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New method of incorporating a body force term into the lattice Boltzmann equation

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Abstract - Electrohydrodynamics requires taking into account the electric forces acting the space charges in liquid. A new general way to incorporate a body force term into the LBE is proposed. The new method is universal and is valid for arbitrary lattices used in LBE models and for any space dimension. Correct incorporation of body-force action into LBE methods is extremely important for multiphase and multicomponent systems and also for thermal LBE models.

1 Introduction

The lattice Boltzmann equation (LBE) method [1,2] is known as a powerful tool for modeling complex fluid systems and has been actively developed in recent years. It has been widely applied in computer simulations of complex fluid flows, including multiphase and multicomponent ones. The advantages of the LBE method are the simplicity of the algorithm, the possibility of parallel computations, and an easy implementation of boundary conditions.

In many problems, fluid flows occur in the presence of body forces (for example, electrohydrodynamic flows [3,4]). In all variants of the LBE method, the mass and momentum conservation laws are satisfied exactly owing to an appropriate choice of equilibrium distribution functions. Nevertheless, all known methods of incorporation of body force term into LBE method [5-11] were shown to be valid only to the first order in $\Delta\mathbf{u} = \mathbf{F}/\rho \cdot \Delta t$. Here $\Delta\mathbf{u}$ is the change in velocity for time step due to body force. This results in incorrect values of one-particle velocity distribution functions. This is important even for isothermal LBE models for which the energy equation is not considered. Indeed, the deviations in internal energy from the value that should precisely correspond to the temperature $\theta = 1/3$ for isothermal LBE models may result in changes in density (or pressure) in the region of fluid where body force acted earlier.

The body force term in correct form is extremely important for electrohydrodynamics, and, especially, for multicomponent and multiphase systems, because the magnitude of body force and, consequently, the values of $\Delta\mathbf{u}$ are sufficiently high in a region of interface layers.

2 LBE model

In the LBE method, single particle distribution functions N_k are used as variables. In the absence of body forces, the evolution equation has the form

$$N_k(\mathbf{x}+\mathbf{c}_k\Delta t, t+\Delta t) = N_k(\mathbf{x},t) + \Omega_k(N(\mathbf{x},t)). \quad (1)$$

Here Ω_k is the collision operator, $\mathbf{c}_k$ are the particle velocities, Δt is the time step (lattice vectors are $\mathbf{e}_k = \mathbf{c}_k\Delta t$). The fluid density ρ and the velocity $\mathbf{u}$ at the node can be calculated as $\rho = \sum_{k=0}^{b} N_k$ and $\rho\mathbf{u} = \sum_{k=0}^{b} \mathbf{c}_k N_k$. For the collision operator, it is common to use the Bhatnagar–Gross–Krook (BGK) approximation: $\Omega_k(N) = (N_k^{eq} - N_k)/\tau$, which represents simple relaxation to local equilibrium [12].

The equilibrium Maxwell–Boltzmann velocity distribution function has the form

$$f^{eq}(\mathbf{u}) = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{(\xi-\mathbf{u})^2}{2\theta}\right). \quad (2)$$

Here ξ is the microscopic velocity of the molecules, D is the space dimension, and $\theta = kT/m$ is the reduced temperature. For isothermal LBE models of fluid, the expansion of equilibrium distribution functions in series in $\mathbf{u}$ depends on the density and velocity as

$$N_k^{eq}(\mathbf{u}) = \rho w_k \left(1 + \frac{\mathbf{c}_k\mathbf{u}}{\theta} + \frac{(\mathbf{c}_k\mathbf{u})^2}{2\theta^2} - \frac{\mathbf{u}^2}{2\theta}\right). \quad (3)$$

The vectors $\mathbf{c}_k$ and the coefficients w_k depend on specific lattice. The lattice should be symmetric enough to ensure that the tensors are isotropic [13,14]. In any specific variant of the LBE method, the main part of the momentum flux tensor must take the form

$$\Pi_{ij}^{(0)} = \sum_{k=0}^{b} c_{ki}c_{kj} N_k^{eq} = p\delta_{ij} + \rho u_i u_j, \quad (4)$$

where p is the pressure and δ_{ij} is the Kronecker delta.

