PHYSICAL REVIEW A VOLUME 45, NUMBER 8 15 APRIL 1992

Recovery of the Navier-Stokes equations using a lattice-gas Boltzmann method

Hudong Chen,* Shiyi Chen,† and William H. Matthaeus
Bartol Research Institute, University of Delaware, Newark, Delaware 19716
(Received 14 August 1991)

It is known that the Frisch-Hasslacher-Pomeau lattice-gas automaton model and related models possess some rather unphysical effects. These are (1) a non-Galilean invariance caused by a density-dependent coefficient in the convection term and (2) a velocity-dependent equation of state. In this paper, we show that both of these effects can be eliminated exactly in a lattice Boltzmann-equation model.

PACS number(s): 47.10.+g

Although the lattice-gas automaton method has provided a fast and efficient way for solving partial-differential equations, there exist some fundamental problems in this method in simulating realistic fluid flows obeying the Navier-Stokes equations. Besides its intrinsic noisy character which makes the computation accuracy difficult to achieve, it contains certain properties even in the fluid limit. As a result, its possible advantage over other conventional computational methods is greatly obscured. Unless these problems are resolved, the lattice-gas automaton method can hardly be used as a satisfactory tool for doing numerical computations for fluids.

A typical lattice-gas model consists of identical particles on a two-dimensional (2D) hexagonal or a 4D face-centered hypercubic lattice (FCHC). If all the particles have the same speed and obey Fermi statistics, then the allowed collisions, restricted by mass and momentum conservation, lead to a Fermi-Dirac single-particle equilibrium distribution [1]:

$$f_a^{\mathrm{eq}}=\frac{1}{1+e^{\alpha+\boldsymbol{\beta}\cdot\hat{\mathbf{e}}_a}} \tag{1}$$

where $a=1,\ldots,b$ and $\hat{\mathbf{e}}_a$ is the particle velocity in the a direction. α and $\boldsymbol{\beta}$ are determined by the conservation laws. In the case of small velocity, it can be shown that the above distribution can be expanded in powers of velocity $\mathbf{u}$ as

$$f_a^{\mathrm{eq}}=\frac{\rho}{b}+\frac{\rho D}{c^2 b}\hat{\mathbf{e}}_a\cdot\mathbf{u}+\rho\frac{D(D+2)}{2c^4 b}g(\rho)Q_{aij}u_i u_j+O(u^3) \tag{2}$$

where $Q_{aij}=\hat{e}_{ai}\hat{e}_{aj}-(1/D)\delta_{ij}$. For a one-speed lattice-gas model of lattice dimension D, $g(\rho)=(D/D+2)(b-2\rho)/(b-\rho)$. In the above, ρ and $\mathbf{u}$ are the averaged particle density per site and the fluid velocity, respectively. In addition, c is the particle speed which is equal to one lattice unit per lattice time for a hexagonal lattice, and is equal to $\sqrt{2}$ lattice units for FCHC, while b ($=6$ for a hexagonal lattice, $=24$ for FCHC) is the total number of states on a lattice site [1].

The lattice-gas fluid momentum equation in the small velocity limit can be written explicitly as follows:

$$\partial_t(\rho\mathbf{u})+\nabla\cdot[\rho g(\rho)\mathbf{u}\mathbf{u}]=-\nabla p+\nabla\cdot[\nu\nabla(\rho\mathbf{u})]+\nabla[\zeta\nabla\cdot(\rho\mathbf{u})], \tag{3}$$

where the pressure $p=c_s^2\rho[1-g(\rho)\mathbf{u}^2/c^2]$ with $c_s^2=c^2/D$ and ν and ζ are the kinematic viscosity and the bulk viscosity, respectively. From the above we see that the lattice-gas fluid momentum equation cannot be reduced to the Navier-Stokes equation in general because of two fundamental problems. The first is the non-Galilean invariance property due to the density dependence of the convection coefficient $g(\rho)$. This limits the validity of the lattice-gas method only to a strict incompressible regime. Second, the pressure has an explicit and unphysical velocity dependence. This effect causes unphysical fluid kinetic energy oscillations even in a uniform density case [2,3]. It should be mentioned that, by adapting multispeeds in a lattice-gas model, both of the above nonphysical properties have been greatly reduced but not completely eliminated [4].

Unlike a lattice-gas model, a lattice Boltzmann-equation (LBE) model is not noisy so that the accuracy is easily controlled [5]. More importantly, we show in this paper that both of the nonphysical properties mentioned above can be completely eliminated in a rather straightforward way in a LBE. Therefore, the resulting fluid equations derived from the LBE model presented below exactly obey the realistic fluid equations for any density distribution.

