On the cubic velocity deviations in lattice Boltzmann methods

2006 J. Phys. A: Math. Gen. 39 3127

(http://iopscience.iop.org/0305-4470/39/12/019)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 3127–3136 doi:10.1088/0305-4470/39/12/019

On the cubic velocity deviations in lattice Boltzmann methods

Gábor Házi and Péter Kávrán

KFKI Atomic Energy Research Institute, Budapest, Hungary

Received 25 November 2005, in final form 7 February 2006
Published 8 March 2006
Online at stacks.iop.org/JPhysA/39/3127

Abstract

The macroscopic equations derived from the lattice Boltzmann equation are not exactly the Navier–Stokes equations. Here the cubic deviation terms and the methods proposed to eliminate them are studied. The most popular two- and three-dimensional models (D2Q9, D3Q15, D3Q19, D3Q27) are considered in the paper. It is demonstrated that the compensation methods provide only partial elimination of the deviations for these models. It is also shown that the compensation of Qian and Zhou (1998 *Europhys. Lett.* **42** 359) using the compensation parameter $K = 1$ in a D2Q9 or D3Q27 model can eliminate all the cross terms perfectly, but the deviation terms $\partial_x \rho u_x^3$, $\partial_y \rho u_y^3$ and $\partial_z \rho u_z^3$ still survive the compensation.

PACS numbers: 47.45.−n, 02.60.−x, 05.50.+q, 47.11.+j

1. Introduction

The lattice Boltzmann method is a relatively novel simulation technique in the field of computational fluid dynamics. Although the method can be used to solve a wide variety of macroscopic equations, it was originally proposed to model the incompressible Navier–Stokes equations in the low Mach number limit [2].

Macroscopic equations can be derived from the lattice Boltzmann equation through a Chapman–Enskog expansion. The derivation yields not exactly the incompressible Navier–Stokes equations. One part of the deviations can be considered as a kind of truncation error and can be reduced by increasing the resolution of the simulation just as for conventional finite difference schemes. The other part is often referred to as the compressibility error because it can be reduced by decreasing the Mach number (unless it is a relevant parameter of the problem in question). One contribution for the compressibility error comes from a cubic term not being present in the Navier–Stokes equations but appears in the macroscopic equations derived from the lattice Boltzmann equation. Recently, it has been demonstrated that the third-order deviation terms can reduce the accuracy of the lattice Boltzmann method, for instance, in the initial stage of two-dimensional decaying turbulence [3].

First, Qian and Orszag derived the deviation term for an athermal lattice Boltzmann model [4]. Weimar and Boon proposed a deviation free model with 13 lattice links to study reactive flows [5]. Chen *et al* [6] studied third-order effects in thermal lattice Boltzmann models. They proposed model parameters for a two-dimensional model with 16 lattice links and showed that this model is free of the third-order velocity deviation. Considering athermal situations Qian and Zhou [1] presented a two-dimensional model with 17 lattice links (D2Q17), and proposed a method to eliminate the third-order velocity deviation term.

It is worth emphasizing that all the methods mentioned above share some properties, e.g., next-neighbouring lattice sites are used during the streaming step. The question arises naturally: is it possible to eliminate the cubic deviation term in simple models (e.g. in a two-dimensional nine-velocity D2Q9 model), where we consider only neighbouring sites during the propagation?

To answer the question, the compensation of Qian and Zhou is revised in details. First, we derive the compensation parameter for the D2Q17 model. We show analytically that there is no parameter with real value, which can make a perfect elimination for a D2Q17 model. However, we also demonstrate that using the parameters of Qian and Zhou, part of the deviation terms can be compensated and as a consequence, when studying simple shear flows, one can draw the faulty reasoning that the compensation is perfect. Most importantly, we show that using the same compensation parameter one can achieve partial compensation for the simpler two-dimensional nine-velocity (D2Q9) and the three-dimensional 15- (D3Q15), 19- (D3Q19) and 27-velocity (D3Q27) models. Numerical examples are presented to support our analytical results. Based on these results we also discuss the range of problems where the various models can be applied.

2. The lattice Boltzmann method

The lattice Boltzmann equation can be written as follows:

$$f_{\sigma,i}(\mathbf{x} + c_{\sigma,i\alpha}\delta, t + \delta) - f_{\sigma,i}(\mathbf{x}, t) = \Omega_{\sigma,i}(\mathbf{x}, t), \tag{1}$$

where $f_{\sigma,i}$ is the one particle velocity distribution function, $c_{\sigma,i\alpha}$ is the lattice vector, δ is the time step, Ω is the collision operator, σ is the particle velocity group and i is the index of the lattice links. The simplest form of the collision operator is given by

$$\Omega_{\sigma,i}(\mathbf{x}, t) = -\frac{1}{\tau}\left[f_{\sigma,i}(\mathbf{x}, t) - f_{\sigma,i}^{\mathrm{eq}}(\mathbf{x}, t)\right]. \tag{2}$$

This so-called Bhatnagar–Gross–Krook (BGK) operator prescribes a simple relaxation process towards local equilibrium.