For the two-dimensional nine-velocity D2Q9 model [15] ($|\mathbf{c}_k| = 0$, 1 or $\sqrt{2}$) on a square lattice, the coefficients are $w_0 = 4/9$, $w_{1-4} = 1/9$, and

$w_{5-8} = 1/36$. We used also the one-dimensional D1Q3 model with three values of the velocity $\mathbf{c}_k = -1$, 0, and +1 ($w_0 = 2/3$, $w_{1,2} = 1/6$). For both models the appropriate value of temperature is $\theta = 1/3$. The reduced relaxation time τ defines the kinematic viscosity $\nu = \theta(\tau - 1/2)$.

3 Body force

During the time step, a body force changes the momentum of a fluid at a node by $\Delta\mathbf{p} = \mathbf{F}(\mathbf{x},t)\Delta t$. The corresponding change of the velocity is equal to $\Delta\mathbf{u} = \mathbf{F}/\rho \cdot \Delta t$.

Let us consider a uniform flow with density ρ and velocity $\mathbf{u}$ for which the velocity distribution function is equilibrium (2). One can show that after action of a short pulse of uniform field $\mathbf{F}$, the flow should remain uniform and the velocity distribution should be simply shifted by a value $\Delta\mathbf{u}$, remaining equilibrium, but with a new value of the mean velocity $\mathbf{u} + \Delta\mathbf{u}$. For the LBE method, this implies that $N_k(\mathbf{x}, t+\Delta t)$ should be equal to $N_k^{eq}(\mathbf{u}+\Delta\mathbf{u})$ if initially $N_k(\mathbf{x},t) = N_k^{eq}(\mathbf{u})$.

3.1. Exact difference method for the continuous Boltzmann equation

The continuous Boltzmann equation (CBE) with collision integral Ω has the form

$$\frac{\partial f}{\partial t} + \xi\nabla f + \mathbf{a}\nabla_\xi f = \Omega, \qquad (5)$$

where $f(\mathbf{x},\xi,t)$ is the single particle distribution function in phase space $(\mathbf{x},\xi)$ and $\mathbf{a} = \mathbf{F}(\mathbf{x},t)/\rho$ is the acceleration due to the action of the force.

It is very difficult to evaluate correctly the term $\nabla_\xi f$ for a nonequilibrium distribution function bearing in mind following transformation of it to form appropriate for LBE. Nevertheless, one can approximately write $\nabla_\xi f \approx \nabla_\xi f^{eq}$ since the main part of the distribution function f is f^{eq}. In this approximation, the explicit expression was obtained in [7] from (2)

$$\mathbf{a}\nabla_\xi f^{eq} = -\frac{\mathbf{a}(\xi - \mathbf{u})}{\theta} f^{eq}. \qquad (6)$$

On the other hand, we noticed [16] that the relation $\nabla_\xi f^{eq} = -\nabla_\mathbf{u} f^{eq}$ is valid for any form of equilibrium distribution function (including the Maxwell–Boltzmann equilibrium distribution function (2)) because all of them must depend only on the difference $(\xi - \mathbf{u})$ to ensure the Galilean invariance. The full derivative (at constant density ρ) in a frame of reference that moves with the fluid velocity $\mathrm{d}f^{eq}(\mathbf{u}(\mathbf{r}(t),t))/\mathrm{d}t = \nabla_\mathbf{u} f^{eq} \cdot (\partial\mathbf{u}/\partial t + \nabla\mathbf{u}\cdot d\mathbf{r}/dt)$ is equal to the change of the distribution function due to the action of the force $\mathbf{a}\nabla_\mathbf{u} f^{eq}$.

Hence, equation (5) now becomes [16]

$$\frac{\partial f}{\partial t} + \xi\nabla f - \frac{\mathrm{d}f^{eq}}{\mathrm{d}t} = \Omega. \qquad (7)$$

Here the body force term is written as the full derivative along the Lagrange coordinate df^{eq}/dt at constant density ρ. This form of the continuous Boltzmann equation is preferred over approximation (6) because it exactly converts equilibrium distribution functions to equilibrium ones after the action of the force. In this particular case, the collision term $\Omega = 0$ because the velocity distribution remains equilibrium.

