Optimal initial condition for lattice-gas hydrodynamics

S. Chen, Zhen-Su She,* L. C. Harrison, and Gary D. Doolen
Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
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A method for minimizing the unphysical oscillations in simple lattice-gas hydrodynamic models is presented. Numerical simulations of two types of shear flows are reported that illustrate the usefulness of this method.

I. INTRODUCTION

Lattice-gas methods have been used to simulate Navier-Stokes fluids and many other physical systems.[1–3] These methods fully exploit the properties of discreteness and local interactions. Several reports have recently pointed out some problems of these methods.[4,5] In particular, Dahlburg, Montgomery, and Doolen[5] found unphysical energy oscillations in a lattice gas simulating Kolmogorov free decay flows, whose kinetic energy should decrease monotonically. In their paper, it was correctly explained that the cause of this phenomena is an unphysical compressibility contained in the equation of state of the lattice gas. In this paper, we propose a procedure for choosing initial conditions which minimize these oscillations. We illustrate this procedure using the FHP-I model[1,6] for simplicity.

II. DESCRIPTION OF THE UNPHYSICAL OSCILLATION

The lattice gas theory is based on an asymptotic expansion with two small parameters; the Mach number, and $\epsilon = 1/S$, where S is the characteristic size of the supercell over which spatial averages are taken. For lattice-gas calculations, these parameters are finite, introducing fluctuations in macroscopic quantities. These fluctuations propagate at the sound speed ($1/\sqrt{2}$ in FHP-I model).

The dependence of pressure p on density n and velocity u has the form[6]

$$p = (n/2)[1 - g(n)(u^2/c^2)] \ . \tag{1}$$

Here c is the particle propagation speed (1 for the FHP-I model) and $g(n) = (n-3)/(n-6)$. For convenience, we separate the density into two parts,

$$n = n_0 + n' \ , \tag{2}$$

where n_0 is a constant and n' is the density fluctuation.

As seen from Eq. (1), the low-speed regions have higher pressures for constant density. If we initialize a constant density ($n'=0$) and a nonuniform velocity, a spatially nonuniform pressure results. This nonuniform pressure is the driving force which causes the fluid to redistribute its density. As time evolves, the density fluctuation n' becomes positive in the higher-speed regions and negative in the lower-speed regions. Damped periodic oscillations in n' can occur. We demonstrate this behavior in the FHP-I model with a uniform initial density, an x-direction velocity distribution, $u_x = U_0 \sin(2\pi y/L)$, and $u_y = 0$ (Kolmogorov flow). Here L is the width of the flow. For $U_0 = 0.2$, we show in Fig. 1(a), the density distribution at three times during the first oscillation. For all plots, n_0 is 1.2 particles per cell, 2048×2048 cells are used, and the supercell size is 64×2048 cells.

The importance of this oscillation phenomenon is best illustrated when we use $U_0 = 0.3$. In Fig. 2, we show the time evolution of the normalized streamwise kinetic energy $E_x = \sum_V n u_x^2$, where V denotes the whole periodic box. We see that the kinetic energy of the system can sometimes increase unphysically in this force-free decay flow (the dashed line in Fig. 2). In Fig. 3, we show the time evolution of the cross-stream kinetic energy, $E_y = \sum_V n u_y^2$. Notice that the oscillation frequency of the energy in the streamwise component is half that of cross-stream component. Both oscillation periods can be understood as follows: we separate velocities into two parts, a constant part and a fluctuating part,