The macroscopic quantities are obtained from the distribution functions by taking their suitable moments

$$\rho = \sum_{\sigma,i} f_{\sigma,i}, \qquad \rho u_\alpha = \sum_{\sigma,i} c_{\sigma,i\alpha} f_{\sigma,i}. \tag{3}$$

The local equilibrium distribution function plays a crucial role in the lattice BGK models. Here we use the form proposed by Qian and Zhou [1]:

$$f_{\sigma,i}^{\mathrm{eq}} = \rho w_{\sigma,i}\left[1 + \frac{u_\gamma c_{\sigma,i\gamma}}{c_s^2} + \frac{u_\gamma u_\zeta}{2c_s^4}\left(c_{\sigma,i\gamma}c_{\sigma,i\zeta} - c_s^2\delta_{\gamma\zeta}\right) + K\frac{u_\gamma u_\zeta u_\eta c_{\sigma,i\gamma}}{6c_s^6}\left(c_{\sigma,i\zeta}c_{\sigma,i\eta} - 3c_s^2\delta_{\zeta\eta}\right)\right], \tag{4}$$

where $w_{\sigma,i}$ is the lattice weight and c_s is the speed of sound. Hereupon the repeated Greece indices imply summation.

The above form of the local equilibrium distribution is a low Mach number expansion of the Maxwell–Boltzmann distribution. For athermal simulations terms are kept only up to second order, because it is sufficient to assure conservation of mass and momentum [7]. Third-order terms have to be taken into account for conservation of energy in thermal models. On the other hand, it is obvious that we need to work with third-order terms even in an athermal model, if we want to influence the third-order deviations. The role of the parameter K is to control the appearance of the third-order terms, assuring the cancellation of the deviation terms.

It is worth mentioning that specifying somewhat more general form of the equilibrium distributions, both the models of Weimar and Boon [5] and Chen *et al* [6] provide more freedom in the parameter choice of the equilibrium distributions. The following form of the equilibrium is used in the model of Weimar and Boon [5]:

$$f_{\sigma,i}^{\mathrm{eq}} = \rho w_{\sigma,i}\left[1 + \frac{u_\gamma c_{\sigma,i\gamma}}{c_s^2} + \frac{u_\gamma u_\zeta}{2c_s^4}\left(c_{\sigma,i\gamma}c_{\sigma,i\zeta} - c_s^2\delta_{\gamma\zeta}\right) + E_i\frac{u_\gamma u_\zeta u_\eta c_{\sigma,i\gamma}}{6c_s^6}\left(c_{\sigma,i\zeta}c_{\sigma,i\eta} - 3F_i c_s^2\delta_{\zeta\eta}\right)\right]. \tag{5}$$

Note that this form differs from the model of Qian and Zhou only in the treatment of the third-order terms, which here can be controlled by two parameters (E_i, F_i) instead of one (K). In the thermal model of Chen *et al* [6] practically the same form as (5) is used. The only difference is that those authors considered the expansion up to fourth order and in this way the deviation terms of the energy equations become accessible, too. So the model of Qian and Zhou reduces to the model of Chen *et al* for $E_i = K$ and $F_i = 1$.

In lattice Boltzmann models the lattice has to be sufficiently symmetric, ensuring the necessary isotropy in macroscopic level. The suitable lattices yield vanishing odd-rank tensors and isotropic even-order tensors up to sixth and fourth rank for thermal and athermal simulations, respectively.

These constraints can be expressed as follows: $T_\alpha^{(1)} = T_{\alpha\beta\gamma}^{(3)} = T_{\alpha\beta\gamma\zeta\eta}^{(5)} = 0$ and

$$T_{\alpha\beta}^{(2)} = \sum_{\sigma,i} w_{\sigma,i}c_{i\alpha}c_{i\beta} = \Psi_2\delta_{\alpha\beta}, \tag{6}$$

$$T_{\alpha\beta\gamma\zeta}^{(4)} = \sum_{\sigma,i} w_{\sigma,i}c_{i\alpha}c_{i\beta}c_{i\gamma}c_{i\zeta} = \Phi_4\Delta_{\alpha\beta\gamma\zeta} + \Psi_4(\delta_{\alpha\beta}\delta_{\gamma\zeta} + \delta_{\alpha\gamma}\delta_{\beta\zeta} + \delta_{\alpha\zeta}\delta_{\beta\gamma}), \tag{7}$$

