J. Fluid Mech. (2009), *vol.* 628, *pp.* 299–309. © 2009 Cambridge University Press
doi:10.1017/S002211200900665X Printed in the United Kingdom

Lattice Boltzmann method with self-consistent thermo-hydrodynamic equilibria

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(Received 27 November 2008 and in revised form 16 February 2009)

Lattice kinetic equations incorporating the effects of external/internal force fields via a shift of the local fields in the local equilibria are placed within the framework of continuum kinetic theory. The mathematical treatment reveals that in order to be consistent with the correct thermo-hydrodynamical description, temperature must also be shifted, besides momentum. New perspectives for the formulation of thermo-hydrodynamic lattice kinetic models of non-ideal fluids are then envisaged. It is also shown that on the lattice, the definition of the macroscopic temperature requires the inclusion of new terms directly related to discrete effects. The theoretical treatment is tested against a controlled case with a non-ideal equation of state.

1. Introduction

Lattice implementations of discrete-velocity kinetic models have gained considerable interest in the last decade as efficient tools for the theoretical and computational investigations of the physics of complex flows (Shan & Chen 1993; Ladd 1994; Swift, Osborn & Yeomans 1995; He & Luo 1997; Qi 2006; Gonnella, Lamura & Sofonea 2007; Li & Wagner 2007). An important class of discrete-velocity models for ideal fluid flows, the lattice Boltzmann models (Benzi, Succi & Vergassola 1992; Chen & Doolen 1998; Wolf Gladrow 2000), can be derived from the continuum Boltzmann (BGK) equation (Bathnagar, Gross & Krook 1954), upon expansion in Hermite velocity space of the single particle distribution function $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$, describing the probability to find a molecule at space–time location $(\boldsymbol{x}, t)$ and with velocity $\boldsymbol{\xi}$ (He & Luo 1997; Martys, Shan & Chen 1998; Shan & He 1998; Shan, Yuan & Chen 2006). As a result, the corresponding lattice dynamics acquire a more systematic justification in terms of an underlying continuum kinetic theory.

The main goal of this paper is to extend such systematic link between continuum and lattice formulation to the case of thermo-hydrodynamical fluctuations in non-ideal fluids under the action of external (say gravity) and/or internal forces. In particular, we shall show that if the effects of the force field are taken into account via a uniform shift of the momentum in the equilibrium distribution, as proposed in Shan & Chen (1993), the evolution for the total kinetic energy needs to be corrected as well. A viable possibility is to introduce an *ad hoc* shift in the temperature field entering

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https://doi.org/10.1017/S002211200900665X Published online by Cambridge University Press

the local equilibrium. By doing so, the total kinetic energy recovers the correct thermo-hydrodynamical evolution.

Let us consider the usual continuum, D-dimensional, Boltzmann BGK equation

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\nabla f+\boldsymbol{g}\cdot\nabla_{\xi} f=-\frac{1}{\tau}(f-f^{(0)});\qquad f^{(0)}(\boldsymbol{\xi};\rho,\theta,\boldsymbol{u})=\frac{\rho}{(2\pi\theta)^{D/2}}\mathrm{e}^{-|\boldsymbol{\xi}-\boldsymbol{u}|^2/2\theta},\quad(1.1)$$

where $\boldsymbol{g}$ represents an acceleration field and τ a relaxation time towards the local equilibrium $f^{(0)}$. This local equilibrium will depend on the local density ρ, momentum $\rho\boldsymbol{u}$ and temperature θ.

We will show that, as far as the macroscopic evolution of the hydrodynamical fields is concerned, it is possible to renormalize the action of the force $\rho\boldsymbol{g}$ only in terms of a suitable *shift* of the local Maxwellian equilibrium distribution appearing in (1.1): $f^{(0)}(\boldsymbol{\xi};\rho,\theta,\boldsymbol{u})\to\bar{f}^{(0)}(\boldsymbol{\xi};\rho,\bar{\theta},\bar{\boldsymbol{u}})$. The new – shifted – Boltzmann formulation is

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\nabla f=-\frac{1}{\tau}(f-\bar{f}^{(0)});\qquad \bar{f}^{(0)}(\boldsymbol{\xi};\rho,\theta,\boldsymbol{u})=\frac{\rho}{(2\pi\bar{\theta})^{D/2}}\mathrm{e}^{-|\boldsymbol{\xi}-\bar{\boldsymbol{u}}|^2/2\bar{\theta}}.\quad(1.2)$$

