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Negative-Viscosity Lattice Gases

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A new irreversible collision rule is introduced for lattice-gas automata. The rule maximizes the flux of momentum in the direction of the local momentum gradient, yielding a negative shear viscosity. Numerical results in 2D show that the negative viscosity leads to the spontaneous ordering of the velocity field, with vorticity resolvable down to one lattice-link length. The new rule may be used in conjunction with previously proposed collision rules to yield a positive shear viscosity lower than the previous rules provide. In particular, Poiseuille flow tests demonstrate a decrease in viscosity by more than a factor of 2.

KEY WORDS: Lattice gases; cellular automata; viscosity; turbulence.

1. INTRODUCTION

Scientists studying turbulence in fluid dynamics have often turned to computer simulations for insight not readily attainable by analytic theories or laboratory experiments. Simulations of turbulence have remain limited, however: current capabilities allow computations of flows at Reynolds numbers that are only a fraction of those realized in nature.

Motivated in part by the realization of these issues, Frisch, Hasslacher, and Pomeau (FHP)[1] recently introduced lattice-gas automata for the numerical solution of the incompressible Navier–Stokes equations. The lattice gas is a discrete model of a fluid in which identical particles of equal mass populate a regular lattice, obey simple collision rules, and travel to neighboring sites at each time step. Although this discrete model captures only the gross characteristics of true molecular dynamics, the macroscopic behavior of the gas is currently understood to be very close to the Navier–Stokes equations.[2–4]

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So that turbulence may be simulated efficiently by lattice gases, considerable effort has been devoted to the search for collision rules that yield the smallest possible viscosity and therefore the largest possible Reynolds number. Rule optimization has been pioneered by Hénon.[5–7] As he points out, when the simple 2D FHP gas is implemented with collisions that satisfy reversibility (more precisely, "semi-detailed balance"), the rules which minimize viscosity are straightforward to find. However, for 3D lattice gases[8] the overhelming number of possible collisions makes finding the optimal reversible rules considerably more subtle. Hénon has therefore created a general scheme for optimization, the results of which have been successfully applied in ref. 9.

Here I adopt an alternative approach to the minimization of viscosity. The collisions of this new model are irreversible and depend on the local, microscopic momentum gradient. Simply stated, collisions occur such that they results in the maximum possible flux of momentum in the direction of the momentum gradient. This behavior is, of course, contrary to the classical view of molecular viscosity as a mechanism which acts to diffuse momentum. Consequently, the model has as a possible outcome the appearance of a nonphysical negative viscosity. Importantly, the new, negative-viscosity collision rules may be statistically mixed with the old, positive-viscosity rules to yield a positive viscosity which is smaller than that obtained from previously published schemes. As an example, I present a numerical result demonstrating a decrease in viscosity by more than a factor of 2 for a 2D model.

2. THE RULE

The negative-viscosity collision rule is essentially a generalization of the rule used in ref. 10 to model surface tension in a fluid composed of two components, say, a "red" phase and a "blue" phase. In that model, collisions are designed to maximize the flux of color in the direction of the color gradient. For certain choices of parameters, the red phase separates from the blue phase, and surface tension is found at the interfaces. The mechanism for phase separation arises because the diffusivity of the minority phase in a mixture is negative, as has been confirmed by both theoretical prediction and numerical simulation.[11]

The negative-viscosity rule is a tensorial extension of the two-phase rule: instead of directing the flux of color up the color gradient in a two-phase fluid, the new rule directs the flux of momentum up the momentum gradient in a single-phase fluid. Thus, the diffusivity of momentum—the kinematic viscosity—can be negative.

I use the 2D FHP hexagonal lattice gas as an example (generalization

to 3D is straightforward). The moving-particle velocities at a site are numbered from 1 to 6, with $\mathbf{c}_j = (\cos(2\pi j/6), \sin(2\pi j/6))$. A fixed number m of identical but distinguishable rest particles is also allowed at each site; thus, $\mathbf{c}_{6+k} = 0$, $k = 1,..., m$.