Since the velocity change in a time interval Δt is equal to $\Delta\mathbf{u} = \mathbf{a}\Delta t$, we obtain

$$\mathbf{a}\nabla_\xi f\,\Delta t = -(f^{eq}(\rho,\mathbf{u}+\Delta\mathbf{u}) - f^{eq}(\rho,\mathbf{u})). \qquad (8)$$

Here we note that the last expression is exact even for a finite change of velocity $\Delta\mathbf{u}$ if the distribution was locally equilibrium before the action of the force. Hence, this method can be called the exact difference method (EDM) for the continuous Boltzmann equation.

3.2. Exact difference method for LBE

After discretization of the continuous Boltzmann equation (7) in velocity space, as it was done in [8,9,17,18], we obtain the exact difference method for LBE models in form

$$N_k(\mathbf{x}+\mathbf{c}_k\Delta t, t+\Delta t) = N_k(\mathbf{x},t) + (N_k^{eq}(\mathbf{u}(\mathbf{x},t)) - N_k(\mathbf{x},t))/\tau + \Delta N_k. \qquad (9)$$

Here the changes of the distribution functions ΔN_k due to the force are equal to the difference of the equilibrium distribution functions at the constant density ρ

$$\Delta N_k = N_k^{eq}(\rho,\mathbf{u}+\Delta\mathbf{u}) - N_k^{eq}(\rho,\mathbf{u}). \qquad (10)$$

If initially $N_k(\mathbf{x},t) = N_k^{eq}(\mathbf{u}_0)$, then using this method, we obtain desired result $N_k(\mathbf{x},t+\Delta t) = N_k^{eq}(\mathbf{u}_0+\Delta\mathbf{u})$. This means that, indeed, the distribution function in a local region of space is simply shifted by a value $\Delta\mathbf{u}$ under the action of the body force, remaining equilibrium. This is valid for arbitrary values of τ. Hence, we propose a new method of incorporating the body force term into the LBE that ensures that the equilibrium distribution function remains exactly equilibrium after the action of the uniform force, although the LBE is a discrete method. Thus, we derived the exact difference method (EDM) for LBE.

Moreover, because this method is valid for the continuous Boltzmann equation for an arbitrary form of the collision integral, our method (9), (10) proposed for LBE models is valid not only for the collision operator with single relaxation time (BGK) but also for collision operators of arbitrary form.

One can exactly rewrite equations (9) and (10) in another form. Let us take into account action of the body force before execution of the collision operator

$$N_k^*(\mathbf{x},t+\Delta t) = N_k(\mathbf{x},t) + \Delta N_k. \quad (11)$$

Next, the effect of collision operator is calculated:

$$N_k(\mathbf{x},t+\Delta t) = N_k^*(\mathbf{x},t+\Delta t) + (N_k^{eq}(\mathbf{u}+\Delta\mathbf{u}) - N_k^*(\mathbf{x},t+\Delta t))/\tau. \quad (12)$$

Conceptually, this approach is similar to the method of splitting in physical processes which was used for finite-difference equations [19]. In this form of our method, the collision operator acts on the distribution functions after the body force term. This commutative property indicates that the accuracy of our method is second order in time.

In [20,21], it was shown that the LBE method (1) has second-order accuracy in both space and time due to a special form of the discretization error. Hence, it is very important that our method of incorporating the body force term into the LBE method is also second-order accurate in time.

For the specific form of equilibrium distribution functions (3), the body force term (10) can be written as

$$\Delta N_k = \rho w_k\left(\frac{\mathbf{c}_k - \mathbf{u}}{\theta} + \frac{(\mathbf{c}_k\mathbf{u})}{\theta^2}\mathbf{c}_k\right)\Delta\mathbf{u} + \rho w_k\left(\frac{(\mathbf{c}_k\Delta\mathbf{u})^2}{2\theta^2} - \frac{(\Delta\mathbf{u})^2}{2\theta}\right). \quad (13)$$

Nevertheless, the body force term in the form (10) is more general and more convenient for numerical implementations.

3.3. Chapman–Enskog expansion

The Chapman–Enskog expansion is the common tool to derive the macroscopic hydrodynamic equations that correspond to specific LBE method.