The first result of the paper is to show that in order to recover the correct thermo-hydrodynamic behaviour, the shifted local velocity and temperature must take the following form:

$$\bar{\boldsymbol{u}}=\boldsymbol{u}+\tau\boldsymbol{g},\qquad \bar{\theta}=\theta-\tau^2 g^2/D.\quad(1.3)$$

The idea of shifting momentum has been pioneered for the case of a driving force due to internal, self-consistent interactions, which depend on the system configuration, typically the density field distribution. Such kind of extension has proven instrumental to the succesful formulation of lattice kinetic theory of isothermal non-ideal fluids (Shan & Chen 1993), in which one is concerned with the isothermal hydrodynamic evolution of density and momentum alone.

Here we extend it further to the important case of thermo-hydrodynamic fluctuations. Indeed, the use of shifted equilibria has many immediate and important methodological consequences: (i) it provides an elegant way to incorporate the force effects, thereby dispensing with the need of taking derivatives of the distribution function in velocity space; (ii) it allows a systematic derivation of lattice kinetic equations for non-ideal fluids with (pseudo) potential energy interactions (Martys *et al.* 1998; Guo, Zheng & Shi 2002; Shan *et al.* 2006); (iii) it highlights the need of including a suitable redefinition of the hydrodynamical fields on the lattice, in order to recover the correct continuum limit of the thermo-hydrodynamical equations for density, momentum and total kinetic energy $\mathscr{K}$. Here and throughout, by continuum thermo-hydrodynamic limit we refer to the following set of macroscopic equations (repeated indices are summed upon):

$$\left.\begin{aligned}&\partial_t\rho+\partial_i(\rho u_i)=0,\\&\partial_t(\rho u_k)+\partial_i(P_{ik})=\rho g_k,\\&\partial_t\mathscr{K}+\tfrac{1}{2}\partial_i q_i=\rho g_i u_i,\end{aligned}\right\}\quad(1.4)$$

where P_{ik} and q_i are momentum and energy fluxes (still unknown at this level of description). More precisely, we shall show that the above equations can be obtained *exactly* from the previous continuum Boltzmann equation with shifted equilibrium (1.2). This would not be the case for the energy evolution, if the momentum is the only shifted quantity in (1.2). Moreover, we will show that if the external forcing is of conservative type, i.e. can be written as the gradient of a function depending only

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on the local density, the total energy, kinetic plus internal, is conserved when the proper temperature shift is considered. The relevance of such a continuum kinetic theory is mainly motivated by the final goal of formulating lattice versions of the Boltzmann equations for non-ideal fluids, including thermo-hydrodynamic effects. In fact, in lattice formulations, the need of representing velocity degrees of freedom through a limited set of discrete speeds raises the problem of a correct and efficient implementation of the continuum velocity-streaming operator $\boldsymbol{g}\cdot\nabla_\xi f$. We shall show that shifted equilibria in the continuum representation have a well-defined lattice analogue, so that the lattice counterpart of the continuum description (1.2) can be obtained through the usual lattice Boltzmann discretization,

$$f_l(\boldsymbol{x}+\boldsymbol{c}_l\Delta t, t+\Delta t) - f_l(\boldsymbol{x}, t) = -\frac{\Delta t}{\tau}(f_l(\boldsymbol{x}, t) - f_l^{(0)}(\boldsymbol{x}, \rho^{(L)}, \bar{\boldsymbol{u}}^{(L)}, \bar{\theta}^{(L)})), \tag{1.5}$$

where the subscript l runs over the discrete set of velocity on the lattice $\boldsymbol{c}_l$, and the superscript L indicates that the macroscopic fields are now defined in terms of the lattice Boltzmann populations:

$$\rho^{(L)} = \sum_l f_l; \qquad \rho^{(L)}\boldsymbol{u}^{(L)} = \sum_l \boldsymbol{c}_l f_l; \qquad D\rho^{(L)}\theta^{(L)} = \sum_l |\boldsymbol{c}_l - \boldsymbol{u}^{(L)}|^2 f_l.$$