The configuration at a site where a collision occurs is denoted by $n = \{n_i\}$, $1 \leqslant i \leqslant 6 + m$, where $n_i = 1$ if the ith velocity cell is occupied, and 0 if it is not. The configuraition at the nearest-neighbor site in direction $\mathbf{c}_j$ is denoted by $n^j = \{n_i^j\}$. The momentum-gradient tensor $G_{\alpha\beta}$ is then defined as

$$G_{\alpha\beta} = \tfrac{1}{2} \sum_j \mathbf{c}_{j\alpha} \sum_i n_i^j \mathbf{c}_{i\beta} \tag{1}$$

where Greek letters represent vector or tensor indices and Roman letters indicate particle velocities. Note that $G_{\alpha\beta}$ is just the discrete analog of $\partial_\alpha(\rho u_\beta)$, the momentum gradient in a continuum fluid.

The ith velocity cell's contribution to the flux of α momentum in the β direction (or vice versa) is $n_i \mathbf{c}_{i\alpha} \mathbf{c}_{i\beta}$. The sum of the flux of each component of momentum in the direction of that component's gradient is thus $n_i \mathbf{c}_{i\alpha} \mathbf{c}_{i\beta} G_{\alpha\beta}$ (summation over repeated Greek indices is assumed). The simplest model of a negative viscosity is then one in which the collision rule $n \to n'$ is such that the sum over the gradient-directed momentum fluxes,

$$\sum_i n_i' \mathbf{c}_{i\alpha} \mathbf{c}_{i\beta} G_{\alpha\beta} \tag{2}$$

is maximum, subject to the contraints of mass and momentum conservation.

Such a scheme indeed produces the desired results. However, collisions directed up the gradient $G_{\alpha\beta}$ maximize not only shear, but also compression (or dilatation) as well. Since only the shear viscosity is of interest, I use instead the traceless momentum gradient

$$G'_{\alpha\beta} = G_{\alpha\beta} - \tfrac{1}{2} \delta_{\alpha\beta} G_{\gamma\gamma} \tag{3}$$

which is the same form used in classical derivation of the shear viscosity.[13]

The momentum flux of interest is then given by

$$F(n) = \sum_i n_i \mathbf{c}_{i\alpha} \mathbf{c}_{i\beta} G'_{\alpha\beta} \tag{4}$$

The result of a collision is determined by solving

$$F(n') = \max_{n''} F(n'') \tag{5}$$

subject to the constraints of mass conservation,

$$\sum_i n_i'' = \sum_i n_i \tag{6}$$

and momentum copnservation,

$$\sum_i \mathbf{c}_i n_i'' = \sum_i \mathbf{c}_i n_i \tag{7}$$

Equations (5)–(7) thus constitute the negative-viscosity rule. If more than one n' satisfies these equations, then the outcome of a collision is chosen randomly from the set of all possible solutions. After the collisions have occurred, each particle n_i' advances with velocity $\mathbf{c}_i$.

Several remarks are now appropriate. First, note that the second term on the right-hand side of Eq. (3) may affect the solution of Eq. (5) only via the creation or destruction of rest particles. Accordingly, I have chosen to use an 8-bit model with $m=2$ rest particles per site. Second, note that, although the elements of $G_{\alpha\beta}$ may change upon rotation of the coordinate axes, the rule given by equations (5)–(7) is statistically isotropic. To implement this rule, I have found it sufficient to simply compute the sign of each element of $G_{\alpha\beta}$. These four terms, together with a number specifying the mass and momentum invariants, are then input to a table that gives the outcome of a collision.

3. NUMERICAL EXPERIMENTS

3.1. Unforced Flow

Figure 1 illustrates a typical result with the 8-bit negative-viscosity model. There is an average of 3.2 particles per site on a 32×32 lattice. The initial condition was a net momentum of zero at each lattice site, and thus zero momentum in total; the boundaries are periodic in both directions. No forces have been applied. The flow vectors represent the momentum flux at each site averaged over 25 time steps beginning at time step 2000. (The flow is indeed unsteady, but only at a time scale much slower than one time step.) No spatial averaging has been performed.