$$T_{\alpha\beta\gamma\zeta\eta\theta}^{(6)} = \sum_{\sigma,i} w_{\sigma,i}c_{i\alpha}c_{i\beta}c_{i\gamma}c_{i\zeta}c_{i\eta}c_{i\theta} = \Phi_6\Delta_{\alpha\beta\gamma\zeta\eta\theta} + \Psi_6\sum_{k,cp_k\{\alpha,\beta,\ldots,\theta\}}\delta_{\alpha\beta}\Delta_{\gamma\zeta\eta\theta} + \Gamma_6\sum_{k,cp_k\{\beta,\gamma,\ldots,\theta\}}\delta_{\alpha\beta}T_{\gamma\zeta\eta\theta}^{(4)}, \tag{8}$$

where δ, Δ are

$$\delta_{\alpha\beta} = \begin{cases}1 & \alpha = \beta\\ 0 & \text{otherwise},\end{cases}$$

$$\Delta_{\alpha\beta\gamma\zeta} = \begin{cases}1 & \alpha = \beta = \gamma = \zeta\\ 0 & \text{otherwise},\end{cases}$$

$$\Delta_{\alpha\beta\gamma\zeta\eta\theta} = \begin{cases}1 & \alpha = \beta = \gamma = \zeta = \eta = \theta\\ 0 & \text{otherwise}\end{cases}$$

and

$$cp_k : I = \{a_1, a_2, \ldots, a_j, \ldots, a_n\} \rightarrow I_{cp} = \left\{i_{a_1}, i_{a_2}, \ldots, i_{a_j}, \ldots, i_{a_n}\right\},$$
$$i_{a_j} = a_{(j+k)} \bmod(n).$$

All other parameters are lattice specific constants.

For a specific lattice one can usually simplify the above expressions. For the models considered in this paper (D2Q9, D2Q17, D3Q15, D3Q19, D3Q27) direct computation can be used for the calculation of (8) obtaining c_s^2 when all indices are the same and c_s^4 when there are four identical indices and the remaining indices are different e.g. (*yyyyxx*).

Consequently one can express the sixth-order tensor (8) as follows:

$$T^{(6)}_{\alpha\beta\gamma\theta\zeta\eta} = \Phi_6 \Delta_{\alpha\beta\gamma\zeta\eta\theta} + \Psi_6 P_{\alpha\beta\gamma\theta\zeta\eta},$$

where

$$\begin{aligned} P_{\alpha\beta\gamma\theta\zeta\eta} = {} & \delta_{\alpha\beta}\Delta_{\gamma\zeta\eta\theta} + \delta_{\alpha\gamma}\Delta_{\beta\zeta\eta\theta} + \delta_{\alpha\zeta}\Delta_{\beta\gamma\eta\theta} + \delta_{\alpha\eta}\Delta_{\beta\gamma\zeta\theta} + \delta_{\alpha\theta}\Delta_{\beta\gamma\zeta\eta} + \delta_{\beta\gamma}\Delta_{\alpha\zeta\eta\theta} \\ & + \delta_{\beta\zeta}\Delta_{\alpha\gamma\eta\theta} + \delta_{\beta\eta}\Delta_{\alpha\gamma\zeta\theta} + \delta_{\beta\theta}\Delta_{\alpha\gamma\zeta\eta} + \delta_{\gamma\zeta}\Delta_{\alpha\beta\eta\theta} + \delta_{\gamma\eta}\Delta_{\alpha\beta\zeta\theta} \\ & + \delta_{\gamma\theta}\Delta_{\alpha\beta\zeta\eta} + \delta_{\zeta\eta}\Delta_{\alpha\beta\gamma\theta} + \delta_{\zeta\theta}\Delta_{\alpha\beta\gamma\eta} + \delta_{\eta\theta}\Delta_{\alpha\beta\gamma\zeta}. \end{aligned}$$

3. Two-dimensional models

The lattice vectors **c** and the weights $w_{\sigma,i}$ of a D2Q9 model are specified in [7]. The speed of sound in this model is given by $c_s = 1/\sqrt{3}$.