Using the body force term in form (10) and performing a Taylor expansion of equilibrium distribution functions $N_k^{eq}(\rho,\mathbf{u}+\Delta\mathbf{u})$ in series in $\Delta\mathbf{u} = \mathbf{a}\Delta t = \mathbf{F}\Delta t/\rho$, we obtain

$$\Delta N_k = \left(\Delta t + \frac{\Delta t^2}{2}\left(\mathbf{a}\frac{\partial}{\partial\mathbf{u}}\right)\right)\left(\mathbf{a}\frac{\partial N_k^{eq}}{\partial\mathbf{u}}\right) + O(\Delta u^3). \quad (14)$$

Taking into account a small parameter $\Delta t = \varepsilon$ (lattice Knudsen number), expansion of distribution functions $N_k = N_k^{(0)} + \varepsilon N_k^{(1)} + \varepsilon^2 N_k^{(2)} + \ldots$ and also definition $\partial/\partial t = \partial/\partial t_1 + \varepsilon\partial/\partial t_2$, we obtain Chapman–Enskog multi-scale expansion of LBE method (9). We used the general constraints for distribution functions $\sum N_k^{eq} = \rho$, $\sum \mathbf{c}_k N_k^{eq} = \rho\mathbf{u}$, $\sum N_k^{(1)} = 0$, $\sum N_k^{(2)} = 0$ and $\sum \mathbf{c}_k N_k^{(1)} = 0$.

In the zero order of the parameter ε, we have $N_k^{(0)} = N_k^{eq}$. In the first order of the parameter ε, we obtain

$$\frac{\partial N_k^{eq}}{\partial t_1} + \mathbf{c}_k\nabla N_k^{eq} = -\frac{N_k^{(1)}}{\tau} + \mathbf{a}\frac{\partial N_k^{eq}}{\partial\mathbf{u}}. \quad (15)$$

Performing the summation over all possible directions $\mathbf{c}_k$ in the equation (15), we obtained

$$\frac{\partial\rho}{\partial t_1} + \nabla(\rho\mathbf{u}) = 0. \quad (16)$$

Multiplying equations (15) by vector $\mathbf{c}_k$ and summing over all possible directions $\mathbf{c}_k$, we obtain

$$\frac{\partial\rho\mathbf{u}}{\partial t_1} + \nabla(\Pi_{ij}^{(0)}) = \rho\mathbf{a}, \quad (17)$$

where the momentum flux tensor for several isothermal models LBE (for example, D1Q3 and D2Q9) has the form $\Pi_{ij}^{(0)} = \rho\theta\delta_{ij} + \rho u_i u_j$, and $\theta = 1/3$. Thus, we obtained the Euler equations (16) and (17) in the first order of Chapman–Enskog expansion in the parameter ε for isothermal case.

In the second order of the parameter ε, after some algebra using (15), we have

$$\frac{\partial N_k^{eq}}{\partial t_2} + \left(1 - \frac{1}{2\tau}\right)\left(\frac{\partial N_k^{(1)}}{\partial t_1} + \mathbf{c}_k\nabla N_k^{(1)}\right) = -\frac{N_k^{(2)}}{\tau} - \frac{1}{2}\left(\frac{\partial}{\partial t_1} + \mathbf{c}_k\nabla - \left(\mathbf{a}\frac{\partial}{\partial\mathbf{u}}\right)\right)\left(\mathbf{a}\frac{\partial N_k^{eq}}{\partial\mathbf{u}}\right). \quad (18)$$

The last additional terms that depend on vector $\mathbf{a}$ relate to body force.

After summing over all possible directions $\mathbf{c}_k$ in (18) we combine it with (16), and then obtain the equation

$$\frac{\partial\rho}{\partial t} + \nabla(\rho\mathbf{u}) = -\frac{\Delta t}{2}\nabla(\rho\mathbf{a}). \quad (19)$$

If we redefine the vector of velocity $\tilde{\mathbf{u}}$ specified at half time step $\Delta t/2$ as $\rho\tilde{\mathbf{u}} = \sum \mathbf{c}_k N_k^{eq} + \mathbf{F}\Delta t/2$ [10], we obtain the continuity equation

$$\frac{\partial\rho}{\partial t}+\nabla(\rho\tilde{\mathbf{u}})=0. \qquad (20)$$

