velocity is discrete, the energy at each site is simply the scalar sum of the (moving) mass $E_i = \sum_{j=1}^{6} N_{i,j}$. After the collision, there is only moving mass in directions $\hat{a}_i$ and $\hat{b}_i$. The mass that does not move is, thus, added to the rest mass and is, directly after the collision, the difference between the sum of the incoming masses and the two outgoing masses. Although the linear momentum has been conserved, this is not true for the energy. In this step, energy is, thus, really dissipated.

At the acceleration step of the update, a fraction γ of the rest mass is accelerated. A fraction ν is sent in the two main directions $\hat{a}_i$ and $\hat{b}_i$, and the rest is evenly distributed in all six directions.

$$N'''_{i,a} = \frac{\nu N''_{i,a} N''_{i,0}}{N''_{i,a} + N''_{i,b}} \tag{8}$$

$$N'''_{i,b} = \frac{\nu N''_{i,b} N''_{i,0}}{N''_{i,a} + N''_{i,b}} \tag{9}$$

$$N'''_{i,x} = \frac{1-\nu}{6} N''_{i,0} \qquad x \in [1,6]. \tag{10}$$

As long as ν is larger than zero (i.e. it is non-negative), the particles are mainly accelerating in the same directions as they are moving. We used a value of $\nu \approx 0.01$ in the simulations. The collision itself will also strongly align the particles.

3. Boundary conditions and convection

One can easily imagine what will happen when a system like the one described above is simulated with periodic boundaries. After the system has been randomly initiated, the vector sum of $N_{i,j}$ over all sites i will give the total linear momentum of the whole system. This is a preferred direction, and the interactions described above will decrease movements in other directions. Movements along this preferred direction will be amplified by the acceleration step and, as a result, all particles will move in this one direction. Simulations of the model give this result, which is also the case of the model of Vicsek *et al* [2].

The boundaries that we use are reflecting, and are made by letting the resulting linear momentum $\boldsymbol{p}_i$ change its direction at the wall sites so that the angle of the outgoing momentum is the same as the angle of the incoming momentum. In systems with the type of mechanical interaction described above, the presence of walls is crucial to the emergence of convection. Other forms of convection-like behaviour might have other origins. There are examples of termites running around in a—seemingly meaningless—circle for a whole day. Such a phenomenon, as we see it, originates from the cooperative character of the termites. Once the circle is closed, by chance each termite will follow its fellow runner

in front of him, and as long as they cannot see or figure out that they are all running in a circle, they will continue to do so.

4. Simulations

The actual simulations were made on a Connection Machine CM-200. A random initial configuration can be made by assigning to each $N_{i,n}$ a number between 0 and 1. This is how we choose the initial configuration if nothing else is stated. Thereafter, the updating rule described above is applied to all sites simultaneously. We use hexagonal boundaries so that no lattice direction is preferred with respect to the others.

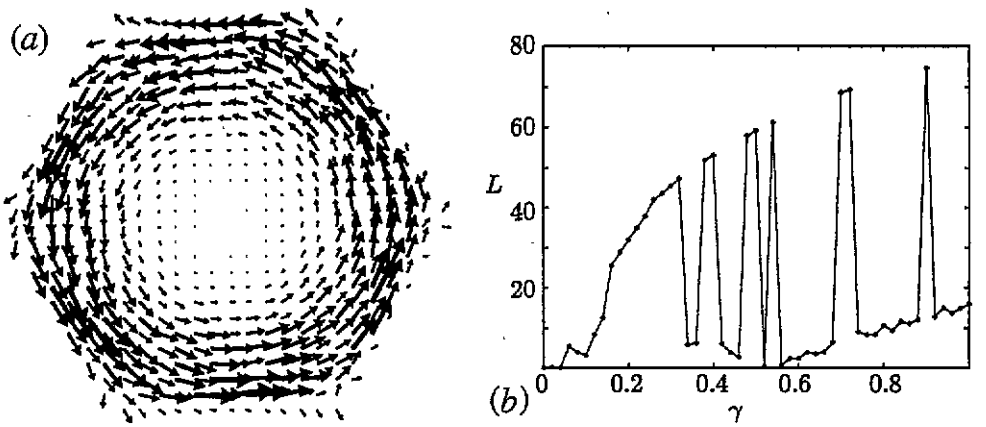

Figure 2. Snapshot and rotation strength from convection on a 128 × 128 lattice. (*a*) A typical snapshot of the convecting system. $\eta = 0.5$, $\gamma = 0.28$, $\nu = 0.01$. The snapshot is taken after 3000 iterations. (*b*) Absolute value of the angular momentum *versus* the parameter γ. $\eta = 0.5, \nu = 0.01$. For γ between 0.15 and 0.33, stable convection is found. The behaviour is meta-stable.

Figure 2(*a*) shows a typical snapshot of convection in the system after a few hundred iterations. The arrows correspond to the resulting momenta p_i. In order to produce a somewhat clearer picture, not all vectors are displayed. A strong and stable convection can be seen. The main characteristic of the convection is the angular momentum L. If the vector from the centre† of the system to site i is R_i, and the linear momentum is p_i at this site, the strength of the rotation is the angular momentum (proportional to the square root of the energy)

$$L\hat{z} = \sum_i R_i \times p_i. \tag{11}$$

Depending on the orientation, L can take both positive and negative values; it will always be parallel to the z-axis since both R_i and p_i lie in the x–y plane.

With this measure we can make a quantitative investigation to decide whether convection is present or not. The absolute value of the time average of L will then provide information on how strong the convection is. We made separate runs for different values of γ, while keeping the other parameters constant. Figure 2(*b*) shows the convection strength *versus* γ. For very low values of γ, the system seems to be rather diffusive. Then, for a higher energy input γ_c^1, the rotation starts and gets stronger for higher γ up to a certain value γ_c.