Substituting the **c** and $w_{\sigma,i}$ parameters into (6) and (7) one can show that $\Psi_2 = c_s^2$, $\Phi_4 = 0$, $\Psi_4 = c_s^4$ and the coefficients of the sixth-order tensor can be obtained by solving

$$\Phi_6 + 15\Psi_6 = c_s^2, \qquad \Psi_6 = c_s^4, \tag{9}$$

yielding finally

$$\Phi_6 = c_s^2 - 15c_s^4. \tag{10}$$

The lattice vectors **c** of the D2Q17 model of Qian and Zhou were specified in [1].

The lattice weights need to be found subject to conservation of mass and momentum, isotropy of the stress tensor and Galilean invariance in macroscopic level. Using these constraints and the lattice relations (6)–(8) it is easy to derive the following equations for the weights:

$$2w_1 + 4w_2 + 8w_3 + 16w_4 = \Psi_2, \tag{11}$$

$$w_0 + 4(w_1 + w_2 + w_3 + w_4) = 1, \tag{12}$$

where $\Psi_2 = c_s^2$,

$$2w_1 + 4w_2 + 32w_3 + 64w_4 = 3\Psi_4, \tag{13}$$

$$4w_2 + 64w_4 = \Psi_4, \tag{14}$$

where $\Psi_4 = c_s^4$, $\Phi_4 = 0$,

$$2w_1 + 4w_2 + 128w_3 + 256w_4 = \Phi_6 + 15\Psi_6, \tag{15}$$

$$4w_2 + 256w_4 = \Psi_6 \tag{16}$$

and Φ_6, Ψ_6 will be determined later on.

Equations (11)–(16) form an equation system with six unknowns $(w_0, \dots, w_5, c_s)$. Satisfying this system by choosing suitable model parameters, one can derive the following macroscopic equations through a Chapman–Enskog expansion:

$$\begin{aligned} &\partial_t \rho + \partial_\alpha(\rho u_\alpha) = 0, \\ &\partial_t(\rho u_\beta) + \partial_\alpha(\rho u_\alpha u_\beta) = -\partial_\beta\big(\rho c_s^2\big) + 2\nu\partial_\alpha(\rho S_{\alpha\beta}) + O(u^3), \end{aligned} \tag{17}$$

where the strain rate tensor is defined as follows:

$$S_{\alpha\beta} = \tfrac{1}{2}(\partial_\alpha u_\beta + \partial_\beta u_\alpha)$$

and the kinematic viscosity is given by

$$\nu = \delta c_s^2\big(\tau - \tfrac{1}{2}\big).$$

4. Perfect compensation of the nonlinear deviation

The macroscopic equations (17) are accurate up to second order in δ and the momentum equation has an unphysical third-order velocity term [1]:

$$\partial_\gamma \rho u_\alpha u_\beta u_\gamma. \tag{18}$$

The deviation terms can be significant when the density gradient or the velocity is high, such as in relatively high Mach number flows.

In order to eliminate the deviation terms, Qian and Zhou [1] proposed to choose a proper model parameter K. Accordingly, we have to satisfy the following equation:

$$\partial_\gamma \rho u_\alpha u_\beta u_\gamma = -\frac{K}{6c_s^6}\partial_\theta \rho u_\gamma u_\zeta u_\eta\big(T^{(6)}_{\alpha\beta\gamma\theta\zeta\eta} - 3c_s^2\delta_{\zeta\eta}T^{(4)}_{\alpha\beta\gamma\theta}\big). \tag{19}$$

From (19), substituting the lattice relations (7), (8), simplifying and considering the case $\alpha = \beta = x$ a long but simple equation can be derived without loss of generality. The equation implies that the following relations have to hold for a perfect elimination of the cubic term in 2D:

$$K\left(\frac{\Phi_6}{6c_s^6} + 15\frac{\Psi_6}{6c_s^6} - \frac{3}{2}\right) = 1, \qquad \frac{\Psi_6}{6c_s^6} - \frac{1}{2} = 0, \qquad \frac{\Psi_6}{2c_s^6} - \frac{1}{2} = 1. \tag{20}$$

The solution of this system is given by

$$K = 1, \qquad \Psi_6 = 3c_s^6, \qquad \Phi_6 = -30c_s^6. \tag{21}$$

That is, for a complete elimination of the cubic term in 2D we have to use the compensation parameter $K = 1$ and equations (11)–(16) have to be solved by using the parameters given by (21).

Unfortunately, there is no solution with real roots for (11)–(16) and the parameters obtained above. Therefore, a perfect elimination is not possible for a D2Q17 model. The same conclusion can be achieved in the case of a D2Q9 model. Indeed, we have found relation (10) and for the commonly used D2Q9 relations in (21) cannot be satisfied.

Note that the problem with this kind of compensation is that one has only two free parameters and three equations (20). To overcome this problem one has to introduce an additional parameter which makes (20) well determined. This approach is used in both [5] and [6].

