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LETTER TO THE EDITOR

Triangular versus square lattice gas automata for the analysis of two-dimensional vortex fields

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Abstract. The consequences of the lack of isotropy of the momentum flux tensor of the Hardy–Pomeau–De Pazzis (HPP) fluid are discussed. It is shown that this lack of isotropy is tantamount to introducing a force which is incompatible with a correct evolution of two-dimensional vortex configurations. In addition, a qualitative discussion is presented on the physical reasons why this problem can be cured by moving to the six-link lattice introduced by Frisch, Hasslacher and Pomeau (FHP).

Lattice gas models obeying cellular automata (CA) rules constitute a subject of growing interest for the simulation of complex hydrodynamic phenomena. In fact, with suitable restrictions on the crystallographic symmetries of the lattice, and by taking the appropriate spatial averages, various fluid dynamical equations are obtained which describe the macroscopic behaviour of the lattice gas as a continuum system. Since the cellular automata rules are intrinsically discrete and only involve logical operations, a new and fairly different simulation strategy is therefore offered. The simplest lattice gas model, currently referred to as HPP (Hardy–Pomeau–De Pazzis) [1], involves a regular square lattice, holding up to four particles per site, each endowed with a unit mass and unit speed along one of the four directions defined on the lattice. The dynamics of the HPP automaton is invariant under all the transformations which conserve the square lattice, namely mirror symmetries with respect to a lattice line, discrete translations and rotations of $\frac{1}{2}\pi$. Unfortunately, this latter symmetry is not sufficient to ensure the isotropy of the resulting macroscopic equations. As first shown by Frisch *et al* [2], this isotropy can be recovered by replacing the HPP square lattice with a triangular lattice in which each site is connected to its neighbours through six links angularly spaced by $\frac{1}{3}\pi$. For this reason, all the hydrodynamical simulations in this domain are now currently performed with hexagonal lattices, usually referred to as FHP (Frisch–Hasslacher–Pomeau) model. However, as far as we know, no specific analysis of the practical consequences of this anisotropy on the evolution of two-dimensional vortex configurations has ever been presented, so that one may wonder whether at least the qualitative aspects of this evolution can be studied with the HPP automaton in spite of its lack of isotropy. To this purpose, we reformulate the HPP momentum equation as the correct Euler equation plus a forcing term which embodies the effects of the lack of isotropy. We find that this forcing term indeed rapidly drives the fluid close to an equilibrium situation which is essentially a direct product of two separate one-dimensional equilibria. This is achieved via a sort of ballastic instability of the vortices, which are first turned into quasisquare structures and subsequently die out because of the inability of pressure gradients to prevent kinematic losses on the edges.

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As is well known [3], the fluid dynamic picture of a fluid may be conceived as the gluing of local thermodynamic equilibria characterised by slowly varying parameters, typically the fluid density $\rho(x_i, t)$ and speed $u_i(x_k, t)$. These two quantities fulfil macroscopic equations which, in the inviscid limit, can be cast in conservative form as follows:

$$\partial_t \rho + \partial_i \rho u_i = 0 \tag{1}$$

$$\partial_t \rho u_i + \partial_k P_{ik} = 0 \tag{2}$$

where ∂_t is the temporal derivative, ∂_i, $i = 1, 2$, the spatial gradient and P_{ik} is the momentum flux tensor. The first of these two equations represents mass conservation (the continuity equation) while the second one is the equation of motion of the fluid, i.e. the Euler equation. In a real fluid the momentum flux tensor takes the form

$$P_{ik} = \rho u_i u_k + p\delta_{ik} \tag{3}$$

where p is the scalar pressure and δ_{ik} is the usual Kronecker delta function. It is not difficult to show that (3) represents the most general form of an isotropic tensor in dimension $D = 2$.

Note that in the frame moving with the fluid, the above expression reduces to a diagonal tensor, so that the familiar Pascal law is recovered; in fact the quadratic component $u_i u_k$ stems from the translational symmetry related to the principle of Galilean invariance. In a lattice gas, such a symmetry is broken and this results in the appearance of a density-dependent extra factor $G(\rho)$ in front of the quadratic term.