$$u_x = u_x^{(0)} + u_x^{(1)} \ ,$$
$$u_y = u_y^{(0)} + u_y^{(1)} \ . \tag{3}$$

For Kolmogorov flow, $u_y^{(0)} = 0$ and $u_x^{(1)} \ll u_x^{(0)}$. We as-

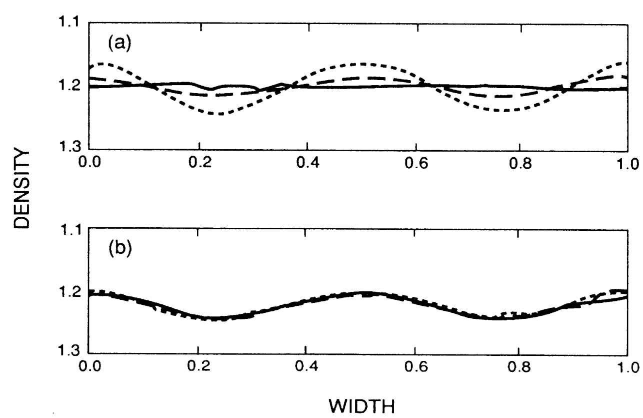

FIG. 1. Density distribution (particles per cell) of the Kolmogorov flow at times: $T=0$, $\frac{1}{4}$, and $\frac{1}{2}$ of the oscillation period with initial velocity of 0.2: (a) at constant initial density; (b) at constant initial pressure.

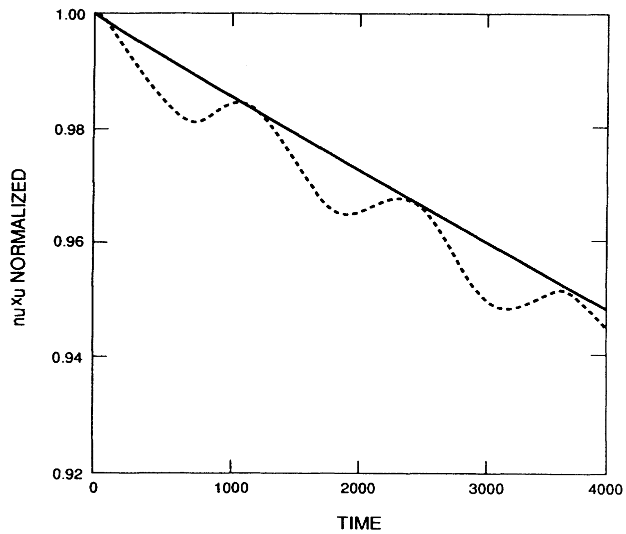

FIG. 2. Streamwise kinetic energy for Kolmogorov decay flow vs time in cell update units. The dashed line describes the behavior for constant initial density. The solid line describes constant initial pressure. For both cases, the maximum velocity is 0.3.

sume that the fractional fluctuation of density and velocity are the same order of magnitude and have the same propagation speed, i.e., the sound speed

$$n' = \delta n + \bar{n}\exp[i(kx - \omega t)] ,$$
$$u_x^{(1)} = \delta u_x + \bar{u}_x \exp[i(kx - \omega t)] , \quad (4)$$
$$u_y = \delta u_y + \bar{u}_y \exp[i(kx - \omega t)] .$$

Here, δn, δu_x, and δu_y are the fluctuations due to the finite-size supercell average. Wavelength equals $2\pi/k$ and frequency equals $2\pi\omega$. $\bar{n}$, $\bar{u}_x$, and $\bar{u}_y$ are the amplitudes of the perturbations corresponding to propagation waves. From the dashed line in Fig. 3, we see that the oscillation due to the pressure wave sits on the top of a background caused by the supercell average. We see that, for example, these two groups of fluctuations have the same order of magnitude.