Their approach is based on the fact that the Navier–Stokes equations can be obtained without cubic deviations, as far as the equilibrium distribution function satisfies the following relations:

$$\sum_{\sigma,i} f_i^{(0)} = \rho, \tag{22}$$

$$\sum_{\sigma,i} c_{\sigma,i\alpha} f_i^{(0)} = \rho u_\alpha, \tag{23}$$

$$\sum_{\sigma,i} c_{\sigma,i\alpha} c_{\sigma,i\beta} f_i^{(0)} = p\delta_{\alpha\beta} + \rho u_\alpha u_\beta, \tag{24}$$

$$\sum_{\sigma,i} c_{\sigma,i\alpha} c_{\sigma,i\beta} c_{\sigma,i\theta} f_i^{(0)} = \rho u_\alpha u_\beta u_\theta + p\partial_\theta (u_\theta \delta_{\alpha\beta} + u_\alpha \delta_{\beta\theta} + u_\beta \delta_{\alpha\theta}). \tag{25}$$

The last constraint assures the cancellation of the cubic deviation terms. Indeed, as a result of the Chapman–Enskog expansion one arrives at the following form of the non-equilibrium stress tensor (see, e.g., [11] for details):

$$\Pi_{\alpha\beta}^{(1)} = -\tau\left[\partial_{t_0} \rho u_\alpha u_\beta - c_s^2 \delta_{\alpha\beta} \partial_\gamma \rho u_\gamma + \partial_\theta S_{\alpha\beta\theta}\right],$$

where

$$\partial_\theta \sum_{\sigma,i} c_{\sigma,i\alpha} c_{\sigma,i\beta} c_{\sigma,i\theta} f_i^{\text{eq}} = \partial_\theta S_{\alpha\beta\theta} = c_s^2 (\delta_{\alpha\beta} \partial_\gamma \rho u_\gamma + \partial_\beta \rho u_\alpha + \partial_\alpha \rho u_\beta).$$

The first term of the non-equlibrium stress can be simplified using the first-order equations of the expansion, the Euler equations, obtaining

$$\partial_{t_0} \rho u_\alpha u_\beta = -u_\beta \partial_\gamma \rho u_\alpha u_\gamma - u_\beta \partial_\alpha \rho c_s^2 - u_\alpha \partial_\beta \rho c_s^2 - \rho u_\alpha u_\gamma \partial_\gamma u_\beta.$$

Using this relation the non-equilibrium stress tensor can be rewritten as follows:

$$\Pi_{\alpha\beta}^{(1)} = -\tau \left[\begin{array}{c} -u_\beta \partial_\gamma \rho u_\alpha u_\gamma - u_\beta \partial_\alpha \rho c_s^2 - u_\alpha \partial_\beta \rho c_s^2 - \rho u_\alpha u_\gamma \partial_\gamma u_\beta \\ - c_s^2 \delta_{\alpha\beta} \partial_\gamma \rho u_\gamma + \partial_\theta S_{\alpha\beta\theta} \end{array}\right]. \tag{26}$$

In order to cancel the third-order terms we add the term $\partial_\theta \rho u_\alpha u_\beta u_\theta$ to $\partial_\theta S_{\alpha\beta\theta}$, so that the following condition has to be fulfilled:

$$\sum_{\sigma,i} c_{\sigma,i\alpha} c_{\sigma,i\beta} c_{\sigma,i\theta} f_i^{\text{eq}} = \rho u_\alpha u_\beta u_\theta + S_{\alpha\beta\theta} = \rho u_\alpha u_\beta u_\theta + p\partial_\theta (u_\theta \delta_{\alpha\beta} + u_\alpha \delta_{\beta\theta} + u_\beta \delta_{\alpha\theta}).$$

This is the condition for the equilibrium, which has to be applied in order to eliminate the cubic velocity deviation. It was originally introduced by Chen *et al* [6] and later used by Weimar and Boon [5].

Using the lattice relations (6)–(8), it can be verified that the equilibrium distribution proposed by Chen *et al* [6] and used up to third order also by Weimar and Boom can satisfy this constraint by suitable model parameters. In contrast the equilibrium distribution of Qian and Zhou [1] does not do it.