Following the general theory exposed in [4], it is easy to verify that in the HPP lattice gas the momentum flux tensor is

$$P_{ik}^{\mathrm{HPP}} = p\delta_{ik} + \rho G(\rho)(u^2 - v^2)\sigma_{ik} \tag{4}$$

where u and v stand for the x and y components of the velocity vector u_i, σ_{ik} is the Pauli matrix $\sigma_{ik} = \delta_{ik}(-1)^{(i+1)}$ and G is the coefficient arising from the lack of translational symmetry. From this expression we see that the 'pressure' component $p\delta_{ik}$ is the same as in a real fluid, while the quadratic part is not. This means tht the lack of isotropy of the HPP tensor leaves the linear modes unaffected (such as the sound waves observed in the early cellular automata simulations [5]) but is likely to significantly alter the non-linear fluid regime.

To give a quantitative insight in this direction, we find it convenient to rewrite the HPP tensor as a sum of the lattice Navier–Stokes tensor, i.e. (3) with the quadratic term premultiplied by a factor G, plus a 'spurious' tensor T_{ik} which is meant to account for all the physical effects related to the lack of isotropy of the HPP model. By comparing equation (3), modified as mentioned above, and equation (4), one obtains

$$T_{ik} = -\rho G \tilde{u}_i \tilde{u}_k \tag{5}$$

where the tilde denotes the interchange between x and y directions so that $\tilde{u}_1 = u_2 \equiv v$ and $\tilde{u}_2 = u_1 \equiv u$. After this, the motion equation for the momentum can be written as

$$d_t \rho u_i + \partial_i p = \partial_k T_{ki} \equiv f_i \tag{6}$$

where $d_t \equiv \partial_t + G u_k \partial_k$ is the substantial derivative taken along the fluid path and f_i the spurious force associated with the lack of isotropy (hereafter called the HPP force). This force can be written explicitly as follows:

$$f_i = \rho G s \tilde{u}_i \tag{7}$$

where $s = u_y + v_x$ is the strain term describing the deformation of a fluid element under tangential stresses.

Let us now consider the following isotropic vortex configuration:

$$u = -yR(r) \qquad v = xR(r) \qquad (r^2 = x^2 + y^2) \tag{8}$$

where $R(r)$ is a suitable shape function describing the spatial structure of the vortex. For this configuration, we immediately obtain

$$s = (y^2 - x^2)\, \mathrm{d}R/\mathrm{d}r. \tag{9}$$

Discarding the possibility that $\mathrm{d}R/\mathrm{d}r = 0$ (we assume $R(r)$ a monotonically decreasing function of r), we see that the condition $s = 0$ can only be met along the bisectrices of the plane, where both the components of the HPP force vanish. From the above expressions, we also see that along the coordinate axes the force is aligned with the axes themselves and points towards the origin, i.e. the centre of the vortex.

Complete information on the topology of the HPP force can be obtained by examining its flow lines, defined by the requirement $\boldsymbol{f} \times \mathrm{d}\boldsymbol{l} = 0$, i.e. $\mathrm{d}y/\mathrm{d}x = f_y/f_x$. This yields the following path equation:

$$yx = \text{constant} \tag{10}$$

which shows that the spurious force is distributed along hyperbolic paths, symmetric about the bisetrices of the x,y plane, with an intensity which is maximum along the coordinate axes and zero on the bisetrices. As already noticed, along the coordinate axes the force is centripetal, i.e. it points towards the origin and tends therefore to compress the vortex. It is also useful to identify those paths along which the kinetic energy of the fluid is left unaffected by the spurious force. For this, the requirement is $\boldsymbol{f} \cdot \mathrm{d}\boldsymbol{l} = 0$, which is $\mathrm{d}y/\mathrm{d}x = -f_x/f_y$. This yields

$$y^2 - x^2 = \text{constant}. \tag{11}$$

Hence, in order for its kinetic energy to be unaffected by the presence of the HPP force generated by the circular vortex, the fluid should move along hyperbolic paths: manifestly we have run against a topological conflict!