Multiplying equation (18) by vector $\mathbf{c}_k$ and summing over all possible directions and then combining it with (17), we obtain, by analogy, the Navier–Stokes equation for isothermal LBE models for redefined velocity $\tilde{\mathbf{u}}$

$$\frac{\partial\rho\tilde{\mathbf{u}}}{\partial t}+\nabla(\tilde{\Pi}^{(0)})=\rho\mathbf{a}+\nu\frac{\partial}{\partial x_j}\left(\rho\left(\frac{\partial\tilde{u}_j}{\partial x_i}+\frac{\partial\tilde{u}_i}{\partial x_j}\right)\right)$$
$$+\nu\frac{\partial}{\partial x_j}\left(u_j\frac{\partial\rho}{\partial x_i}+u_i\frac{\partial\rho}{\partial x_j}\right) \qquad (21)$$
$$+\left(\tau-\frac{1}{2}\right)\frac{\partial}{\partial x_j}\left(u_iu_j\frac{\partial\rho}{\partial t_1}\right),$$

where $\nu=\theta(\tau-1/2)\Delta t$. Here $\tilde{\Pi}_{ij}^{(0)}=\rho\theta\delta_{ij}+\rho\tilde{u}_i\tilde{u}_j$ is the redefined momentum flux tensor. Thus, we have the system of Navier-Stokes equations (20) and (21) in the second order of Chapman–Enskog expansion in the parameter ε.

Last two extraneous terms in (21) are usual deviations of Chapman–Enskog expansion for LBE models from Navier-Stokes equation due to compressibility of liquid. Sometime, these terms are usually neglected to obtain the LBE methods for nearby incompressible fluids [8,9] or can be taken into account for compressible fluids in finite-difference form. No any additional incorrect terms appeared due to presence of body force. This fact is outstanding advantage of our exact difference method.

3.4. Methods of explicit derivative

In another class of models [7-9], the body force term (6) was directly used, assuming that it is constant during the time step. In this case, the change of the distribution function due to the action of a short pulse of the force takes the form

$$\Delta N_k=\frac{(\mathbf{c}_k-\mathbf{u})\Delta\mathbf{u}}{\theta}N_k^{eq}(\mathbf{u}). \qquad (22)$$

This class of body force terms can be called the method of explicit derivative (MED).

Usually the zero or first order expansion in series in $\mathbf{u}$ was used. In the first order we have

$$\Delta N_k=\rho w_k\left(\frac{\mathbf{c}_k-\mathbf{u}}{\theta}+\frac{(\mathbf{c}_k\mathbf{u})}{\theta^2}\mathbf{c}_k\right)\Delta\mathbf{u}. \qquad (23)$$

In the case of second order expansion of (22) in series in $\mathbf{u}$, the situation will not be better.

The main disadvantage of this method is the lack of terms of the second order in $\Delta\mathbf{u}$ (compare with (13)). This leads to an incorrect form of the body force work. For example, the body force work is equal to zero for a fluid that was initially at rest.

Let us introduce the value of deviation of this method (23) from the exact difference method (10)

$$\Delta R_k=-\frac{\rho w_k}{2\theta}\left(\frac{(\mathbf{c}_k\Delta\mathbf{u})^2}{\theta}-(\Delta\mathbf{u})^2\right). \qquad (24)$$

3.5. Method of modifying the BGK collision term

In [5,6], the action of body forces was taken into account by means of modification of the BGK collision operator (MCO) in the evolution equation:

$$N_k(\mathbf{x}+c_k\Delta t,t+\Delta t)=N_k(\mathbf{x},t)$$
$$+(N_k^{eq}(\mathbf{u}+\Delta\mathbf{u}_+)-N_k(\mathbf{u}))/\tau, \qquad (25)$$

where $\Delta\mathbf{u}_+=\Delta\mathbf{u}\cdot\tau$.

Unfortunately, the method (25) is valid only in linear approximation in $\Delta\mathbf{u}$. For isothermal LBE method using (3), one can obtain

$$\Delta N_k=N_k^{eq}(\mathbf{u}+\Delta\mathbf{u})-N_k^{eq}(\mathbf{u})$$
$$+\frac{\rho w_k}{2}\left(\frac{(\mathbf{c}_k\Delta\mathbf{u})^2}{\theta^2}-\frac{(\Delta\mathbf{u})^2}{\theta}\right)(\tau-1). \qquad (26)$$

Hence, the deviation from EDM is equal to

$$\Delta R_k=-\frac{\rho w_k}{2\theta}\left(\frac{(\mathbf{c}_k\Delta\mathbf{u})^2}{\theta}-(\Delta\mathbf{u})^2\right)(1-\tau). \qquad (27)$$

Only in the case $\tau=1$, does this deviation vanish and, therefore, for fluid that was initially in the state $N_k=N_k^{eq}$, the velocity distribution remains equilibrium after the action of the body force. But if τ is fixed, one cannot vary the viscosity $\nu=1/6$.

