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Cellular Automata Modeling of Physical Systems

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one sees that the physical quantity associated with the wave number k is the total number of particle $\rho_0 = \sum_r \rho(r) = N$.

Equation 3.10 has another solution for $\exp(i\omega\tau) = -1$ which is

$$\cos(k\lambda) = -1 \tag{3.44}$$

Within the possible range of values of k, this implies that $k\lambda = \pi$. Therefore, in our dynamics, there is a quantity which changes its sign at each iteration. The quantity associated with $k\lambda = \pi$ is

$$\rho_{\pi/\lambda} = \sum_{r \in lattice} \rho(r,0) e^{-i\pi(r/\lambda)} \tag{3.45}$$

Thus,

$$\rho_{\pi/\lambda} = N_{\text{even}} - N_{\text{odd}} \tag{3.46}$$

where N_{even} and N_{odd} denote the total number of particles on even and odd lattice sites, respectively. Our result is easily explained by the following fact: all particles entering an even site at time t will move to an odd site at time $t+1$, and conversely. Therefore, there is no interaction, at any time, between particles that are not located on the same odd or even sublattice. Particle conservation holds independently for each sublattice and our system actually contains two non-interacting subsystems. This feature is known as the checkerboard invariant.

This spurious invariant may have undesirable effects in reaction-diffusion processes, such as the annihilation reaction $A + A \to 0$ in which two particles entering the same site are removed with a probability p_{reaction}. If the odd and even sublattices are not well distinguished, the amount of A particles will eventually reach a constant concentration because no reaction can take place between particles on different sublattices.

3.2 The FHP model

The FHP rule is a model of a two-dimensional fluid which was introduced by Frisch, Hasslacher and Pomeau [31], in 1986. We show here how the fully discrete microscopic dynamics maps onto the macroscopic behavior of hydrodynamics. Due to the nonlinearity of the rule, the calculation will be much more complex than in the case of the one-dimensional diffusion rule discussed in the previous section.

3.2.1 The collision rule

The FHP model describes the motion of particles traveling in a discrete space and colliding with each other, very much in the same spirit as the HPP lattice gas discussed in section 2.2.5. The main difference is that, for isotropy reasons that will become clear below, the lattice is hexagonal (i.e. each site has six neighbors, as shown in figure 3.1).

The FHP model is an abstraction, at a microscopic scale, of a fluid. It is expected to contain all the salient features of a real fluid. It is well known that the continuity and

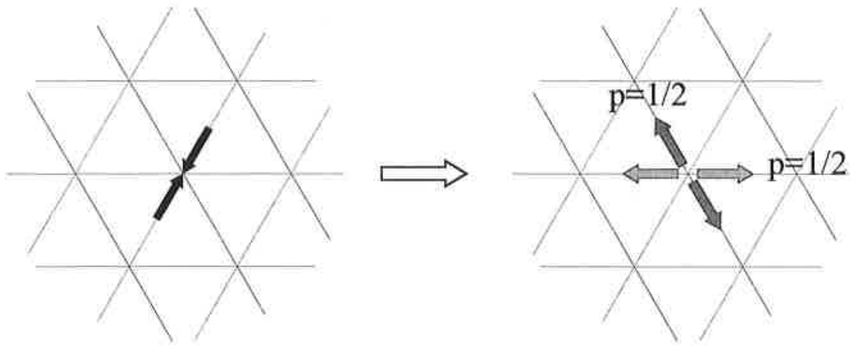

Figure 3.1: *Two-body collision in the FHP model. On the right part of the figure, the two possible outcomes of the collision are shown in dark and light gray, respectively. They both occur with probability* 1/2.

Navier–Stokes equations of hydrodynamics express the local conservation of mass and momentum in a fluid. The detailed nature of the microscopic interactions does not affect the form of these equations but only the values of the coefficients (such as the viscosity) appearing in them. Therefore, the basic ingredients one has to include in the microdynamics of the FHP model are the conservation of particles and momentum after each updating step. In addition, some symmetries are required so that, in the macroscopic limit where time and space can be considered as continuous variables, the system is isotropic.