5. Partial compensation of the nonlinear deviation

It can be shown that satisfying relations (20), part of the deviations can be eliminated and the only remaining deviation term is $\partial_x \rho u_x^3$ (and $\partial_y \rho u_y^3$ considering $\alpha = \beta = y$) in 2D. Consequently, a partial elimination can be achieved by choosing $\Psi_6 = 3c_s^6$, which is just the case for a D2Q9 model $\left(3c_s^6 = c_s^4\right)$. Furthermore, we can determine the coefficient of the remaining deviation term from equation (20) as follows:

$$\left(\frac{\Phi_6}{6c_s^6} + 15\frac{\Psi_6}{6c_s^6} - \frac{3}{2}\right) - 1 = 1.$$

Accordingly, using a D2Q9 model with a compensation parameter $K = 1$ part of the deviation terms are perfectly eliminated and the remaining error terms are not influenced at all.

Now, let us consider the D2Q17 model.

In the previous section we found no way to obtain model parameters satisfying the system of equations (11)–(16). However, using the model parameters presented by Qian and Zhou (e.g. $c_s^2 = 0.374\,0845$) one can find that the equation system is satisfied with the value $\Phi_6 = -1.752\,9650$. With this value the coefficient of the remaining error term can be written as follows:

$$\left(\frac{K\Phi_6}{6c_s^6} + 15\frac{K\Psi_6}{6c_s^6} - \frac{3K}{2}\right) - 1 = -0.581\,01,$$

which means that using the model of Qian and Zhou part of the deviations are cancelled perfectly, but still some deviation terms remain.

6. Three-dimensional models

Let us consider now popular three-dimensional models. The lattice vectors and weights of the D3Q15, D3Q19 and D3Q27 models can be found, e.g., in [10]. The speed of sound is given by $c_s = 1/\sqrt{3}$ for all these models.

Substituting the parameters of the above-mentioned three-dimensional models into (6) and (7) one can show that the same relations can then be obtained for the D2Q9 model, i.e. $\Psi_2 = c_s^2$, $\Phi_4 = 0$, $\Psi_4 = c_s^4$ and $\Phi_6 = c_s^2 - 15c_s^4$. Substituting the lattice relations (7) and (8) into (19), simplifying and considering the case $\alpha = \beta = x$, a simple equation can be derived without loss of generality. Just as for the D2Q9 model, the equation implies that relations (20) should be satisfied supplementing by an additional constraint: $K/2 = 0$. Since this constraint contradicts the first equation in (20), therefore, a perfect compensation is not possible in such models. However, using similar arguments then in the two-dimensional models, we can reduce the deviations in three-dimensional models, too.

That is, with the choice of $K = 1$ we can reduce the value of the cross terms. The reduction is perfect in the case of the D3Q27 model, but it is only partial for D3Q15 and D3Q19 models. Besides these deviations we still have the terms $\partial_x \rho u_x^3$, $\partial_y \rho u_y^3$ and $\partial_z \rho u_z^3$, which will not be affected at all by the compensation. It is worth mentioning that in the three-dimensional models studied the more general form of the compensation (5) does not help to further reduce the deviations. It is worth noting that the same conclusion can be achieved by simply considering the constraint (25).

7. Numerical results

7.1. Decaying shear flow

In [1], the effect of the compensation was demonstrated by simulating shear flow in a moving frame, measuring the effective viscosity, which is influenced by the third-order deviation term. It has been shown that the effective viscosity does not change with the frame velocity when the compensation is in action.

The decaying shear flow in a moving frame is specified by the following velocity and pressure (density) fields:

$$u_x = A, \qquad u_y = B\cos(x - At)\,\mathrm{e}^{-\nu t}, \qquad \rho = \text{const},$$

where A determines the frame velocity.

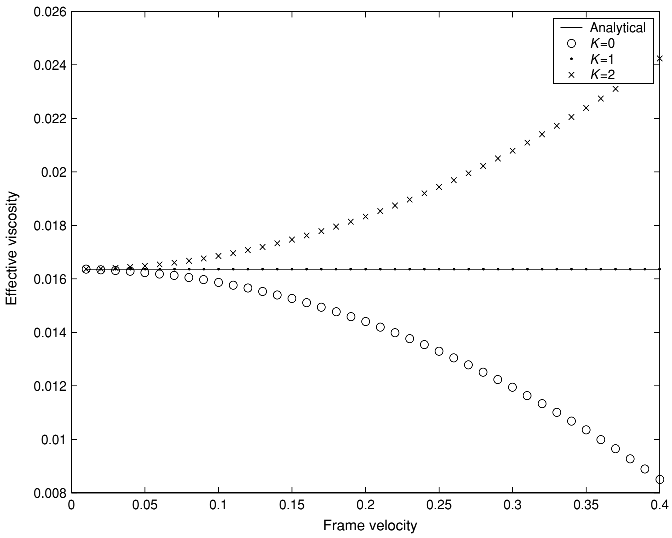

Figure 1. Effective viscosity in a D2Q9 model using various frame velocities and compensation parameters.

