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Lattice BGK Models for Navier-Stokes Equation.

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Abstract. – We propose the lattice BGK models, as an alternative to lattice gases or the lattice Boltzmann equation, to obtain an efficient numerical scheme for the simulation of fluid dynamics. With a properly chosen equilibrium distribution, the Navier-Stokes equation is obtained from the kinetic BGK equation at the second-order of approximation. Compared to lattice gases, the present model is noise-free, has Galileian invariance and a velocity-independent pressure. It involves a relaxation parameter that influences the stability of the new scheme. Numerical simulations are shown to confirm the speed of sound and the shear viscosity.

Recently, lattice gases have attracted much attention since models were proposed to simulate fluid flows: the FHP for 2D [1] and the FCHC [2] for 3D have been shown to satisfy the incompressible Navier-Stokes equation. Other models have been designed to allow the numerical simulation of a variety of physical situations and their properties have been studied in great details [3]. Typically, all lattice gas models are built with the following ingredients: a regular lattice, on each node a set of variables $\{n_i\}$, $i \in \{1, \ldots, b\}$, describes the population of b given velocities c_i. The dynamics is divided into two steps: streaming from node to node according to the velocity c_i and redistribution of the populations at each node during the collision step. To represent some physical situation, such a model must satisfy the following constraints:

the lattice must be sufficiently symmetric,

basic physical quantities must be conserved (mass, momentum, energy),

local equilibrium exists and depends only upon the conserved quantities.

By now the main advantages of lattice gas techniques are well established:

intrinsic stability,

easy introduction of boundary conditions,

simple numerical codes allowing efficient parallel implementation.

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However, lattice gases suffer from some drawbacks. A fundamental one is statistical noise which results in the need for spatial (or time) averaging (loss in efficiency) and to some interesting physical behaviour like the coupling of statistical fluctuations, due to the nonlinearity of the governing equations, that leads to a divergence of transport coefficients in low dimensions [4]. In addition lattice gases usually are not Galilean invariant (presence of a so-called $g(\rho)$ density-dependent factor in the nonlinear advection term of the Navier-Stokes equation), they have a velocity-dependent pressure and they present spurious invariants that correspond to unphysical hydrodynamical quantities.

These difficulties can be cured as their origins are well understood. The Fermi-Dirac (or alternatively Bose-Einstein) statistics causes $g(\rho)$ to depend upon the density. However, in the discrete kinetic theory [5] where the gas is Maxwellian, $g(\rho)$ does not depend upon the density. The pressure dependence upon the velocity is related to g when g is different from unity. The regular lattice structure on which the particles reside produces the nonphysical invariants. Such quantities are scalar and they influence the dynamics through the pressure term, but their production by shock waves and boundary conditions is not yet clear.

In order to solve some of these difficulties, there exist three similar more or less efficient ways using modifications of the collision step. The first one was proposed by McNamara and Zanetti [6], who used the mean population of particles instead of the Boolean variables of lattice gases. (n_i is now a real variable between 0 and 1 instead of 0 or 1.) The expression for the collision step uses the same expression as in the Boolean counterpart which leads to the use of polynomials in the n_i that have as many terms as there are effective collisions. This is unpractical for anything but extremely simple cases and in particular rules out the consideration of the 3D FCHC model. The second one was proposed by Higuera, Succi and Benzi [7], who used a linearized expression for the collision term, the so-called enhanced collision, with a matrix whose elements depend only on the angle of two interacting particles. This method was generalized to the 3D FCHC model. These two versions of lattice Boltzmann equations suppress completely the statistical noise and control the initial spurious invariants easily. However the problems related to the density-dependent g and to the velocity-dependent pressure are unsolved because the preceding authors dealt with Fermi gases. The third way was studied by Qian, d'Humières and Lallemand [8, 9], who used Maxwellian particles that violate the semi-detailed balance of binary collisions and introduced more populated rest particles. Thus they obtained noise-free models with Galileian invariance and a velocity-independent pressure. Some universal expressions for the speed of sound and viscosities were obtained for all dimensions. One-dimensional shock waves were studied and compared to the results of the classic characteristic method [9]. The detailed choice of collision terms for 2D model is complicated and 3D collision rules are not yet worked out [8]. The last two ways of modifying lattice gases for simulating fluid flows may cause numerical instability.