As in the case of the HPP model, the microdynamics of FHP is given in terms of Boolean variables describing the occupation numbers at each site of the lattice and at each time step (i.e. the presence or the absence of a fluid particle). The FHP particles move in discrete time steps, with a velocity of constant modulus, pointing along one of the six directions of the lattice. The dynamics is such that no more than one particle enters the same site at the same time with the same velocity. This restriction is the exclusion principle; it ensures that six Boolean variables at each lattice site are always enough to represent the microdynamics.

In the absence of collisions, the particles would move in straight lines, along the direction specified by their velocity vector. The velocity modulus is such that, in a time step, each particle travels one lattice spacing and reaches a nearest-neighbor site.

Interactions take place among particles entering the same site at the same time and result in a new local distribution of particle velocities. In order to conserve the number of particles and the momentum during each interaction, only a few configurations lead to a non-trivial collision (i.e a collision in which the directions of motion have changed). For instance, when exactly two particles enter the same site with opposite velocities, both of them are deflected by 60 degrees so that the output of the collision is still a zero momentum configuration with two particles (see figure 3.1). As shown in figure 3.1, the deflection can occur to the right or to the left, indifferently. For symmetry reasons, the two possibilities are chosen randomly, with equal probability.

Another type of collision is considered: when exactly three particles collide with an

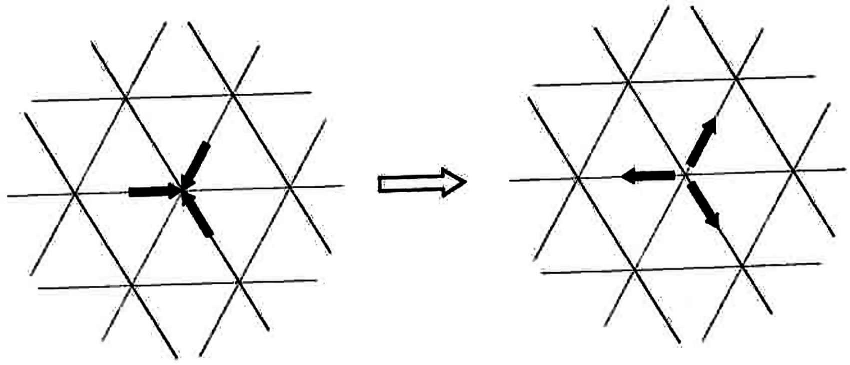

Figure 3.2: *Three-body collision in the FHP model.*

angle of 120 degrees between each other, they bounce back to where they come from (so that the momentum after the collision is zero, as it was before the collision). Figure 3.2 illustrates this rule. Several variants of the FHP model exist in the literature [3], including some with rest particles (models FHP-II and FHP-III).

For the simplest case we are considering here, all interactions come from the two collision processes described above. For all other configurations (i.e those which are not obtained by rotations of the situations given in figure 3.1 and 3.2) no collision occurs and the particles go through as if they were transparent to each other.

Both two- and three-body collisions are necessary to avoid extra conservation laws. The two-particle collision removes a pair of particles with a zero total momentum and moves it to another lattice direction. Therefore, it conserves momentum along each line of the lattice. On the other hand, three-body interactions deflect particles by 180 degrees and cause the net momentum of each lattice line to change. However, three-body collisions conserve the number of particles within each lattice line.

In the FHP rule, particles interact only at the lattice sites. It is tempting to think of this dynamics as snapshots, at integer clock cycles, of a continuous time evolution on a lattice. Between two consecutive time steps, the particles move along the lattice links. Strictly speaking, we may ask what happens to them when they cross each other on a lattice link. It is not specified in the model and somewhat irrelevant from the technical point of view. If we want a precise picture of what occurs along the lattice links, we may either imagine that the particles are transparent to each other or, since particles are indiscernible, that they collide half way and bounce back.

