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Noise and compressibility in lattice-gas fluids

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Computations are reported in which the hexagonal lattice gas is used to simulate two-dimensional Navier-Stokes shear flows. Limitations associated with noise in the initial loading and compressible effects associated with a velocity-dependent equation of state arise and interact with each other. A relatively narrow window in density and flow speed exhibits physical behavior.

The purpose of this paper is to remark upon some potentially nontrivial limitations which may somewhat restrict the use of cellular automata as fluid simulation tools. In particular, we discuss the two-dimensional hexagonal lattice gas. This model has recently been proposed as a simulator of two-dimensional Navier-Stokes flows[1–4] and of two-dimensional magnetohydrodynamics.[5] Some related considerations have been remarked upon by Orszag and Yakhot[6] at a more abstract level.

There are two interacting limitations which we wish to describe and then illustrate with the Shimomura-Doolen computer code. The first and more obvious one concerns the restrictions that must be placed on the density and fluid velocity in order that the Navier-Stokes equation itself shall be an accurate approximation to the macrodynamics of the cellular automaton. Unless the particle number density n is less than 3 particles per hexagon, the equation of motion acquires a strong and unphysical density dependence through a factor $(3-n)/(6-n)$ in the advective term.[1,2] In addition, the fluid velocity $\mathbf{u}$ must satisfy $u^2 \ll 1$ (low Mach number) in order that the conventional criteria[7,8] for incompressible flow be met. The macroscopic equations of the hexagonal lattice gas seem not to be close to any recognized description of compressible flow when the density gradients become significant.[2]

The joint requirements of $n<3$ and $u \ll 1$ raise statistical questions connected with the smooth representation of macroscopic fluid variables from the microscopic random loading. Even at the level of producing acceptable initial conditions for the macroscopic velocities and densities, these can be severe, independently of questions of time evolution. The random density variations δn and velocity variations $\delta\mathbf{u}$ are essentially governed by the Poisson distribution. For instance, $\delta n/n$ is roughly $N_{ss}^{-1/2}$, where N_{ss} is the number of particles per supercell. (A supercell is a region of the plane containing many adjacent hexagons over which the microvariables are averaged to give fluid variables.) The largest array of supercells which will fit comfortably into the core memory of, say, the CRAY XMP is $(64)^2$ supercells of $(64)^2$ hexagons each. (This resolution can be improved with currently available solid-state disk memories.)

If $n \cong 1$ per hexagon is taken as typical of densities which are less than 3, this implies $N_{ss}^{-1/2}$ is of the order of 1.6%. An initial condition which we have studied intensively is the initial shear flow velocity $\mathbf{u}=u_0\hat{e}_x\sin(ky)$. This initial condition should lead to simple viscous decay with no distortion of the spatial profile. We will argue later that the second limitation to be described restricts u_0 to be $\lesssim 0.1$. A $|\delta\mathbf{u}|$ of the order of 1%, which also results from supercells of $(64)^2$ hexagons at a density of $n \cong 1$ thus implies at least a 10% error in representing the velocity field $\mathbf{u}(\mathbf{x};t=0)$, and more away from its maximum. This would not be considered acceptable accuracy for, say, a spectral method computation.

We illustrate by noting what random initialization will provide for the shear flow initial condition $\mathbf{u}(\mathbf{x};t=0)=u_0\hat{e}_x\sin y$, with periodic boundary conditions, at nearly uniform density. At $n=0.9$ per hexagon, we obtained $\delta n/n \cong 1.2\%$ with $(64)^2$ hexagons per supercell, $\delta n/n \cong 0.8\%$ at $(128)^2$, and $\delta n/n \cong 0.6\%$ at $(256)^2$. For $u_0=0$, these three typical loadings led to rms values of δu_x (x-component of macroscopic velocity) of 0.0109, 0.0077, and 0.0054, respectively. These fluid velocity fluctuations are of the same typical magnitudes as those about $u_0=0.1 \ll 1$, for the same n. This implies an error near the maximum of $\mathbf{u}$ of about 10%, 7.7%, and 5.4%, respectively, with *larger* fractional errors away from the maxima. Only the $(64)^2$ case of these three resolutions is realistic under present circumstances.