In the expression (1.5), the Boltzmann equilibrium (see Nie, Shan & Chen 2008 for its explicit expression) is computed with shifted momentum and temperature as follows:

$$\bar{\boldsymbol{u}}^{(L)} = \boldsymbol{u}^{(L)} + \tau\boldsymbol{g}, \qquad \bar{\theta}^{(L)} = \theta^{(L)} + \Delta\theta. \tag{1.6}$$

After some algebra, it can be shown that the temperature shift $\Delta\theta$ can be expressed in closed form as a function of the lattice time step Δt:

$$\Delta\theta = \frac{\tau(\Delta t - \tau)g^2}{D} + O(\Delta t)^2 + \cdots. \tag{1.7}$$

Moreover, in order to recover the thermo-hydrodynamical equations

$$\left.\begin{aligned} &\partial_t\rho^{(H)} + \partial_i\left(\rho u_i^{(H)}\right) = 0, \\ &\partial_t\left(\rho^{(H)}u_k^{(H)}\right) + \partial_i\left(P_{ik}^{(H)}\right) = \rho^{(H)}g_k, \\ &\partial_t\mathscr{K}^{(H)} + \tfrac{1}{2}\partial_i q_i^{(H)} = \rho^{(H)}g_i u_i^{(H)} \end{aligned}\right\} \tag{1.8}$$

the hydrodynamical fields can be computed in terms of a closed expansion to all orders in Δt and also in terms of a suitable lattice operator. For example, density is left unchanged, $\rho^{(H)} = \rho$, while the first non-trivial correction to momentum is given by the well-known pre- and post-collisional average (Buick & Greated 2000)

$$\boldsymbol{u}^{(H)} = \boldsymbol{u}^{(L)} + \frac{\Delta t}{2}\boldsymbol{g}$$

as well as by a new, non-trivial, correction to the temperature field

$$\theta^{(H)} = \theta^{(L)} + \frac{(\Delta t)^2 g^2}{4D}.$$

First, we notice that in the limit $\Delta t \to 0$, the lattice formulation for both shifted fields and hydrodynamical fields goes back to the continuum one, as it should. Second, the continuum formulation in terms of shifted fields indicates a straightforward link with the discrete variables via the Hermite–Gauss expansion (Shan *et al.* 2006). Third, and

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maybe more important for applications, we emphasize that in order to achieve a self-consistent thermo-hydrodynamical description in the lattice (1.8), both momentum – as it was known – and temperature, acquire discrete corrections.

2. Shifted continuum equilibrium

In this section we deal with the macroscopic properties of a continuum model (1.2). The main goal is to renormalize the effects of the forcing term $\boldsymbol{g}\cdot\nabla_\xi f$ in (1.1) via a suitable local equilibrium with shifted fields:

$$\bar{\boldsymbol{u}} = \boldsymbol{u} + \Delta\boldsymbol{u}(\boldsymbol{g},\tau); \qquad \bar{\theta} = \theta + \Delta\theta(\boldsymbol{g},\tau). \tag{2.1}$$

It is well known (Bathnagar *et al.* 1954; Wolf Gladrow 2000) that the usual definition of Boltzmann equation with explicit forcing given in (1.1) leads to the exact macroscopic equations (1.4) with the averaged fields given by

$$\rho = \int \mathrm{d}\xi f; \qquad \rho\boldsymbol{u} = \int \mathrm{d}\xi\boldsymbol{\xi} f; \qquad \mathscr{K} = \frac{1}{2}(\rho D\theta + \rho u^2) = \frac{1}{2}\int \mathrm{d}\xi\xi^2 f. \tag{2.2}$$

The momentum and energy fluxes

$$P_{ij} = \int \mathrm{d}\xi\xi_i\xi_j f, \qquad q_i = \int \mathrm{d}\xi\frac{\xi^2}{2}\xi_i f$$

on the left-hand side of the equations in (1.4) need to be closed, a task which is usually accomplished via the Chapman–Enskog expansion (see below). In order to derive (1.4) from (1.1) it is indeed sufficient to notice that the collision operator $-(1/\tau)(f - f^{(0)})$ preserves mass, momentum and total kinetic energy, as long as the local equilibrium is expressed in term of the macroscopic fields, ρ, $\boldsymbol{u}$, θ; i.e. whenever, besides the definition (2.2), the local equilibrium carries the same mass, momentum and energy of the actual distribution, namely

$$\rho = \int \mathrm{d}\xi f^{(0)}; \qquad \rho\boldsymbol{u} = \int \mathrm{d}\xi\boldsymbol{\xi} f^{(0)}; \qquad \mathscr{K} = \frac{1}{2}(\rho D\theta + \rho u^2) = \frac{1}{2}\int \mathrm{d}\xi\xi^2 f^{(0)}. \tag{2.3}$$