A LBE for simulating fluid adapts essentially all lattice-gas kinetic rules except it uses real numbers instead of integers and neglects the particle-particle correlations [5]. Basically, in a LBE, we solve the following kinetic equation:

$$f_a(\mathbf{x}+\hat{\mathbf{e}}_a,t+1)=f_a(\mathbf{x},t)+\Omega_a, \tag{4}$$

where f_a is a positive single-particle distribution function. The collision integral Ω_a, which contains only local informations, satisfies mass and momentum conservation at each lattice site. Therefore, a LBE still preserves the advantage of doing parallel computing. In addition, the requirement for using Fermi statistics is no longer necessary. This provides much more freedom in the functional form of the equilibrium distribution. This can be understood intuitively. A particle in a LBE can be viewed as a package of infinite subparticles of mass approximately zero. It can be infinitely separated. Thus, there are infinitely more ways of doing collisions satisfying the mass and momentum conservation compared with those in a

lattice-gas automaton model. Consequently, it can produce basically any desired equilibrium distribution as long as we select the collisions properly. For instance, we can immediately see that the non-Galilean invariance problem can be completely eliminated if the system has the following equilibrium distribution,

$$f_a^{eq}=\frac{\rho}{b}+\frac{\rho D}{c^2 b}\hat{\mathbf{e}}_a\cdot\mathbf{u}+\rho\frac{D(D+2)}{2c^4 b}Q_{aij}u_i u_j\,, \tag{5}$$

which is just the lattice-gas equilibrium distribution in the small velocity limit with $g(\rho)=1$. There are many choices of the collision integral Ω_a that could generate this equilibrium distribution, but the simplest one is to have a linearized form [6], with a single relaxation time [7]

$$\Omega_a=-\frac{1}{\tau}(f_a-f_a^{eq})\,. \tag{6}$$

The distributions f_a and f_a^{eq} correspond to the identical values of ρ and $\mathbf{u}$ at each lattice site, and f_a^{eq} can be chosen to have either the functional form (5) or any other form. The constant τ, which is generally required to be greater than one half, on the basis of stability analysis, determines the single relaxation time scale for approach to the desired equilibrium distribution. The single-relaxation-time collision integral is not only easy to implement computationally, but possesses some other desirable features. For instance, it produces a particle-density-independent viscosity [7]. Since the equilibrium distribution has $g(\rho)=1$, we immediately see that the resulting fluid equations are fully Galilean invariant for any particle density distribution.

The elimination of the velocity dependence of the pressure, however, is not possible with a one-speed LBE. This is because the equilibrium distribution given above is unique for a one-speed LBE in order to satisfy the requirements of mass and momentum conservation as well as the Galilean invariance. However, in a one-speed model particle-number conservation and energy conservation are equivalent, therefore, the flow energy corresponding to $\mathbf{u}$ must diminish the random kinetic energy and therefore the pressure. Consequently, one-speed models must admit a pressure decrease with the increase of velocity. We show below that this velocity-dependence effect can be eliminated if we include rest particles in a LBE.

Physically, introducing the rest particles is like having included a particle reservoir. At a given spatial location where there is relatively higher fluid velocity, the part of pressure due to the moving particles becomes relatively smaller. At such a position, we allow rest particles to be excited and transformed isotropically into moving particles so that the pressure is increased and restored to its proper value. As a consequence, the overall pressure does not depend explicitly on velocity but on the total particle density only.

If we include rest particles, then, in addition to the lattice Boltzmann equations given above for the moving particles (with speed c), we have an equation governing the evolution of the rest particles:

$$f_0(\mathbf{x},t+1)=f_0(\mathbf{x},t)+\Omega_0\,, \tag{7}$$

where Ω_0 can also be chosen to have a linearized single relaxation time form, $\Omega_0=-(1/\tau)(f_0-f_0^{eq})$. Moreover, we have freedom to assume that the equilibrium distribution for the moving particles has the general form,

$$f_a^{eq}=d+\frac{\rho D}{c^2 b}\hat{\mathbf{e}}_a\cdot\mathbf{u}+\rho\frac{D(D+2)}{2c^4 b}\hat{e}_{ai}\hat{e}_{aj}u_i u_j+\gamma\mathbf{u}^2\,, \tag{8}$$

and the equilibrium distribution for the rest particles has the form

$$f_0^{eq}=d_0+\gamma_0\mathbf{u}^2\,. \tag{9}$$

The coefficients γ, γ_0, d, and d_0 can be used for eliminating the velocity dependence of the pressure, and for satisfying the following constraint relations derived from the conditions of mass and momentum conservation:

$$\rho=d_0+bd\,, \tag{10}$$

$$\gamma_0+\rho\frac{(D+2)}{2c^2}+b\gamma=0\,. \tag{11}$$

Using the above equilibrium distributions, the ideal part of the momentum flux tensor can be shown to be

$$\Pi_{ij}=\sum_a(\hat{\mathbf{e}}_a)_i(\hat{\mathbf{e}}_a)_j f_a^{eq}=\frac{bc^2}{D}d\delta_{ij}+\rho u_i u_j+\left(\frac{\rho}{2}+\frac{bc^2}{D}\gamma\right)\mathbf{u}^2\delta_{ij}\,, \tag{12}$$

which, when substituted into the resulting fluid momentum equation, again satisfies the requirement of Galilean invariance as in the one-speed LBE above. However, it can also be seen immediately that in this latter model the velocity dependence of the pressure is eliminated if we let $\gamma=-\rho D/2bc^2$.

Solving the constraint relations we further get that $\gamma_0=-\rho/c^2$. The choice of d_0 is, however, rather arbitrary. This remaining freedom is useful in generating some additional desirable properties. For the purpose of simplicity, we use $d_0=\rho_0/(b+1)$ in this paper, where the constant ρ_0 is the averaged particle density [=(total particle number)/(total lattice sites)]. Since d_0 is a constant, d is seen to be linearly dependent on the total particle density ρ the same way as in the one-speed LBE. As a consequence, the fluid equations will be exactly the same as those derived from the one-speed LBE (with the same sound speed), except that the pressure is now related correctly to the total particle density only, having a form of an isothermal ideal gas,

$$p=c_s^2\rho\,. \tag{13}$$

Therefore, we have completely obtained the correct Navier-Stokes fluid equations for arbitrary particle densities through the pressure-corrected LBE (PCLBE).

The code for the present model, similar to others [8] is simple and efficient. The measurement of the viscosity gives at least four significant figures compared with the analytic results through two-dimensional channel flow and the Couette flow. A number of two- and three-dimensional applications of the present model, including two-dimensional back-step flow, three-dimensional Baltrami flow, and Green-Taylor vortex and three-dimen-

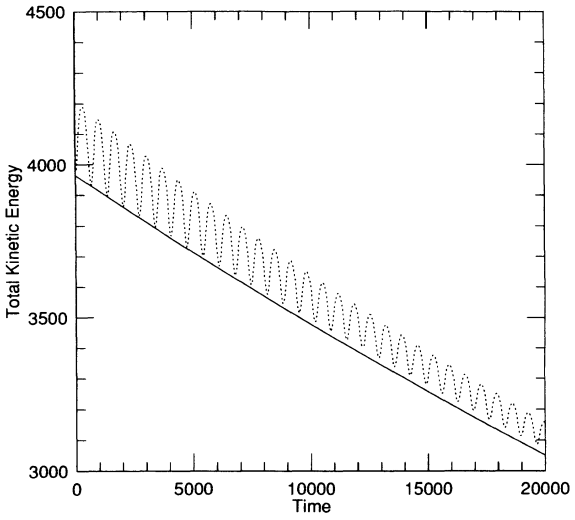

FIG. 1. Numerical results of free decay of the total fluid kinetic energy $U=\frac{1}{2}\int_v \rho \mathbf{u}^2$ as a function of time obtained by solving two LBEs. The solid line is the result from the PCLBE and the dotted line is from the one-speed LBE (both in the lattice unit). The lattice size for these computations is 40×1000 lattice sites. Periodic boundary conditions in both x and y directions. The initial velocity is $u_y=0$ and $u_x=0.3\sin[(2\pi/1000)y]$ in the unit of the lattice particle speed c. The time is scaled with the lattice time unit. The unphysical oscillations in one-speed LBE are completely absent in the PCLBC.