The second class of difficulties arise from the fact that a kinetic theory derivation of the pressure tensor leads to the expression

$$\mathbf{p} \cong \frac{n}{2}\mathbb{1}(1-u^2/2)-\frac{n\mathbf{u}\mathbf{u}}{2} \ . \tag{1}$$

The tensor part of the $\mathbf{u}$ dependence can be absorbed in the advective term of the equation of motion and its distorting effects neutralized by a rescaling of the time, under some circumstances.[1] However, the $u^2/2$ in the scalar part of the pressure cannot be made to disappear. Even when the conventional tests for incompressibility[7,8] are met, the u^2 dependence can lead to unphysical compressible behavior. Particularly for the case of shear flows with nearly uniform density and small $\mathbf{u}\cdot\nabla\mathbf{u}$, the force due to the scalar pressure is

$$-\nabla[(n/2)(1-u^2/2)]\cong(n/4)\nabla u^2 \ . \qquad (2)$$

Equation (2) can represent an unbalanced volume force which is the largest one in the problem. Even for rather modest values of $\mathbf{u}$ this force, which is mainly prependicular to $\mathbf{u}$, can launch compressible oscillations which are the most prominent feature of the behavior. An acceleration is produced which accelerates mass toward the crests of u^2 until enough density is built up for it to be repelled. The resulting oscillations superficially resemble sound waves, but have a different physical origin in the velocity-dependent pressure. They are unrelated to the Navier-Stokes equation or processes occurring in a real fluid. To the extent that n *is* uniform and cancels out, Eq. (2) remains as a rather severe constraint on allowable velocity fields.

Initial conditions of the previously alluded to profile, $u_0\hat{e}_x \sin y$ and uniform density, are allowed to evolve using the code. Figure 1(a) shows the space-averaged computed values of nu_x^2 as a function of time for $u_0=0.3$, 0.2, and 0.1, all normalized to the total initial space-

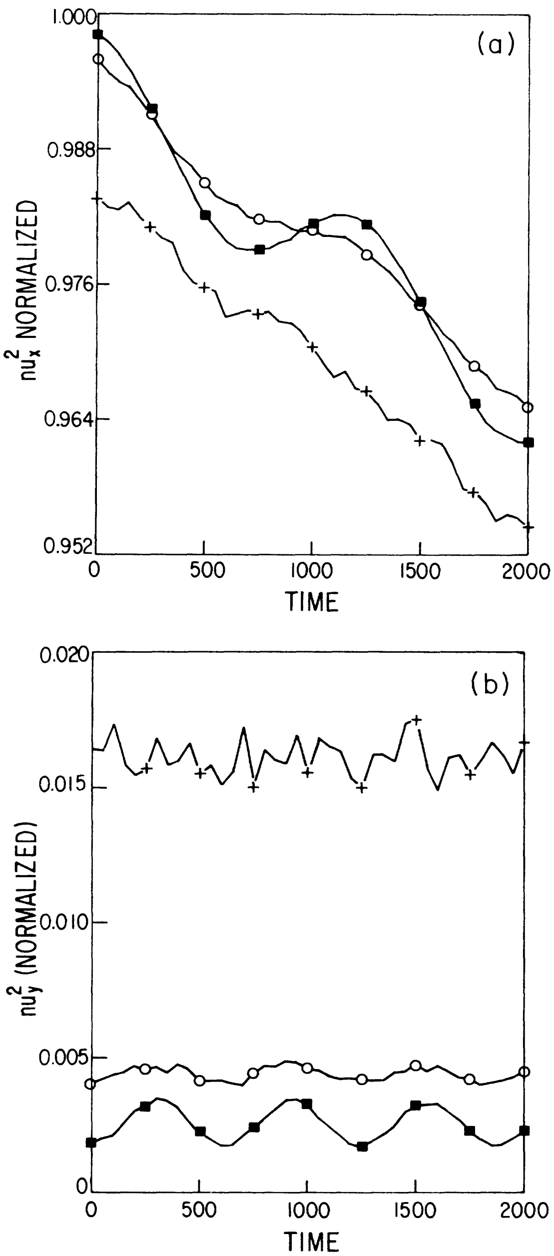

FIG. 1. (a) Streamwise component of the volume-averaged total kinetic energy vs time. Particle density is 1.2, hexagon, with $u_0=0.1$ (crosses), $u_0=0.2$ (open circles), and $u_0=0.3$ (black squares). Energy is expressed as a fraction of the total fluid kinetic energy in both directions. (b) Cross-stream component of kinetic energy for the same three situations as in (a). This quantity should be zero for the Navier-Stokes equation, compressible or incompressible. (Normalization is to the total initial fluid energy.)