To clarify what we mean by 'topological conflict', let us repeat the same procedure with the 'Euler' force $f_i^{\mathrm{E}} \equiv -\rho u_k \partial_k u_i$. One sees that this term results in a purely radial force which adds up to the centrifugal force along the outward normal with no component along the tangential direction, as it must be according to the isotropy requirements. Consequently, the vortex is a force-free path, whose equilibrium is ensured by an inward radial pressure gradient balancing both the Euler and the centrifugal forces. In other words, the vortices are equilibrium structures in that they coincide with coordinate lines of the geometry induced by the Euler force. These coordinate lines (r = constant) are associated with the conservation of the kinetic energy $K = \frac{1}{2}\rho(u^2 + v^2)$, which can play the role of an independent coordinate perfectly equivalent to the radial one. With the same arguments, we see that the natural system induced by the HPP force is qualitatively different: it is in fact a hyperbolic system in which the force-free paths are labelled by the hyperbolic form $K_- = \frac{1}{2}\rho(u_i \sigma_{ij} u_j) \equiv \frac{1}{2}\rho(u^2 - v^2)$, a sort of 'skew' kinetic energy. Along a vortex path, K is conserved whereas K_- undergoes periodic oscillations.

It is now instructive to rewrite (2) for the unknowns K and K_- instead of u and v. By applying the scalar and antiscalar product† of (2) with the velocity vector u_i, we obtain

$$d_t K + u_i \partial_i p = 2\rho G u v s \tag{12}$$

$$d_t K_- + u_i \sigma_{ij} \partial_j p = 0. \tag{13}$$

From these equations we see that K_- indeed evolves as in a real fluid, as it must do since the antiscalar product with the fluid velocity annihilates the HPP force. On the contrary, the kinetic energy is affected by the spurious term on the RHS of (12). The requirement that this spurious term vanishes introduces a sort of macroscopic 'exclusion principle' which forbids the simultaneous presence at the same spatial location of two non-vanishing velocity components.

Thus, of all the possible two-dimensional configurations, this principle singles out those which can be decomposed into a direct product of two decoupled one-dimensional structures along the coordinate axes. If we confine our attention to these configurations, it is clear that the closest one to a circular vortex is a square vortex whose sides are aligned with the coordinate axes. Indeed, by remembering the topology of the HPP force acting on a circle, we see that it tends to transform the circle into a square. Let us therefore assume the following velocity field:

$$u = u(x, y) H(|y| - |x|) \qquad v = v(x, y) H(|x| - |y|) \tag{14}$$

where the notation H stands for the Heavyside step function. Elementary calculations show that the HPP force is always orthogonal to the vortex path and consequently it does not affect its kinetic energy. The Euler force reduces to its one-dimensional components uu_x and vv_y which give rise to singular Dirac delta stretching contributions on the corners of the vortex where the fluid velocity suffers a discontinuity. Consequently, in order for the vortex configuration to be maintained against the ballistic losses induced by the Euler force on the corners, a balancing singularity must also develop in the pressure field. Owing to this singularity, around the corners the inviscid approximation fails completely and higher-order spatial derivatives must be accounted for, no matter how small the fluid viscosity is.

Therefore, we have performed a series of numerical simulations on an IBM 3090 with vector facility in order to ascertain whether the diffusion effects brought about by higher-order derivatives can play some stabilising role. In other words, this means investigating whether the smoothing effects of the collisions can somehow damp out the shortest wavelengths produced by the Euler term, thereby removing the unphysical discontinuities generated by the HPP term.