The question is how to keep some of the advantages of lattice gases and of the lattice Boltzmann equation while overcoming their drawbacks.

To answer this question, we propose a new kind of model which can be used to simulate the Navier-Stokes equation in a simple and efficient way. From computational fluid dynamics, it is known that the method of relaxation has good stability property if the relaxation parameter ω is between 0 and 2. This method can be described simply as follows: if $N(t)$ is a quantity at time t and N_e is its predicted value, then $N(t+1)$ is given by

$$N(t+1) = (1-\omega)N(t) + \omega N_e . \tag{1}$$

It is called subrelaxation if $0 < \omega < 1$ and over-relaxation if $1 < \omega < 2$, and the scheme is linearly stable for $0 < \omega < 2$. Introducing this idea to treat our problem, the natural way to

choose the N_e is to take the equilibrium distribution, a function only of the hydrodynamical quantities, that is the density, momentum, etc. We use this relaxation process to replace the collision term without changing the propagation term, so the evolution equation for the particle density can be written down as

$$N_i(t+1, \boldsymbol{x}+\boldsymbol{c}_i) = (1-\omega) N_i(t, \boldsymbol{x}) + \omega N_{ie}(t, \boldsymbol{x}), \tag{2}$$

where N_i is the density of particle i and $\boldsymbol{c}_i$ its velocity. This formula is very general and can be used for many physical problems in principle. Now we use the equilibrium distribution N_{ie} of the models proposed in [8] as the predicted value

$$N_{ie}(t, \boldsymbol{x}) = t_p \rho \left\{ 1 + \frac{c_{i\alpha} u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta}{2c_s^2} \left(\frac{c_{i\alpha} c_{i\beta}}{c_s^2} - \delta_{\alpha\beta} \right) \right\}, \tag{3}$$

where α and β represent Cartesian coordinates (with implied summation for repeated indices), c_s is the speed of sound, the index p is the square modulus of particle's velocity, and t_p is the corresponding equilibrium distribution for $u = 0$. The t_p's are determined to achieve isotropy of the fourth-order tensor of velocities and Galilean invariance [8]. For the family of models with b velocities on a simple cubic lattice of dimension d (denoted $DdQb$), the values of t_p are given by

Model	t_0	t_1	t_2	t_3
*D*1*Q*3	2/3	1/6	0	0
*D*2*Q*9	4/9	1/9	1/36	0
*D*3*Q*15	2/9	1/9	0	1/72
*D*3*Q*19	1/3	1/18	1/36	0
*D*4*Q*25	1/3	1/36	0	0

Formula (2) is very similar to the lattice Boltzmann equation of Higuera, Succi and Benzi, the main difference is that a single ω replaces the collision matrix. Equation (2) can be considered as a BGK model [10] on a chosen lattice with a properly selected equilibrium distribution. Using the multiscale technique, we can obtain the exact Navier-Stokes equation at the second order of approximation:

$$\partial_t \rho + \partial_\alpha(\rho u_\alpha) = 0, \tag{4}$$

$$\partial_t(\rho u_\alpha) + \partial_\alpha(\rho u_\alpha u_\beta) = -\partial_\alpha(c_s^2 \rho) + \nu \partial_\beta[\partial_\beta(\rho u_\alpha) + \partial_\alpha(\rho u_\beta)], \tag{5}$$

where the speed of sound c_s and the shear viscosity ν are given by

$$c_s = \frac{1}{\sqrt{3}}, \tag{6}$$

$$\nu = \frac{1}{6}\left(\frac{2}{\omega} - 1\right). \tag{7}$$

These two expressions are independent of space dimension (1). We notice that the physical requirement of positive viscosity gives the same condition of stability for ω: $0 < \omega < 2$, as that of the relaxation method.