Note that for this flow the $\partial_x \rho u_x^3$ and $\partial_y \rho u_y^3$ terms vanish by definition; therefore, complete compensation of the cubic deviation can be achieved by a D2Q17 or a D2Q9 model.

In order to demonstrate this fact, we simulated decaying shear flow using different frame velocities. Simulation results are shown in figure 1 for the D2Q9 model (similar figure is shown in the paper of Qian and Zhou for the D2Q17 model). The solid line represents the analytical viscosity.

As one can see in figure 1, the viscosity is velocity *independent* only when the compensation parameter $K = 1$. This parameter can be used for both models and it provides perfect elimination of the cubic terms at least for shear flow simulations. Without compensation or using a compensation parameter $K \neq 1$, one makes the effective viscosity velocity dependent due to the cubic deviations.

7.2. Acoustic waves

In order to test our analytical results further, we considered flows where the $\partial_x \rho u_x^3$ term does not vanish. Such flow, for instance, is a plain sound wave. The performance of the lattice Boltzmann method for the simulation of linear and nonlinear acoustics has been studied by Buick *et al* [8, 9] at low Mach numbers. Here we study the performance of the compensated method simulating sound waves with various amplitudes. So the initial condition is given as follows:

$$u_x = A\frac{c_s}{\rho_0}\sin(x), \qquad u_y = 0, \qquad \rho = \rho_0 + A\sin(x).$$

Simulations were performed using both the D2Q17 and D2Q9 models with and without compensation. The simulation domain is a rectangle with the size NX = 256, NY = 4. In figure 2, the time development of the normalized velocity is shown at the point NX/4 for D2Q17 simulations in which the amplitude of the wave was varied in a range [0.01, 0.2] by the parameter A. The relaxation time is unit. The solid lines show the normalized velocities obtained by a compressible pseudospectral code using the corresponding model parameters.

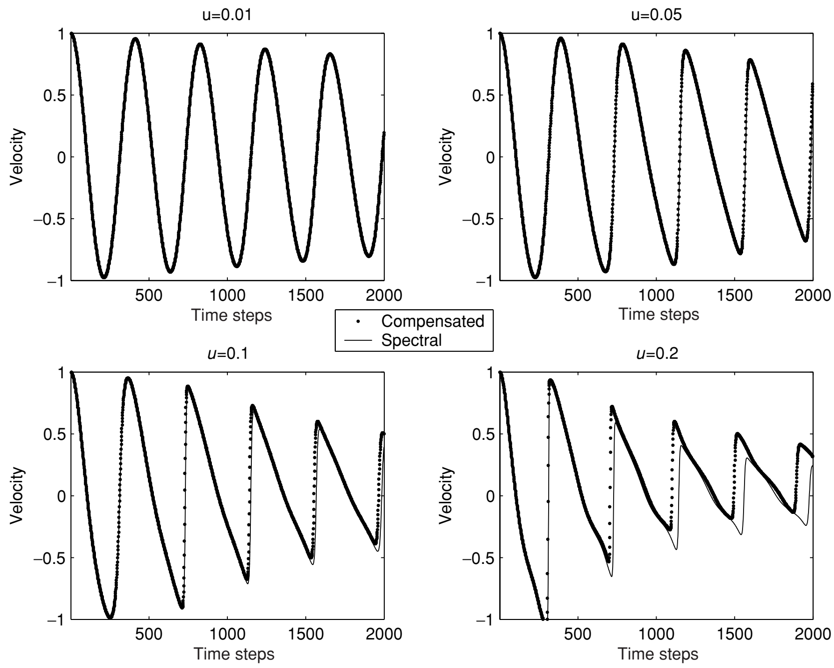

Figure 2. Evolution of the decaying sound waves at the position NX/4 using various initial velocity amplitude (D2Q17 model).

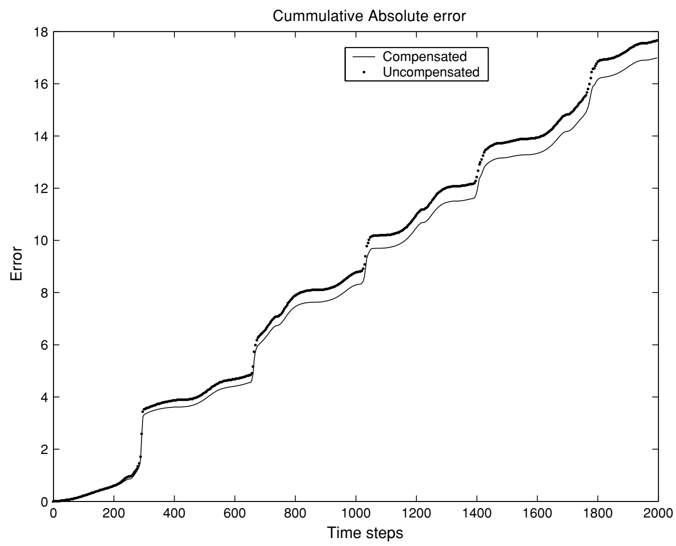

Figure 3. Cummulative absolute error of the standard and compensated methods (D2Q17 model—$u = 0.3$).