The outcome of these simulations was definitely negative and confirmed the dominance of the 'ballistic instability' mentioned above. In other words, what one observes is that the circular vortices are first turned into square structures which subsequently rapidly deplete under the expelling effect of the Euler force. This ballistic instability must be regarded as the most genuine (and catastrophic) manifestation of the lack of isotropy: it provides the system with an eminently quick and efficient route towards a factorised x,y equilibrium incompatible with the existence of a circular vortex.

Before concluding, a few comments on the reasons why the problems of the HPP automaton can be cured by adopting a six-link underlying lattice are in order.

† The antiscalar product is just a scalar product in the metric defined by the matrix σ, i.e. $A^*B \equiv A_i \sigma_{ij} B_j = A_1 B_1 - A_2 B_2$.

As previously shown, the main failure of the HPP fluid is its inability to ensure a proper energy transfer between the x and y axes, a mechanism which is essential for the correct evolution of any genuinely two-dimensional fluid configuration. This inability can be traced back to the properties of the free-streaming and collision operators which govern the microevolution of the lattice gas. Therefore, let us briefly review the basic features of the HPP automaton. On each grid site (i, j) one puts N_{ij} particles $(0 \leq N_{ij} \leq 4)$, each endowed with a unit mass and speed, so that the state on this site can be represented by a quadruplet $(N^1, N^2, N^3, N^4)_{ij}$ where N^s, $s = 1, \ldots, 4$, can take only the values zero or one according to whether the site holds a particle pointing in the direction s or not. Thus, the notation (1111) denotes a fully occupied site, while (0000) indicates the total absence of particles (hole). Conventionally, we assume $s = 1, 2$ corresponding to increasing values of the x, y coordinates, respectively, while $s = 3, 4$ are associated with the propagation in the opposite directions $-x$, $-y$.

Starting from the Boolean field N^s_{ij}, at each site one can define a local particle number (occupation number) and momentum given by

$$N_{ij} = \sum_{s=1}^{4} N^s_{ij} \qquad J_{ij} = \sum_{s=1}^{4} N^s_{ij} \hat{c}_s \tag{15}$$

where $\hat{c}_s$ are four unit vectors pointing along the directions defined on the grid.

The evolution rule is as follows: particles are marched one step ahead in the direction of their speed (free propagation) and collide whenever two particles with opposite speeds meet on the same site (head-on collisions). The effect of the collision is to turn the particles' speed at right angles, provided that the new directions are unoccupied: otherwise nothing happens.

It is easy to verify that the only transitions allowed by the conservation laws (number and linear momentum) and the exclusion principle (no more than one particle at each site for a given direction) are those that transform (1010) into (0101) and vice versa.

These simple prescriptions suffice to construct the free-streaming and collision operators acting upon the Boolean field N^s_{ij}. It is easy to verify that the microdynamics induced by these operators leads to the existence of $L_x + L_y$ invariants of motion, L_x and L_y being the number of gridpoints along x and y. These invariants correspond to the longitudinal gridline momenta (LGM), i.e. the total momentum carried by each gridline along the direction defined by the gridline itself. In the square lattice the gridlines are aligned with the macroscopic axes, so that one simply has

$$J^x_j = \sum_{i=1}^{L_x} (N^1_{ij} - N^3_{ij}) \qquad J^y_i = \sum_{j=1}^{L_y} (N^2_{ij} - N^4_{ij}). \tag{16}$$

The invariance of these quantities can be easily verified with no need of formulae. In fact, in the free-streaming phase, particles only move either along a row (column) or perpendicularly to it: obviously in either case the total momentum along the row (column) is left unchanged. This is equally true for the collision step since only head-on collisions between self-balanced doublets $(J_{ij} = 0)$ are allowed. Note that, since the LGM are essentially one-dimensional invariants, their existence provides the ultimate reason for the inability of the HPP automaton to support truly two-dimensional macroconfigurations.