Note that a fully deterministic FHP model can also be considered, to avoid generating random numbers to select among the possible outcomes of the two-body collision. The usual strategy used for this purpose is to alternate between the two outcomes. One method consist of using time parity (i.e at even time steps, a $n_i n_{i+3}$ collision results in a $n_{i+1}n_{i+4}$ configuration and, at odd time steps, to a $n_{i+5}n_{i+2}$ configuration). Another technique is to add a seventh bit to the automaton state, which acts as a control bit. When this bit is 1, the $n_{i+1}n_{i+4}$ configuration is chosen and the bit is flipped to 0. Conversely, when the seventh bit is 0, the $n_{i+5}n_{i+2}$ output is selected and the control bit is flipped to 1.

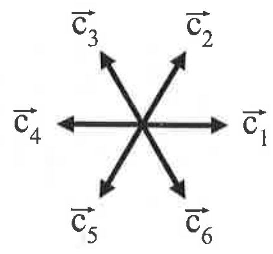

Figure 3.3: *The direction of motion $\vec{c}_i$.*

A deterministic FHP dynamics is interesting also because it guarantees time reversibility invariance, which is a fundamental symmetry of microscopic physics. However, in the rest of this section, we shall consider the probabilistic FHP rule initially described because no macroscopic difference is expected to show up when one dynamics is used in place of the other.

3.2.2 The microdynamics

The full microdynamics of the FHP model can be expressed by evolution equations for the occupation numbers: we introduce $n_i(\vec{r}, t)$ as the number of particles (which can be either 0 or 1) entering site $\vec{r}$ at time t with a velocity pointing along direction $\vec{c}_i$, where $i = 1, 2, ..., 6$ labels the six lattice directions. The unit vectors $\vec{c}_i$ are shown in figure 3.3.

We also define the time step as τ and the lattice spacing as λ. Thus, the six possible velocities $\vec{v}_i$ of the particles are related to their directions of motion by

$$\vec{v}_i = \frac{\lambda}{\tau}\vec{c}_i \tag{3.47}$$

Without interactions between particles, the evolution equations for the n_i would be given by

$$n_i(\vec{r} + \lambda\vec{c}_i, t + \tau) = n_i(\vec{r}, t) \tag{3.48}$$

which expresses that a particle entering site $\vec{r}$ with velocity along $\vec{c}_i$ will continue in a straight line so that, at the next time step, it will enter site $\vec{r} + \lambda\vec{c}_i$ with the same direction of motion. However, due to collisions, a particle can be removed from its original direction or another one can be deflected into direction $\vec{c}_i$.

For instance, if only n_i and n_{i+3} are 1 at site $\vec{r}$, a collision occurs and the particle traveling with velocity $\vec{v}_i$ will then move with either velocity $\vec{v}_{i-1}$ or $\vec{v}_{i+1}$ (note that the operations on index i are taken to be modulo 6). The quantity

$$D_i = n_i n_{i+3}(1 - n_{i+1})(1 - n_{i+2})(1 - n_{i+4})(1 - n_{i+5}) \tag{3.49}$$

indicates, when $D_i = 1$ that such a collision will take place. Therefore,

$$n_i - D_i \tag{3.50}$$

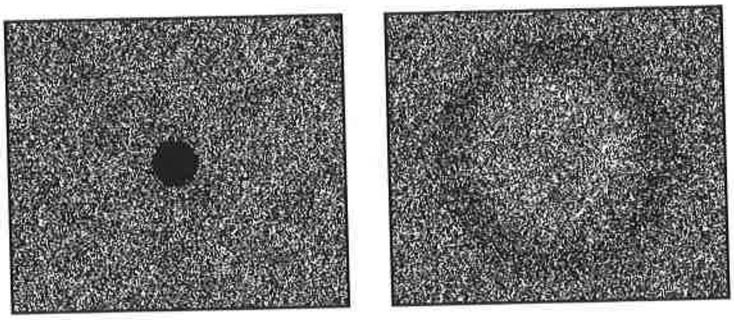

Figure 3.4: *Development of a sound wave in a FHP gas, due to particle overconcentration in the middle of the system.*

is the number of particles left in direction $\vec{c}_i$ due to a two-particle collision along this direction.