3.6. Method of undefined coefficients

In [10], the general form of expansion of body force term in a power series in the particle velocity $\mathbf{c}_k$ was used

$$\Delta N_k=\rho w_k\left(A+\frac{\mathbf{B}\mathbf{c}_k}{\theta}+\frac{\mathbf{C}:(\mathbf{c}_k\mathbf{c}_k-\mathbf{1}\theta)}{2\theta^2}\right)\Delta t. \qquad (28)$$

The undefined coefficients A, $\mathbf{B}$ and $\mathbf{C}$ depend on body force $\mathbf{F}=\rho\mathbf{a}$ and were found as $A=0$, $\mathbf{B}=\mathbf{a}$ and $C_{ij}=a_iu_j+a_ju_i$ to cover the continuity and Navier–Stokes equations in Chapman–Enskog expansion. Actually, the expression (28) is an expansion of (22) in series in $\mathbf{u}$ truncated to first order in $\mathbf{u}$. Thus, in this method as well as in (22), only the terms that are proportional to the first order in $\Delta\mathbf{u}$ (and, consequently, to the first order in force $\mathbf{F}\Delta t$) were taken into account. Hence, this method has the same disadvantages that are appropriate to the method of explicit derivative.

In another model [11] the method of undefined coefficients (28) was used in combination with the method of modifying the collision operator in form

$$N_k(\mathbf{x}+c_k\Delta t,t+\Delta t)=N_k(\mathbf{x},t) + (N_k^{eq}(\mathbf{u}+\Delta\mathbf{u}_+)-N_k(\mathbf{u}))/\tau+\Delta N_k, \quad (29)$$

where ΔN_k is equal to (28), and $\Delta\mathbf{u}_+=\Delta\mathbf{u}/2$. The deviation of this method from the EDM is equal to

$$\Delta R_k=-\frac{\rho w_k}{8\theta\tau}\left(\frac{(\mathbf{c}_k\Delta\mathbf{u})^2}{\theta}-(\Delta\mathbf{u})^2\right) \quad (30)$$

for coefficients found in this work [11].

4 Tests

We performed calculations for fluids with phase transition. For this example, the magnitude of body force and, consequently, the values of $\Delta\mathbf{u}$ is sufficiently high in a region of interface layer between gas and liquid phases. The model of phase transition [5,6] was used. To describe the phase transition in this model the attractive forces were introduced between every neighbor nodes. For one-dimensional case we have

$$\mathbf{F}(\mathbf{x})=G_0\psi(\rho(\mathbf{x}))\sum_k\psi(\rho(\mathbf{x}+\mathbf{e}_k))\mathbf{e}_k, \quad (31)$$

Here $G_0>0$ is the coefficient, $\psi(\rho)$ is the following function [5,6]

$$\psi(\rho)=\rho_0(1-\exp(-\rho/\rho_0)). \quad (32)$$

The equation of state for this isothermal model is

$$P=\rho\theta-G_0\psi^2(\rho), \quad (33)$$

where $\theta=1/3$. Critical point is $G_{0*}=2/3$ and $\rho_*=\rho_0\ln 2$.

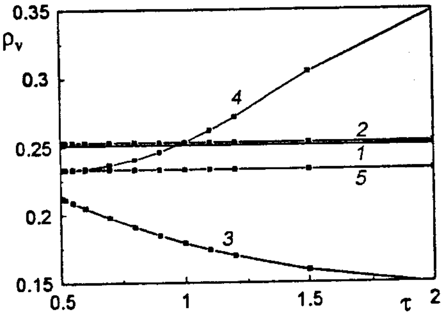

Fig. 1. Vapor density vs. relaxation time τ. *1* – Maxwell rule for (33), *2* – EDM, *3* – MED, *4* – MCO, *5* – Guo et.al. [11] $G_0=0.75$, $\rho_0=1$.

One-dimensional steady state transition layers were calculated at different values of relaxation time τ (Fig. 1). The theoretical values of vapor and liquid densities were calculated using the Maxwell rule for equation of state (33). Only the results obtained by EDM coincide well with the theory and do not depend on relaxation time. Note, the method of modification of collision operator coincides with the EDM at $\tau=1$, and the method [11] coincides with the method of modification of collision operator at $\tau=0.5$.