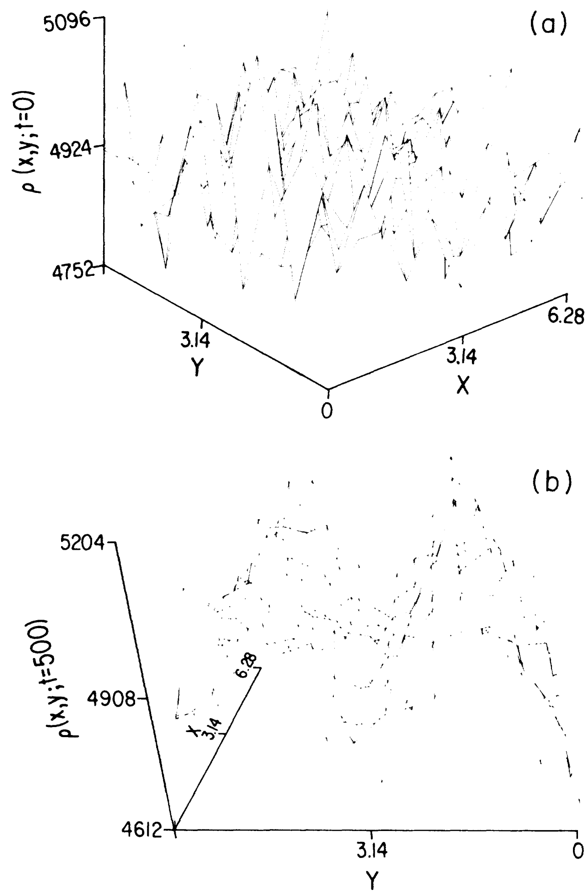

FIG. 2. (a) Density variations due to random loading for $\rho=1.2$ per hexagon and $u_0=0.3$. Supercell mass density ρ is plotted as a function of x and y. (b) Density variations which have developed from the situation shown in (a) as a result of pseudosoundwaves; time is 500 integer time steps. This is the same run that is depicted with black squares in Figs. 1(a) and 1(b).

averaged $n\mathbf{u}^2$. A simple exponential decay is predicted for this quantity from both the compressible and incompressible Navier-Stokes equations, since periodic boundary conditions are imposed. The three curves of Fig. 1(a) display the oscillations which arise, even in this global quantity, when the amplitude u_0 exceeds about 0.1. Figure 1(b) shows the space-averaged nu_y^2 versus t for the same runs: a quantity which is analytically predicted to remain zero, for velocity-independent equations of state. Figure 2 shows three-dimensional perspective plots of the density as a function of x and y for the rather extreme case of $u_0=0.3$. Figure 2(a) shows the initial conditions for which the average percentage variation of $\delta n/n$ is about 1% but with a min-to-max variation of about 7.4%. Figure 2(b) shows $\delta n/n$ at $t=500$ during the resulting evolution, with a $\delta n/n$ about 2.2% and a min-to-max variation of about 12.5%. [A similar oscillation has been obtained with a compressible spectral