† The centre of the system coincides with the centre of the convection cell by stable convection.

For higher energy input, the rotation strength L is either very high or very low, and the same value of γ might give different results for independent runs. This could be explained through the existence of various metastable states. In the cases of high γ where L is low, we did not find very many eddies and whirls. This might be due to the fact that many whirls are superposed, and they cannot be distinguished from each other.

The actual value of γ_c depends on the system size as well as the other parameters η and ν. We found γ_c to be approximately proportional to γ/η. Since the collision mechanism aligns the momenta, we do not expect γ_c to be linearly dependent on ν.

The angular momentum depends on the η and ν in more or less the same way as it depends on the acceleration parameter. In all cases we find the three regions, see figure 3.

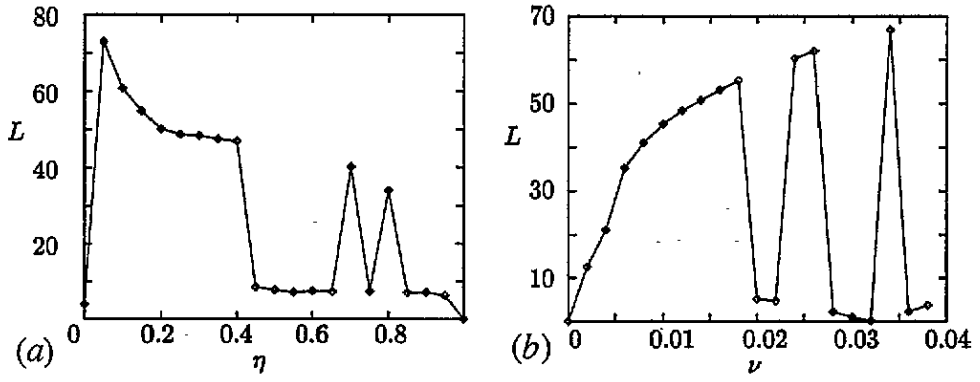

Figure 3. Rotation strength as a function of η and ν from convection on a 128×128 lattice. (*a*) Absolute value of the angular momentum *versus* the parameter η. $\eta = 0.5$, $\gamma = 0.3$, $\nu = 0.01$. (*b*) Absolute value of the angular momentum *versus* the parameter ν. $\eta = 0.5$, $\gamma = 0.3$.

To investigate how the overall behaviour depends on the initial condition, we made simulations starting with convection rolls. To make an initial convection cell, we initiated the vectors p_i perpendicular to R_i and with a magnitude proportional to the distance to the centre. For all γ, the convection stayed stable for as long as we simulated, i.e. up to 10 000 time-steps.

One would further expect that if one makes the system more elongated, two convection cells could appear. A problem here is that the system is no longer symmetric. This means that the result might depend on the orientation of the system on the lattice, since some directions are preferred to others. Still, the effect is strong enough to be observed even in a system where the preferred lattice direction is along the longer side of the system, see figure 4.

The angular momentum clearly depends on the distance from the centre of the convection cell. In figure 5, the average angular momentum is plotted against the distance from the centre of the convection cell. The angular momentum in the centre of the system is very low. From a distance of about 27 lattice spacings from the centre, the angular momentum grows linearly with a slope of 0.046. At a distance of about 50 lattice spacings from the centre, the effect of the walls can be seen, and the angular momentum falls fast. In the six corners of the hexagonal lattice, there are 'pockets' of slower moving particles which accounts for the step-like shape of the right flank in figure 5.

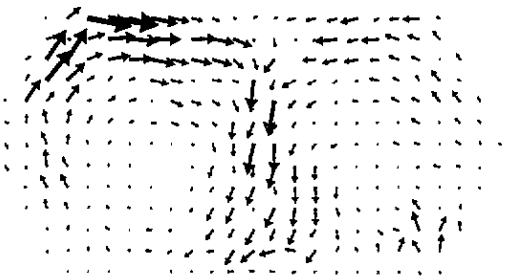

Figure 4. Two cell convection. Size of the lattice is 128×64. $\eta = 0.85$, $\gamma = 0.02$, $\nu = 0.3$

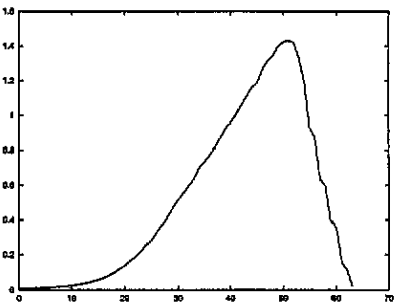

Figure 5. The angular momentum per cell *versus* the distance from the centre after 10 000 iterations. System size is 128×128 sites. $\eta = 0.5$, $\gamma = 1.0$, $\nu = 0.01$

5. Conclusions

We have obtained convection in a simplified model of self-propelling particles. Instead of simulating discrete particles, the model treats densities of mass. Simple mechanisms of collision, acceleration and viscosity, together with reflecting boundaries, are enough to obtain convection. The asymptotic behaviour of the system depends on the initial state. For random initial states we found a phase transition in the acceleration, with the angular momentum as the order parameter. Taken together, this suggests a Reynolds number, $R_e \propto \gamma/\eta$.

Acknowledgments

My most sincere thanks to Hans Herrmann for ideas and discussions, to Harald Puhl for debugging support, and to Gongwen Peng and Stefan Schwarzer for discussions at different stages of this work. The present research was supported by the Swedish Institute and the Swedish Natural Research Council.

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