The coexistence curve is shown in Fig. 2. The deviations of results obtained by method of modification of collision operator, methods of explicit derivative, and method of undefined coefficients [11] from theoretical values are large enough at $G_0>0.7$. Only the results obtained by EDM coincides well with the theory up to $G_0=1$.

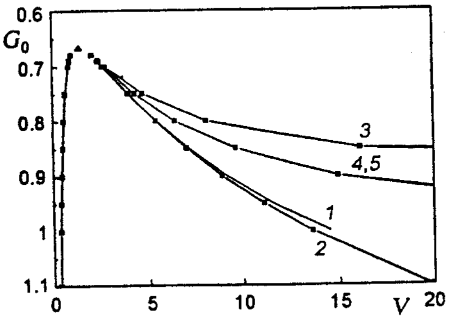

Fig. 2. The coexistence curve for $\tau=0.51$. *1* – Maxwell rule for (33), *2* – EDM, *3* – MED, *4* – MCO, *5* – Guo et.al. [11]. ▲ – critical point. $\rho_0=1$.

5 Discussion and conclusions

A new method (EDM) was proposed that takes into account the action of a body force using the difference of equilibrium distribution functions in form Eq. (10).

In all methods under consideration the terms linear in $\Delta\mathbf{u}$ are equal one to other, and the terms proportional to $\Delta\mathbf{u}^3$ are absent as should be obviously. In all methods the following constraints are exactly correct $\sum R_k=0$, $\sum \mathbf{c}_k R_k=0$. The only difference is in terms proportional to $\Delta\mathbf{u}^2$ (see Eqs. (24), (27), (30)). One could say more that only main coefficients in ΔR_k are different. These deviations from EDM are very important because none of the methods except the exact difference method can precisely convert the locally equilibrium distribution functions into equilibrium ones after action of the locally uniform body force. Indeed, in this case for locally uniform flow, the Maxwell distribution should be simply shifted by a value $\Delta\mathbf{u}$, remaining exactly equilibrium.

The key relation in EDM is the condition $\rho=\text{const}$ for body force term. Using this condition and method of explicit derivative (22) in form

$$\Delta N_k=\frac{(\mathbf{c}_k-\mathbf{u})\Delta\mathbf{u}}{\theta}N_k^{eq}(\rho,\mathbf{u}+\Delta\mathbf{u}/2), \quad (34)$$

the particular form of EDM also could be derived, that exactly coincides with (13).

Thus, all known previous methods of incorporating a body force term into LBE method were shown to be valid only to the first order in $\Delta\mathbf{u}$. The body force term in correct form is extremely important for electrohydrodynamics, and, especially, for multicomponent and multiphase systems, because the magnitude of body force and, consequently, the values of $\Delta\mathbf{u}$ are sufficiently high in a region of interface layers.

Moreover, in the EDM, the values of total energy change, internal energy change and the body force work are exact even for finite time step. The exact difference method is simple enough and the body force term can be incorporated easily into any version of LBE method. At the same time, the number of arithmetical operations does not increase considerably. It is only necessary to calculate the equilibrium distribution functions N_k^{eq} at each node for the second time.

We want to emphasize that our method in form (10) is not an expansion but is a new general way to incorporate the body force term into any variant of lattice Boltzmann equation method. The exact difference method is valid for arbitrary lattices and for any space dimension. It does not depend on specific form (or specific expansion) of equilibrium distribution functions and, consequently, is noticeably simpler than the other methods. Although, the method of modification of collision operator, methods of explicit derivative, and methods of undefined coefficients are well suitable for the most part of liquid flows, there is no one reason to use them now, because the exact difference method is easier for use and is more precise.

The exact difference method is valid also for numerical methods based on non-lattice Boltzmann equation method with fixed set of velocities.

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References

[1] G. R. McNamara and G. Zanetti, "Use of the Boltzmann equation to simulate lattice-gas automata," *Phys. Rev. Lett.*, vol. 61, N 20, pp. 2332–2335, November 1988.

[2] F. J. Higuera and J. Jimenez, "Boltzmann approach to lattice gas simulations," *Europhys. Lett.*, vol. 9, N 7, pp. 663–668, August 1989.