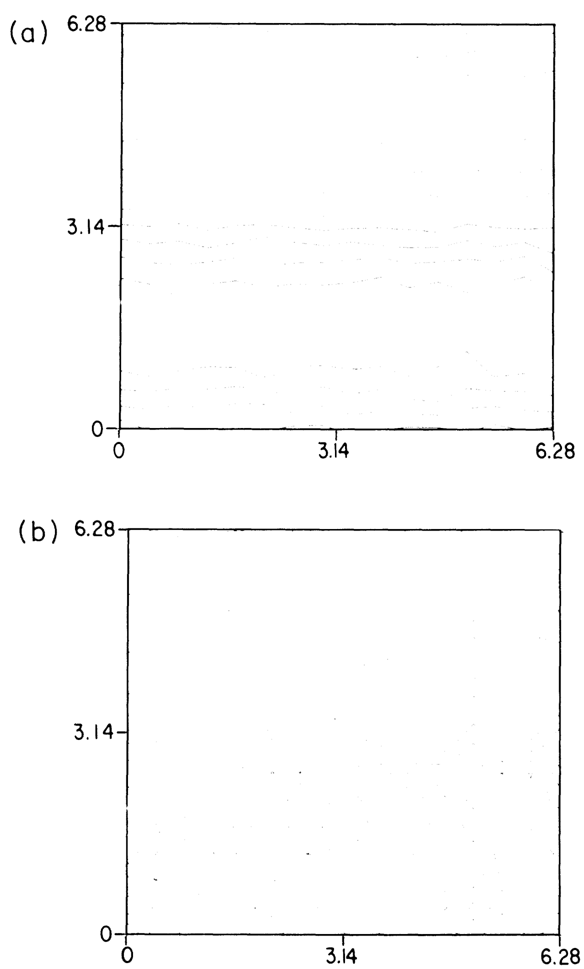

FIG. 3. (a) Contours of $u_x(x,y)=\text{const}$ for $u_0=0.2$. Contours, evaluated at $t=0$ are not straight, but could possibly be said to represent the velocity field desired. Density is 0.9 per hexagon at $(32)^2$ supercells and $(64)^2$ hexagons per supercell. (b) Everything is identical with (a) except that now, $u_0=0.05$. The flow pattern is essentially lost in the noise.

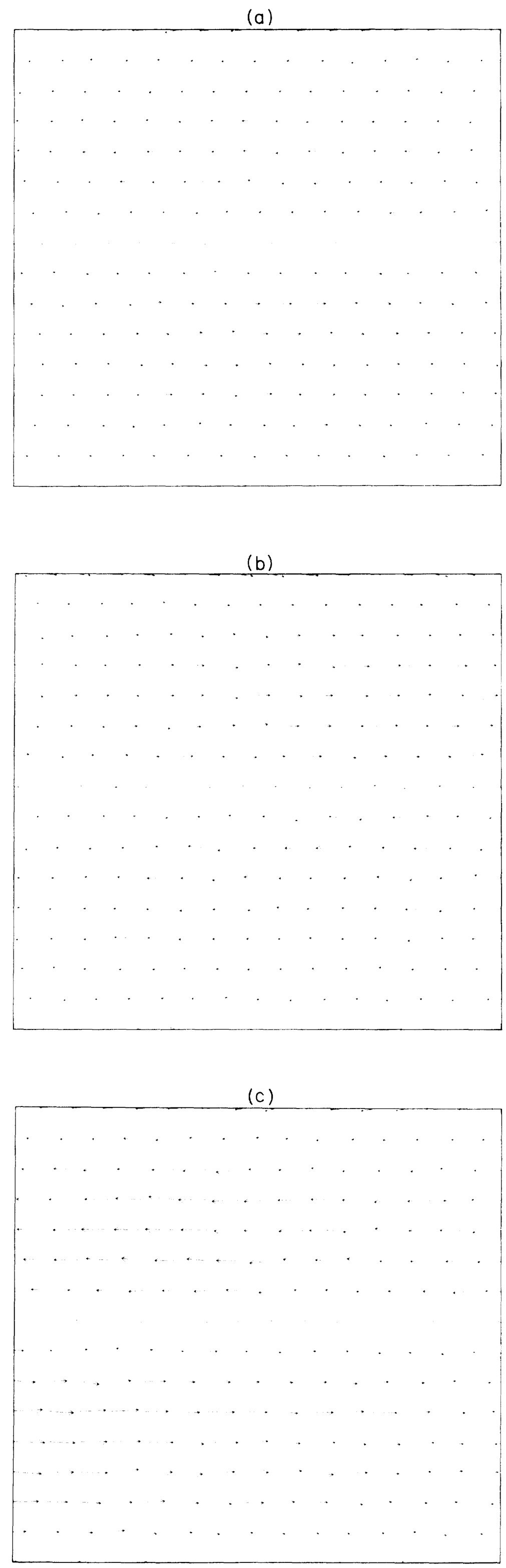

FIG. 4. Arrow plots of the velocity field at three different times in the presence of three-body symmetry scattering only. $u_0=0.5$, density is 1.2 per hexagon. Times are (a) $t=0$; (b) $t=850$; (c) $t=1750$. A totally unphysical oscillation is observed in u_x.

method code, and a pressure tensor given by Eq. (1), independently.] Even if the $\delta n/n$ variation may damp somewhat after several sound-wave transit times, the u-dependent density variations remain important.