The result is a strongly unstable fluid, with structure in the momentum field at the smallest possible scale. Because collisions seek to either maintain or enhance gradients in momentum, the "equilibrium" flow field is one in which the momentum has nearly separated in space; i.e., while the total momentum remains zero, about half the fluid is moving quickly in one direction at the same time the other half is moving quickly in the opposite

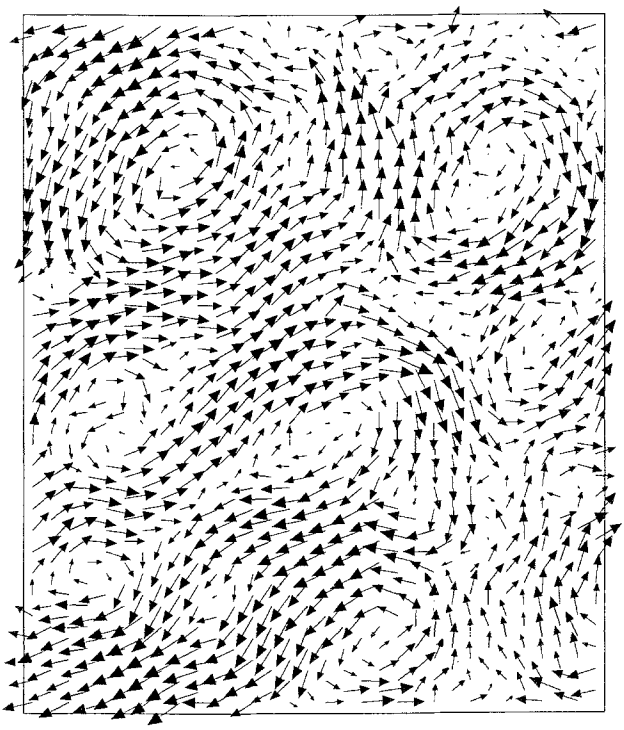

Fig. 1. Momentum flux in the negative-viscosity lattice gas, illustrated after 2000 time steps. Each vector represents the flux of momentum at a single site, averaged over 25 time steps. The initial condition was zero momentum at each site. Boundaries are periodic in both directions.

direction. This separation of momentum, which produces order in the flux field, is the vector-field analog of the separation of mass in the two-phase model of ref. 10.

If a negative viscosity were to exist in nature, velocity gradients would increase without bound. Such behavior is impossible in a lattice gas because the particle velocities are at most one lattice unit per time step. The ability to obtain such a highly resolved picture of the momentum flux by averaging each site over only 25 time steps is probably due to the spatial correlation in velocity induced by the negative viscosity.

3.2. Poiseuille Flow

As mentioned in the introduction, the negative-viscosity rules can be statistically mixed with conventional collision rules to obtain a smaller positive viscosity and thus typical hydrodynamic behavior. I choose as the "conventional" rules collisions that choose randomly from the set of con-

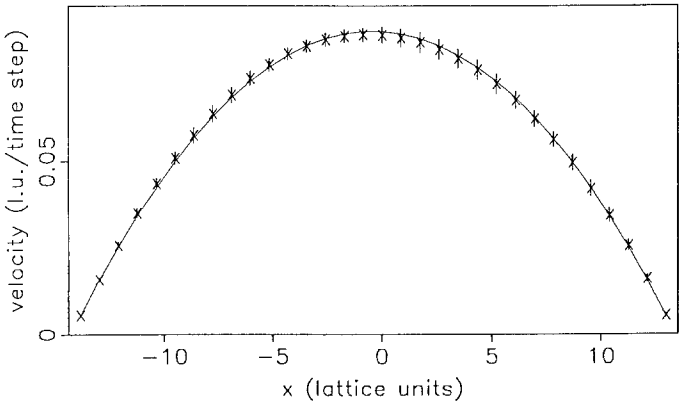

Fig. 2. The results of simulations of Poiseuille flow, compared to the theoretical profile predicted by Eq. (8). The negative-viscosity rules were used with probability $p = 0.45$. The measured viscosity is less than half that of the corresponding collision-saturated model where $p = 0$. Error bars represent one standard deviation from the average of 10 independent simulations performed over 10^5 time steps each.