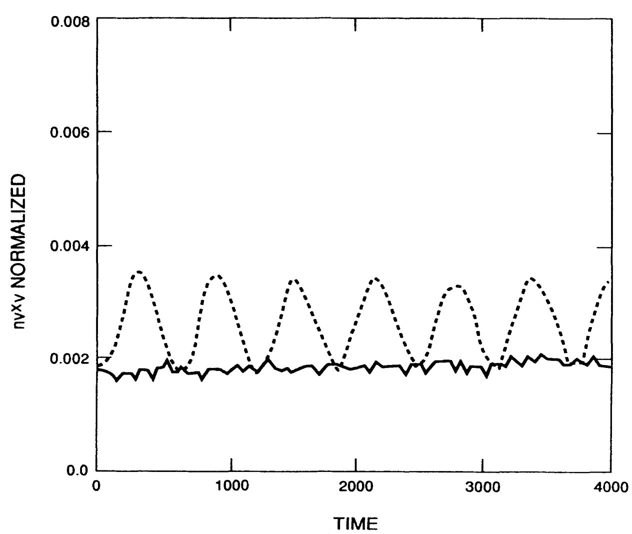

FIG. 3. Cross-stream kinetic energy for the Kolmogorov flow in Fig. 2 (normalized to the total initial streamwise kinetic energy).

Substituting Eqs. (3) and (4) into E_x and E_y, we obtain, to the leading order in n' and $u^{(1)}$,

$$E_x = \sum_V (n_0 u_x^{(0)2} + n' u_x^{(0)2}) ,$$
$$E_y = \sum_V n_0 u_y^{(1)2} . \quad (5)$$

We see that E_x has the oscillation frequency $2\pi\omega$, while E_y has an oscillation frequency $4\pi\omega$. Moreover, $\bar{n}$, $\bar{u}_x$, and $\bar{u}_y$ are directly related to the velocity amplitude through Eq. (1). Hence the oscillation may or may not dominate the exponential decay of the energy. There is no energy increase in the Kolmogorov flows when $U_0 = 0.2$ [see also (5)], but for $U_0 = 0.3$, we see from the dashed line in Fig. 2 that the kinetic energy can increase with time.

In addition, we see that the oscillation behaves like a typical sound-wave process. This can be checked by measuring the propagation speed from the oscillation period of the cross-stream part of the kinetic energy (see Fig. 3). Using the distance between a point of zero velocity and maximum velocity, $l = 256\sqrt{3}$, and the oscillation period $T = 624$, we obtain a speed of propagation, $c = l/T = 0.711$, which is within 1% of the theoretical sound speed.

III. MINIMIZATION OF UNPHYSICAL OSCILLATION BY CHOOSING OPTIMAL INITIAL CONDITIONS

Lattice-gas hydrodynamic equations consist of a continuity equation and the Navier-Stokes equation. They have been derived for incompressible fluids for which $\nabla \cdot \mathbf{u} = 0$. This incompressibility condition combined with the Navier-Stokes equation requires the following Poisson equation for the pressure:

$$\nabla^2 p = -n_0 g(n_0) \nabla \cdot (\mathbf{u} \cdot \nabla \mathbf{u}) . \quad (6)$$

It can be shown that $\nabla \cdot \mathbf{u} = 0$ and (6) are sufficient conditions to satisfy $\partial n / \partial t = 0$ for the initial conditions, ignoring viscous effects. The vanishing of this time derivative is what is required to significantly reduce the effect of the unphysical oscillations.

A. Optimal initial conditions for the Kolmogorov flow

Using (1), the equation of state, we can also write (6) in the following form:

$$\nabla^2 n' = n_0 g(n_0) [-2\nabla \cdot (\mathbf{u} \cdot \nabla \mathbf{u}) + \nabla^2 u^2] . \quad (7)$$

For the Kolmogorov decay flow with a constant initial density, the left-hand side of Eq. (7) vanishes, but the second term on right-hand side does not vanish initially. One method of reducing the unphysical oscillations for energy decay is to require Eq. (7) to be satisfied for the initial condition, for example,