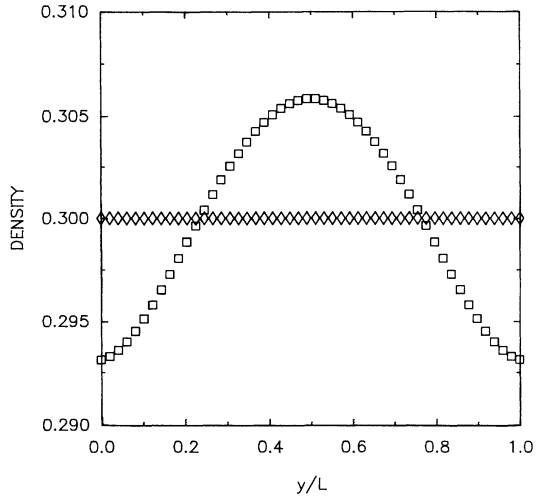

FIG. 2. Numerical results of the particle density distribution across the channel in a driven channel flow. The diamonds represent the steady-state distribution of the particle density, resulting from the solution of the PCLBE; the squares represent the distribution when the unphysical pressure effect is not corrected (one-speed LBE). No-slip boundary conditions are imposed, and the fluid is forced along the channel uniformly with a magnitude $f=0.0001$ per lattice site. The averaged particle density per site is 2.1. The total lattice size is 100×100.

sional turbulent flows, will be shown in the next paper [9]. We now present briefly two numerical tests illustrating the elimination of the velocity dependence of the pressure effects. First, if a LBE exactly solves the Navier-Stokes fluid equations, then the total kinetic energy of fluid $U=\int_V \frac{1}{2}\rho\mathbf{u}^2$ should decay monotonically in time for the case of zero-forcing, periodic boundaries, and a shear flow initial velocity profile, $\mathbf{u}(\mathbf{x},t_0)=u_x(y)\hat{\mathbf{x}}$ with a uniform initial density distribution $\rho(\mathbf{x},t_0)=$const. Two LBE simulations were performed for this case, as shown in Fig. 1. The solid line is the total kinetic energy as a function of time obtained by solving the PCLBE discussed above. It demonstrates that this LBE correctly captures the physical behavior of the Navier-Stokes fluid equations. The dashed line is the total kinetic energy obtained by solving the one-speed LBE above. Although the fluid equations produced from the one-speed LBE are Galilean invariant, the model contains a nonphysical velocity dependence in its pressure. Therefore, its total kinetic energy is shown to have unphysical oscillations [2]. The second test is a channel flow case. If a model correctly reproduces the Navier-Stokes fluid equations, the steady-state particle density across the channel should be uniformly distributed. It is seen that the distribution (diamonds) obtained by simulating PCLBE indeed satisfies this requirement. However, if the unphysical pressure effect is not corrected, the resulting particle density distribution will have a higher value at the center of the channel where the velocity magnitude is greater, as shown by the squares in Fig. 2. This phenomenon is also known in the lattice-gas simulations [10].

We conclude that the present lattice Boltzmann model, by using the single-time relaxation approximation and a particular Maxwell-type distribution in (8) will give the complete Navier-Stokes equations and possibly provide an efficient parallel numerical method for solving various fluid problems. Recent studies on the square lattice by Qian, d'Humiéres, and Lallemand [11] give very similar results.

This work has been supported by NASA Innovative Research Program Grant No. NAGW-1648, and by the U.S. Department of Energy through Grant No. DE-FG02-85ER-53194 at Dartmouth and through Los Alamos National Laboratory. The computations were done on the CM-2 at the Advanced Computing Laboratory at Los Alamos National Laboratory.

*Present address: Department of Physics and Astronomy, Dartmouth College, Hanover, NH 03755.

†Present address: Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545.

[1] U. Frisch, D. d'Humiéres, B. Hasslacher, P. Lallemand, Y. Pomeau, and J.-P. Rivet, Complex Syst. **1**, 649 (1987).

[2] J. Dahlburg, D. Montgomery, and G. Doolen, Phys. Rev. A **36**, 2471 (1987).

[3] S. Chen, Z.-S. She, L. C. Harrison, and G. Doolen, Phys. Rev. A **39**, 2725 (1989).

[4] S. Chen, H. Chen, and G. Doolen, Complex Syst. **3**, 243 (1989).

[5] G. McNamara and G. Zanetti, Phys. Rev. Lett. **61**, 2332 (1988).

[6] F. Higuera and J. Jimenez, Europhys. Lett. **9**, 663 (1989).

[7] S. Chen, H. Chen, D. Martinez, and W. Matthaeus, Phys. Rev. Lett. **67**, 3776 (1991).

[8] S. Succi, R. Benzi, and F. Higuera, Physica D **47**, 219 (1991).

[9] S. Chen, Gary D. Doolen, Xiaowen Shan, and J. Wang (unpublished).

[10] *Lattice Gas Methods for PDEs*, edited by G. Doolen (Addison-Wesley, New York, 1989).

[11] Y. H. Qian, D. d'Humiéres, and P. Lallemand, Europhys. Lett. (to be published).