figurations that conserve mass and momentum, and, if possible, result in an output configuration not equal to the input configuration. (These rules are similar to model III of ref. 12.) The negative-viscosity rule then occurs with probability p, while the other rule occurs with probability $1 - p$.

The gross features of such a scheme are well-tested by simulating Poiseuille flow in a channel. Standard theory (e.g., ref. 13) predicts that the velocity profile is the parabola given by

$$u_y(x) = -\frac{\partial p}{\partial y}\frac{R^2 - x^2}{2\mu} \tag{8}$$

where μ is the dynamic shear viscosity, $\partial p/\partial y$ is the pressure gradient, and the channel walls are taken at $x = \pm R$. To measure the viscosity, I used the square-wave forcing technique of ref. 14 on a 32×64 lattice.[2]

Figure 2 shows the velocity profile obtained with $p = 0.45$ and an average of 3.2 particles per site. Ten simulations with different initial conditions were performed. The data points were obtained by computing the average y velocity at each x location during each time step, averaging these points over 10^5 time steps, and finally taking the mean of the velocity profiles obtained in the 10 simulations. The error bars represent one

[2] Due to coding complications, the clever "Möbius-strip" boundary conditions of ref. 14 could not be used. The square-wave force was thus explicitly modeled with half the lattice forced in the positive y direction, and the other half forced in the other direction. After accounting for sign differences, the profiles in the two channels were then averaged.

standard deviation in the final average of 10 points. The data are compared to the parabolic profile predicted by Eq. (8), where μ was obtained from the average flow rate. The computed value of the dynamic viscosity is $\mu = 0.198 \pm 0.004$ (the kinematic viscosity $\nu = 0.0536 \pm 0.0012$). In contrast, a similar test without the negative-viscosity rule ($p = 0$) yields $\mu = 0.431 \pm 0.006$ ($\nu = 0.117 \pm 0.002$), greater by a factor of 2.2.

Hydrodynamic behavior at viscosities significantly lower than that reported here proved difficult to obtain. Further numerical experiments showed that the viscosity goes negative for p greater than about 0.6.

4. DISCUSSION AND CONCLUSIONS

This study has demonstrated two key points. First, lattice-gas collision rules can be designed to yield a negative viscosity. Second, these new rules can be implemented in such a way as to obtain positive viscosities that are lower than previous rules have provided. Poiseuille flow tests show a decrease in viscosity by more than a factor of 2.

Although this investigation has been purposely phenomenological, analytic study of such a collision rule is possible. It is shown in ref. 11 how a discrete Boltzmann equation may be solved to predict the conditions under which the diffusivity of color goes negative in the two-phase model of ref. 10. Much the same analysis may be performed here to predict where the viscosity changes sign. Further analysis similar to that described in ref. 15 should also be done to ascertain the affects of the loss of semi-detailed balance.

Finally, a practical limitation is worth noting. If a positive viscosity were so small that the dissipation scale were less than a lattice-link length, the hydrodynamic limit of the lattice gas may no longer hold. Instead, one would expect a "grid viscosity" to result from the lattice discretization. Thus, beyond a certain limit in viscosity, increasing the length scale of a simulation may be the only way to increase the Reynolds number. Nevertheless, this new ability to decrease viscosity brings lattice-gas simulations significantly closer to modeling turbulence.

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NOTE ADDED IN PROOF

After the conclusion of this work, Dubrulle, Frisch, Hénon, and Rivet [16] reported results with an irreversible three-dimensional lattice gas model for which a Boltzmann approximation predicts a negative viscosity. Results of simulations, however, do not exhibit a negative viscosity.

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