Let us now see what happens in a six-link lattice. In such a lattice we have six propagation directions (although only two of them are linearly independent since the lattice is two dimensional) and a corresponding set of unit vectors $\hat{c}_s$, $s = 1, \ldots, 6$ (see figure 1). Assuming a macroscopic system of coordinates oriented along $\hat{c}_1$ and $\hat{c}_2$, one has

$$\hat{c}_1 = (1, 0) \qquad \hat{c}_2 = (0, 1) \qquad \hat{c}_3 = (-2\cos\alpha, \sin\alpha) \qquad \hat{c}_{s+3} = -\hat{c}_s \qquad s = 1, \ldots, 3 \quad (17)$$

where α is the angular spacing between the links. Owing to the existence of a third direction of propagation, we have now three possibilities (by symmetry, we restrict ourselves to the case of propagation towards non-decreasing values of j):

$$(i, j) \to (i+1, j)$$
$$(i, j) \to (i, j+1)$$
$$(i, j) \to (i-1, j+1)$$

where the numbering of the grid lines follows the scheme depicted in figure 2.

The first two cases are the strict analogue of the HPP grid in non-orthogonal coordinates, while the third one is peculiar to the six-link grid. It is easy to verify that since the particles undergoing the third type of hopping do carry a net momentum along the gridline they quit (both the contravariant components of $\hat{c}_3$ are different from zero), they give rise to an effective exchange of quanta of momentum between the gridlines which destroys the GLM invariance previously discussed†.

The existence of a third link introduces a considerable amount of extra freedom also in the collision phase. In particular, in addition to two-body head-on collisions (direct analogue of HPP), it is now possible to account for three-body encounters which transform (010101) into (101010) and vice versa. While it is still true that these configurations carry no local momentum, they are nonetheless effective in transferring momentum between the lattice gridlines. Again, this contributes to break the grid invariants.

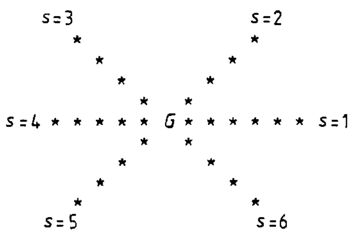

Figure 1. The six links out of a grid point in the FHP lattice.

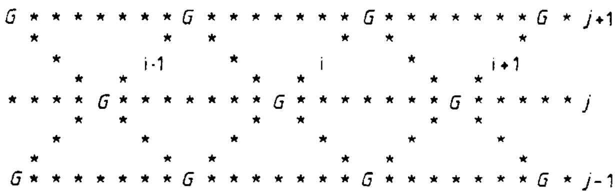

Figure 2. The numbering of grid lines in the FHP lattice.

† We refer here to the direct generalisation of the quantities defined by (16). More specifically J^x and J^y will be replaced by J^x, J^{y1} and J^{y2} where $y1$ and $y2$ are the two vertical oblique directions $s = 2, 3$. So, for example, we have $J_i^{y1} = \Sigma_{j=1}^{L_y} (N_{ij}^2 - N_{ij}^5)$.

Thus in a six-link lattice the LGM cease to be invariant of motion, thereby releasing the degrees of freedom needed to support truly two-dimensional macroscopic configurations. This is the basic physical reason behind the mathematical fact that the momentum flux tensor computed on a six-link lattice displays the correct quadratic component $u_i u_k$, thus allowing a realistic description of non-linear flow regimes which are inaccessible on a four-link lattice.

The fact that the HPP fluid relaxes essentially as a pair of decoupled 1D systems had already been pointed out by Hardy *et al* [1], although in the work of these authors no particular reference to vortex fields as initial conditions was made. In the present work, we have found that the one-dimensional nature of the relaxation becomes manifest from the very early stage of the evolution, thereby preventing even a qualitative study of the vortex dynamics.

We have shown that the anisotropy of the momentum flux tensor of the Hardy-Pomeau-De Pazzis fluid is equivalent to introducing a spurious force which inhibits the correct evolution of two-dimensional vortex structures. In addition, we have presented a few simple arguments which highlight the basic physical reasons why this problem can be circumvented by moving to the six-link lattice introduced by Frisch *et al.*

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