[3] D. A. Medvedev and A. L. Kupershtokh, "Use of the Lattice Boltzmann Equation Method to Simulate Charge Transfer and Electrohydrodynamic Phenomena in Dielectric Liquids," *Proc. 2nd Int. Workshop on Electrical Conduction, Convection, and Breakdown in Fluids*, Grenoble, France, 2000, pp. 60–63.

[4] D. A. Medvedev and A. L. Kupershtokh, "Modeling of electrohydrodynamic flows and micro-bubbles generation in dielectric liquid by lattice Boltzmann equation method," *Proc. 14th Int. Conf. on Dielectric Liquids*, Graz, Austria, 2002, pp. 45–48.

[5] X. Shan and H. Chen, "Lattice Boltzmann model for simulating flows with multiple phases and components," *Phys. Rev. E*, vol. 47, N 3, pp. 1815–1819, March 1993.

[6] X. Shan and H. Chen, "Simulation of nonideal gases and liquid-gas phase transitions by the lattice Boltzmann equation," *Phys. Rev. E*, vol. 49, N 4, pp. 2941–2948, April 1994.

[7] X. He, X. Shan, and G. D. Doolen, "Discrete Boltzmann equation model for nonideal gases," *Phys. Rev. E*, vol. 57, N 1, pp. R13–R16, January 1998.

[8] L.-S. Luo, "Unified theory of lattice Boltzmann models for nonideal gases," *Phys. Rev. Lett.*, vol. 81, N 8, pp. 1618–1621, August 1998.

[9] L.-S. Luo, "Theory of the lattice Boltzmann method: Lattice Boltzmann models for nonideal gases," *Phys. Rev. E*, vol. 62, N 4, pp. 4982–4996, October 2000.

[10] A. J. C. Ladd and R. Verberg, "Lattice-Boltzmann simulations of particle-fluid suspension," *J. Stat. Phys.*, vol. 104, N 5/6, pp. 1191–1251, September 2001.

[11] Z. Guo, C. Zheng, and B. Shi, "Discrete lattice effects on the forcing term in the lattice Boltzmann method," *Phys. Rev. E*, vol. 65, N 4, pp. 046308-1–046308-6, 2002.

[12] P. L.Bhatnagar, E. P. Gross, and M. K. Krook, "A model for collision process in gases. I. Small amplitude process in charged and neutral one-component system," *Phys. Rev.*, vol. 94, N 3, pp. 511–525, May 1954.

[13] S. Wolfram, "Cellular automaton fluids 1: Basic theory," *J. Stat. Phys.*, vol. 45, N 3/4, pp. 471–526, 1986.

[14] Y. Chen, H. Ohashi, and M. Akiyama, "Thermal lattice Bhatnagar–Gross–Krook model without nonlinear deviations in macroscopic equations," *Phys. Rev. E*, vol. 50, N 4, pp. 2776–2783, October 1994.

[15] Y. H. Qian, D. d'Humières, and P. Lallemand, "Lattice BGK models for Navier – Stokes equation," *Europhys. Lett.*, vol. 17, pp. 479–484, February 1992.

[16] A. L. Kupershtokh, "Calculations of the action of electric forces in the lattice Boltzmann equation method using the difference of equilibrium distribution functions," in *Proc. 7th Int. Conf. on Modern Problems of Electrophysics and Electrohydrodynamics of Liquids*, St. Petersburg, Russia, 2003, pp. 152–155.

[17] X. He and L.-S. Luo, "A priori derivation of the lattice Boltzmann equation," *Phys. Rev. E*, vol. 55, N 6, pp. R6333–R6336, June 1997.

[18] T. Abe, "Derivation of the lattice Boltzmann method by means of the discrete ordinate method for the Boltzmann equation," *J. Comp. Phys.*, vol. 131, N 1, pp. 241–246, 1997.

[19] N. N. Yanenko, *The method of fractional steps* (Berlin: Springer), 1967.

[20] J. D. Sterling and S. Chen, "Stability analysis of lattice Boltzmann methods," *J. Comp. Phys.*, vol. 123, N 1, pp. 196–206, 1996.

[21] N. Cao, S. Chen, S. Jin, and D. Martinez, "Physical symmetry and lattice symmetry in the lattice Boltzmann method," *Phys. Rev. E*, vol. 55, N 1, pp. R21–R24, January 1997.