With increasing amplitude the linear theory breaks down and the waves start to take their 'N' shape. The agreement is excellent at low velocities and quite reasonable up to the velocity amplitude 0.1.

Varying the amplitude of the wave we found no effect of the compensation at all for the D2Q9 model. This observation is in line with the analytical results, since we have seen that the compensation does not influence the term $\partial_x \rho u_x^3$ while the cross terms $\partial_x \rho u_x u_y^2$ and $\partial_y \rho u_y u_x^2$ vanish by definition of the flow. The situation is different for the D2Q17 model. Here the coefficient of the term $\partial_x \rho u_x^3$ is changed by the compensation and this effect could be observed in figure 3 where the cumulative absolute error is shown for the standard and the compensated methods.

8. Conclusion

Compensation of the third-order velocity deviations in lattice Boltzmann methods has been studied. It has been shown that using the model originally proposed by Qian and Zhou one can eliminate only *part* of the third-order velocity deviations. We have demonstrated that this compensation also works for D2Q9, D3Q15, D3Q19 and D3Q27 models, using the same control parameter $K = 1$. Unfortunately, the compensation is incomplete for all the models studied.

In the two-dimensional models the terms $\partial_x \rho u_x^3$ and $\partial_y \rho u_y^3$ will survive the compensation. Using a D2Q9 model with compensation, the above terms remain untouched, while in a D2Q17 model these terms can be reduced only slightly. The compensation appears to be complete only for certain 2D numerical problems where these terms do not play any role, such as in simple shear flows used by [1] to demonstrate the efficiency of their method. The remaining deviation terms reduce the accuracy of the solution of acoustic problems as it has been demonstrated through numerical experiments. Concluding, in 2D shear flows one should prefer the D2Q9 model to D2Q17 with the compensation parameter $K = 1$. For acoustic problems we propose to use the model of Weimar and Boon [5], which is free of the cubic deviations.

In the three-dimensional D3Q15 and D3Q19 models the compensation is less efficient, since besides the terms $\partial_x \rho u_x^3$, $\partial_y \rho u_y^3$ and $\partial_z \rho u_z^3$, all cross terms will survive the compensation and their value is only slightly reduced. In the case of the D3Q27 model, the parameter $K = 1$ provides perfect compensation of the cross terms, but even in this model the terms $\partial_x \rho u_x^3$, $\partial_y \rho u_y^3$ and $\partial_z \rho u_z^3$ remain unaffected. The more general form of the compensation (5) cannot provide further reduction of the deviations in these models.

Accordingly, for three-dimensional shear flows the application of the D3Q27 lattice with the compensation parameter $K = 1$ should be used. In three dimensions, one should use one of the models of Chen *et al* [6] in order to eliminate the cubic deviations perfectly.

References

[1] Qian Y H and Zhou Y 1998 *Europhys. Lett.* **42** 359
[2] Chen S and Doolen G D 1998 *Ann. Rev. Fluid Mech.* **30** 329
[3] Hazi G and Jimenez C 2006 *Comput. Fluids* **35** 280
[4] Qian Y H and Orszag S A 1993 *Europhys. Lett.* **21** 255
[5] Weimar J R and Boon J P 1996 *Physica* A **224** 207
[6] Chen Y, Ohashi H and Akiyama M 1994 *Phys. Rev.* E **50** 2776
[7] Qian Y H, d'Humiéres D and Lallemand P 1992 *Europhys. Lett.* **17** 479
[8] Buick J M, Greated C A and Campbell D M 1998 *Europhys. Lett.* **43** 235
[9] Buick J M, Buckley C L, Greated C A and Gilbert J 2000 *J. Phys. A: Math. Gen.* **33** 3917
[10] Mei R, Shyy W, Yu D and Luo L S 2000 *J. Comput. Phys.* **161** 680
[11] Hou S, Zou Q, Chen S, Doolen G D and Cogley A C 1995 *J. Comput. Phys.* **118** 329