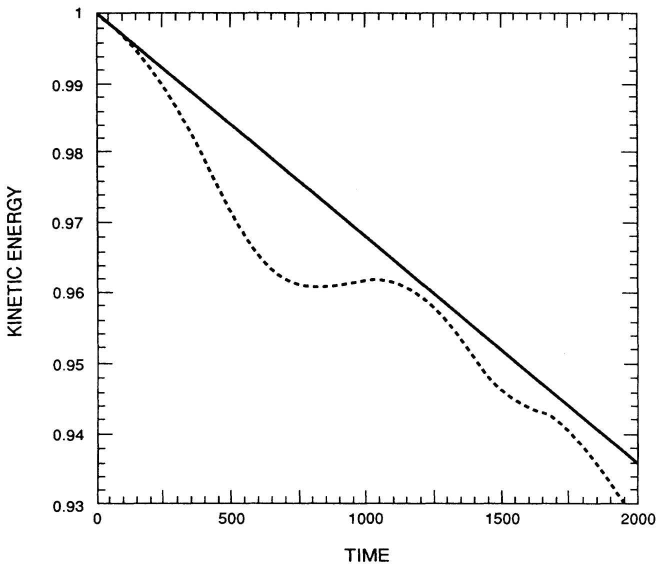

FIG. 4. Normalized total kinetic energy for Green-Taylor vortex with $U_0=0.3$ vs time in cell update units. [solid line for Eq. (10) initial density; dashed line for constant initial density].

$$n'=n_0 g(n_0)u^2 \ . \tag{8}$$

In Fig. 1(b) we show the density distribution at different times, starting from a density distribution given by (8). We can see here only small fluctuations around the initial density due to the finite supercell average. This is a much improved result compared with the large global density oscillations of Fig. 1(a). The initial density (8) produces a constant pressure distribution. There is no initial unbalanced force in the system. In Figs. 2 and 3 we give the streamwise and cross-stream components of energy decay for this Kolmogorov flow (solid lines). The streamwise kinetic energy decays exponentially. The cross-stream energy remains constant. We conclude that by requiring constant initial pressure loading, we can eliminate the unphysical oscillation. Note that the maximum speed here is 0.3 and the Mach number is 0.424.

B. Optimal initial conditions for Green-Taylor vortex flow

For a more general test of the constraint, Eq. (6), we consider a vortex flow with the stream function given by

$$\psi=U_0 \sin(x)\sin(y) \ . \tag{9}$$

We call this a two-dimensional Green-Taylor vortex flow. This flow initializes to a nonuniform pressure, in contrast with the Kolmogorov flow. The solution of (7) gives the following initial density profile:

$$n'=n_0 g(n_0)u^2+n_0 g(n_0)U_0^2\frac{\cos(2x)+\cos(2y)}{2} \ . \tag{10}$$

In Fig. 4 we show the time dependence of the total kinetic energy using (10) as the initial condition. The constant initial density loading gave a large oscillation in the energy decay (dashed line), while the equation (10) initial density decays exponentially (solid line).

IV. CONCLUSIONS

The reduction of unphysical oscillations is important for lattice-gas simulations of incompressible flows, especially at moderate Mach number. If the Kolmogorov decay flows are used to measure the lattice-gas viscosity, large errors in the inferred viscosity can occur if the unphysical oscillations are not properly treated. When the density oscillation in the Kolmogorov flow is eliminated by choosing an optimal initial condition, we obtain a viscosity of 0.682 for density $n=1.2$. This result is within 1% of the theoretical result.[6]

In simulations of incompressible hydrodynamics using lattice-gas methods, Eq. (6) should be approximately satisfied at all times in order to minimize unphysical density oscillations. Because there is no general analytic solution to Eq. (6), it is nontrivial to obtain an optimal initial density loading.

Even though the effects of unphysical oscillations can be significantly reduced by the methods in this paper, it is possible to eliminate the dominant cause of these unphysical oscillations, the u^2 term in the pressure equation, by adding speed two particles.[7] This additional speed model has been shown to decrease the amplitude of the unphysical oscillation in the energy decay even more satisfactorily than the optimal initial condition described in this paper.

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*Present address: Applied and Computational Mathematics, Princeton University, Princeton, NJ 08544.

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