Figure 3 returns to the question of a satisfactory representation of laminar initial conditions for fluid variables. They illustrate the dangers of attempting to achieve nearly imcompressible flows by going to low enough flow speeds u_0. They show contours of constant u_x, which should be straight lines, for $u_0=0.2$ and 0.05 at $t=0$. The noise associated with the finite-size supercell virtually destroys the flow in the latter case.

A final remark concerns still another inequality that needs to be satisfied for the desired fluid behavior to emerge: that the collision mean free path λ_c be much less than a supercell dimension. At low densities, the mean free path for two-body collisions is of the order of $\lambda_c \sim 6/n$. At the densities described here, this is about six hexagon dimensions, safely less than the dimensions of a 32×32 supercell. We illustrate the effects of a too-long λ_c by artificially suppressing the two-body collisions, and allowing whatever relaxation occurs to occur as a consequence of three-body symmetric (3*S*) collisions only.[2] What is shown is the rather extreme case of $u_0=0.5$ with 1.2 particles per hexagon and $(32)^2$-hexagon supercells. The mean free path λ_c and mean collision time can be inferred directly from the computation by counting the collisions that occur and knowing the number of particles. For this case, $\lambda_c \cong 64$. An unphysical oscillation in the sign of the velocity field results, as can be seen from Fig. 4. This effect is reminiscent of echo phenomena, but its origin is not understood in detail; it may be typical of interesting but unphysical regularities to be expected when thermal relaxation is incomplete in the presence of such a high degree of microscopic symmetry.

What appears to have emerged, for the two-dimensional hexagonal lattice gas, is at present a rather narrow window in density and velocity around $n\cong 1$ and $u\cong 0.1$ in which the behavior can seem to be said to be that of an incompressible Navier-Stokes fluid.[9] The need seems to be for substantially larger arrays than are now available with in-core memory simulations, since the uniformly distributed random noise in $\mathbf{u}$ can easily be greater than the $\mathbf{u}$ being simulated, away from the maxima of $\mathbf{u}$. We do not see any easy or early resolution of these limitations, either for hydrodynamics or magnetohydrodynamics. The discussion echos debates of 20 years ago between the random loading and "quiet start" schools of electrostatic particle-in-cell (PIC) plasma simulators.[10] A fully satisfactory resolution to those difficulties has never emerged, in the sense that noise remains a stubborn problem in simulating laminar phenomena such as plasma oscillations.

The resolution of the question of the utility of the lattice gas method for solving the Navier-Stokes equations depends on the computer technology available. To resolve low velocity fields requires a large number of cells, and the current technology dictates the number of cells one can afford to run.

For example, in the two-dimensional hexagonal model the information completely describing ten 2/3 cells can be stored in one 64-bit CRAY word, and independent logical operations on each of the 64 bits can be completed each clock cycle. Because each of the four heads on a CRAY XMP contains two logical vector units, bit logic can be done at the rate of about 10^{11} bits/sec. Because the solid-state disc memory for the CRAY XMP can store 512 000 000 words, about 5×10^9 cells can be modeled. Hence problems with $100\,000\times 50\,000$ cells can be run at the rate of three universe updates per sec, enabling effects which range over 5 orders of magnitude in space to be run in a reasonable time.

In a three-dimensional hydrodynamic model, 24 bits are required per cell. About two cells can be packed in each 64-bit word, allowing 1 000 000 000 cells to fit into CRAY's solid-state disk. Using table look up for the scattering rules and a clever moving algorithm written by Shimomura (private communication), about 50 000 000 cells can be updated each second.

Special-purpose computers constructed with present technology can be made to go to orders of magnitude faster than the serial processors described above. Hence we will probably be unable to determine precisely the utility of the lattice-gas method for some time to come.

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