The stability of the scheme (2) is partially derived from the positivity requirement of the particle density. In order to have the correct nonlinear term in the Navier-Stokes equation, we must truncate the equilibrium distribution just at the second order in velocity (3). For the models that have the same geometries as in [8], we have the positivity conditions for maximum Mach number and the viscosity

$$M \leqslant \begin{cases} \sqrt{2}, & D = 1, \\ \dfrac{\sqrt{5}}{2}, & D \geqslant 2, \end{cases} \tag{8}$$

$$\nu \geqslant \mathrm{Max}\left[0, \sup_{\text{for } N_i > N_{ie}} \left(\frac{N_i - N_{ie}}{N_i} - \frac{1}{6}\right)\right]. \tag{9}$$

The stability conditions concerning the maximum gradient of the hydrodynamical quantities are not yet found, because strong departures from equilibrium (given by eq. (3)) occur in these zone. The higher-order corrections of derivatives to the Navier-Stokes equation are important when the viscosity is approaching zero and this has been demonstrated [11] both analytically and numerically for a one-dimensional 5-particle model.

We use the three-dimensional 15 particles model $D3Q15$ (1 rest particle + 6 particles along the three axis of a cube + 8 diagonal direction particles) to measure the speed of sound and the viscosity as a function of the relaxation parameter ω using the perturbation method on a $128 \times 1 \times 1$ lattice with a small amplitude sinusoidal wave. The excellent agreement between the numerical measurements (points) and the theoretical prediction (solid line) of the shear viscosity is shown in fig. 1 for $0.2 \leqslant \omega < 2.0$. The measured speed of sound agrees

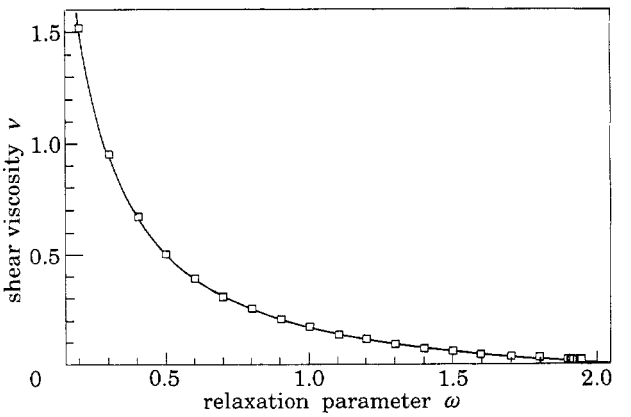

Fig. 1. – The shear viscosity ν as a function of ω for the 15-particle model $D3Q15$, solid line is eq. (7), square points are numerical results.

(1) For the FHP geometry, $t_0 = t_1 = 1/2$, the speed of sound is equal to 1/2 and the factor 6 in eq. (7) must be replaced by 8.

with eq. (6) within $\pm 0.4\%$, while the factor g is equal to unity within $\pm 0.08\%$. When ω is small, the finite size of the lattice gives a big Knudsen number and the results diverges from eqs. (6) and (7) because the system now describes a rarefied gas instead of hydrodynamics.

Now we can make some remarks. In this letter, we have proposed the lattice BGK models as an alternative to the lattice gas models, which can be also interpreted as a relaxation method in computational fluid dynamics. We obtained the exact Navier-Stokes equation at the second order. The gases considered here satisfy Maxwellian statistics while Fermions are used in lattice gas models and the lattice Boltzmann equation. By changing the equilibrium distribution we can deal either with Fermion particles or boson particles as well as with Maxwellian particles. The models overcome some obstacles that are present in lattice gases.

The code used to simulate fluid flows is simple and efficient. Our first numerical simulations did confirm the theoretical predictions. A number of applications of these models will be presented in [11]. We have given some stability conditions on the maximum Mach number and the viscosity but more work remains to be done in the regions of strong spatial gradients. The higher-order corrections in the derivatives involved in the Navier-Stokes equation are important when the viscosisty is close to zero. Recently, we learnt that Koelman studied the special case $\omega = 1$ and gave a test of Karman street simulation [12]. In general, the only physical hypothesis necessary to derive the governing equations is that the dynamics of the physical system can be decomposed into various phenomena that evolve with different time scales, the faster relaxing to equilibrium states depending upon the slower ones, so we hope that a wide range of nonlinear partial differential equations can be simulated in a simple and efficient way on computers by lattice BGK models as proposed in this letter through a properly chosen equilibrium distribution, the choice (3) being just an example which is suitable for fluid dynamics as it leads to the Navier-Stokes equation. Once the complete stability conditions are worked out, this simple scheme may be used as a candidate to construct a specialized Navier-Stokes computer which has a good performances/cost ratio compared to that of general-purpose supercomputer.

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