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CALCULATIONS OF THE ACTION OF ELECTRIC FORCES IN THE LATTICE BOLTZMANN EQUATION METHOD USING THE DIFFERENCE OF EQUILIBRIUM DISTRIBUTION FUNCTIONS

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The lattice Boltzmann equation (LBE) method [1,2] 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, particularly for electrohydrodynamic flows. In [3-6] the LBE method was successfully applied in computer simulations of electrohydrodynamic flows. In this case, it was necessary in addition to take into account the effects due to electric field:

- Convective electrical charge transfer by moving fluid;
- Charge transfer due to conductive currents (for this purpose, it is necessary to calculate the potential of electric field);
- The effect of electric forces on charged fluid in electric field.

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 the second term on the right-hand side 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 [7]. For isothermal fluids, the expansion of equilibrium distribution functions depends on the density and velocity as

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

Here θ is the reduced temperature and the vectors $\mathbf{c}_k$ and the coefficients w_k depend on specific lattice.

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 distribution function is the equilibrium Maxwell–Boltzmann velocity distribution

$$f^{eq}(\mathbf{u}) = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{(\xi - \mathbf{u})^2}{2\theta} \right). \qquad (3)$$

Here ξ is the microscopic velocity and D is the space dimension. Note that this velocity distribution is valid not only for rarefied gases but also for condensed matter [8]. One can show that after action of a short pulse of uniform field $\mathbf{F}$, the flow remains uniform and the velocity distribution is 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 $N_k(\mathbf{x}, t) = N_k^{eq}(\mathbf{u})$.

The ordinary method of modifying the BGK collision operator [9] was shown to be valid only to the first order in $\Delta\mathbf{u}$.

We propose a new method of incorporating the body force term into the LBE that ensures that the equilibrium distribution function remains equilibrium after the action of the force.

Let us take into account action of the body force outside the collision operator

$$N_k(\mathbf{x} + \mathbf{c}_k \Delta t, t + \Delta t) = N_k(\mathbf{x}, t) + (N_k^{eq}(\mathbf{u}(\mathbf{x}, t)) - N_k(\mathbf{x}, t))/\tau + \Delta N_k. \qquad (4)$$

Here the changes of the distribution functions N_k due to the force are equal to the difference of the equilibrium distribution functions

$$\Delta N_k = N_k^{eq}(\mathbf{u} + \Delta\mathbf{u}) - N_k^{eq}(\mathbf{u}). \qquad (5)$$

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 in contrast with ordinary method of modification of collision operator [9]. Thus, for this case, the action of the force is taken into account exactly, although the LBE is a discrete method. Hence, this method can be called the exact difference method (EDM).

Moreover, for EDM in contrast with other known methods [9-11], the equations for kinetic-energy change and for body-force work are satisfied exactly.

The continuous Boltzmann equation has the form

$$\frac{\partial f}{\partial t} + \xi \nabla f + \mathbf{a} \nabla_\xi f = \Omega, \qquad (6)$$

where $f(\mathbf{x}, \xi, t)$ is the single particle distribution function in phase space $(\mathbf{x}, \xi)$, $\mathbf{a} = \mathbf{F}(\mathbf{x}, t)/\rho$ is the acceleration due to the action of the force, and Ω is the collision integral. One can approximately write $\nabla_\xi f \approx \nabla_\xi f^{eq}$ since the main part of the distribution function f is f^{eq}.

The relation $\nabla_{\xi} f^{eq} = -\nabla_{\mathbf{u}} f^{eq}$ is valid for any form of equilibrium distribution function because all of them must depend only on the difference $(\boldsymbol{\xi} - \mathbf{u})$ to ensure the Galilean invariance. The full derivative in a frame of reference that moves with the fluid $\mathrm{d}f^{eq}(\mathbf{u}(\mathbf{r}(t),t))/\mathrm{d}t$ 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 (6) now becomes

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

Thus, we derived the exact difference method (EDM) for the continuous Boltzmann equation. After discretization of the continuous Boltzmann equation in velocity space, as is done in [11-13], we obtain the same method in form (4) for LBE models. Moreover, because this method is valid for the continuous Boltzmann equation for an arbitrary form of the collision integral, our method (4) 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.

The exact difference method is valid for arbitrary lattices and for any space dimension. The 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.

The body-force action term in correct form is extremely important for all variants of the LBE method, especially for thermal LBE models, and also for multiphase and multicomponent systems.

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