Now, when $n_i = 0$, a new particle can appear in direction $\vec{c}_i$, as the result of a collision between n_{i+1} and n_{i+4} or a collision between n_{i-1} and n_{i+2}. It is convenient to introduce a random Boolean variable $q(\vec{r}, t)$ which decides whether the particles are deflected to the right ($q = 1$) or to the left ($q = 0$) when a two-body collision takes place. Therefore, the number of particle created in direction $\vec{c}_i$ is

$$qD_{i-1} + (1-q)D_{i+1} \tag{3.51}$$

Particles can also be deflected into (or removed from) direction $\vec{c}_i$ because of a three-body collision. The quantity which expresses the occurrence of a three-body collision with particles n_i, n_{i+2} and n_{i+4} is

$$T_i = n_i n_{i+2} n_{i+4} (1 - n_{i+1})(1 - n_{i+3})(1 - n_{i+5}) \tag{3.52}$$

As before, the result of a three-body collision is to modify the number of particles in direction $\vec{c}_i$ as

$$n_i - T_i + T_{i+3} \tag{3.53}$$

Thus, according to our collision rules, the microdynamics of the FHP model reads

$$\begin{aligned} n_i(\vec{r} + \lambda\vec{c}_i, t + \tau) \;=\; & n_i(\vec{r}, t) \\ & -D_i + qD_{i-1} + (1-q)D_{i+1} \\ & -T_i + T_{i+3} \end{aligned} \tag{3.54}$$

where the right-hand side is computed at position $\vec{r}$ and time t. These equations are easy to code in a computer and yield a fast and exact implementation of the model. As an example, figure 3.4 illustrates a sound wave in the FHP gas at rest. Although the initial concentration is analogous to the situation of figure 2.13, we observe here a much more isotropic behavior.

3.2.3 From microdynamics to macrodynamics

The macroscopic variables

The physical quantities of interest are not so much the Boolean variables n_i but macroscopic quantities or average values, such as, for instance, the average density of particles and the average velocity field at each point of the system. These quantities are defined from the ensemble average $N_i(\vec{r},t) =< n_i(\vec{r},t) >$ of the microscopic occupation variables. $N_i(\vec{r},t)$ is also the probability of having a particle entering site $\vec{r}$, at time t, with velocity $\vec{v}_i = (\lambda/\tau)\vec{c}_i$.

Following the usual definition of statistical mechanics, the local density of particles is the sum of the average number of particles traveling along each direction $\vec{c}_i$

$$\rho(\vec{r},t) = \sum_{i=1}^{6} N_i(\vec{r},t) \tag{3.55}$$

Similarly, the particle current, which is the density ρ times the velocity field $\vec{u}$, is expressed as

$$\rho(\vec{r},t)\vec{u}(\vec{r},t) = \sum_{i=1}^{6} \vec{v}_i N_i(\vec{r},t) \tag{3.56}$$

Another quantity which plays an important role in the following derivation is the momentum tensor Π, which is defined as

$$\Pi_{\alpha\beta} = \sum_{i=1}^{6} v_{i\alpha} v_{i\beta} N_i(\vec{r},t) \tag{3.57}$$

where the greek indices α and β label the two spatial components of the vectors. The quantity Π represents the flux of the α-component of momentum transported along the β-axis. This term will contain the pressure contribution and the effects of viscosity.

The multiscale and Chapman–Enskog expansion

It is important to show that our discrete world is, at some appropriate scale of observation, governed by admissible equations: the physical conservation laws and the symmetry of the space are to be present and the discreteness of the lattice should not show up. The connection between the microscopic Boolean dynamics and the macroscopic, continuous world has to be established in order to assess the validity of the model.

The starting point to obtain the macroscopic behavior of the FHP automaton is to derive an equation for the N_is. Averaging the microdynamics 3.54 yields

$$N_i(\vec{r}+\lambda\vec{c}_i, t+\tau) - N_i(\vec{r},t) =< \Omega_i > \tag{3.58}$$

where

$$< \Omega_i >= - < T_i > + < T_{i+3} > - < D_i > +\frac{1}{2} < D_{i-1} > +\frac{1}{2} < D_{i+1} > \tag{3.59}$$