When considering the effect of the forcing field embedded within the shifted equilibrium (1.2), the only difference with the previous standard derivation comes from the fact that now the averaged macroscopic fields, when evaluated on the *shifted* equilibrium, *do not* coincide with the hydrodynamical fields defined in terms of the local particle distribution (2.2); i.e. the collision operator, $-(1/\tau)(f - \bar{f}^{(0)})$, preserves momentum and energy only globally and not locally. Still, it is easy to realize that the extra momentum and energy brought by the shifted equilibrium is given by

$$\rho\bar{\boldsymbol{u}} - \rho\boldsymbol{u} = \int \mathrm{d}\xi\boldsymbol{\xi}(\bar{f}^{(0)} - f), \qquad \frac{1}{2}(\rho D\bar{\theta} + \rho\bar{u}^2) - \frac{1}{2}(\rho D\theta + \rho u^2) = \frac{1}{2}\int \mathrm{d}\xi\xi^2(\bar{f}^{(0)} - f) \tag{2.4}$$

and that if we chose the shifted fields as given by expressions (1.3) the exact macroscopic equations (1.4), for density, momentum and kinetic energy evolution, are recovered. To this purpose, it is sufficient to evaluate the first three lowest momenta of (1.2) and use the relations (2.4) and (2.2). This is the first result of the present work.

Let us stress once again that the shift in the temperature only responds to the *need* of cancelling out extra terms on the right-hand side of the third equation in (1.4), which would otherwise result from the momentum shift alone. One may wonder if beside the formal correct unclosed equations (1.4) the two Boltzmann equation

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formulations (1.1) and (1.2) also share the same hydrodynamical behaviour, i.e. if the unclosed momentum and heat fluxes have the same closure. By performing the whole Chapman–Enskog expansion, it can be shown that this is indeed the case, at least up to the second order in the expansion parameter, where dissipative terms in momentum and heat appear. The result of these calculations are sketched in § 4, while all the technical details will be reported elsewhere.

3. Lattice implementation

In this section, we treat the lattice averaged equations and discuss the way that the corresponding shifts in the momentum and temperature fields are affected by the discretization of the algorithm. To this purpose, let us go back to the lattice Boltzmann equation with shifted momentum and temperature given by expression (1.5). First, we Taylor expand the left-hand side of (1.5) and obtain the lattice-series expression

$$D_{l,t} f_l + \frac{\Delta t}{2} D_{l,t}^2 f_l + \frac{(\Delta t)^2}{6} D_{l,t}^3 f_l + \cdots = -\frac{1}{\tau}\left(f_l - f_l^{(0)}\right)$$

with $D_{l,t} = \partial_t + \boldsymbol{c}_l \cdot \nabla$. We can then rewrite (1.5) in a compact form

$$(\mathrm{e}^{\Delta t D_{l,t}} - 1) f_l = \Delta t \mathscr{C}_l \tag{3.1}$$

with $\mathscr{C}_l = -(1/\tau)(f_l - f_l^{(0)})$ the collisional operator. A formal inversion of (3.1) yields

$$D_{l,t} f_l = \frac{\Delta t D_{l,t}}{(\mathrm{e}^{\Delta t D_{l,t}} - 1)} \mathscr{C}_l = \mathscr{C}_l + \left[\frac{\Delta t D_{l,t} \mathrm{e}^{-\Delta t D_{l,t}}}{(1 - e^{-\Delta t D_{l,t}})} - 1\right] \mathscr{C}_l,$$

where the left-hand side is recognized as the generating function of Bernoulli polynomials (Gradshtein & Ryzhik 2000). Let us also introduce the operator $\mathscr{L}_{l,\Delta t}$, defined by the Taylor expansion in $D_{l,t}\Delta t$:

$$\begin{aligned} D_{l,t}\mathscr{L}_{l,\Delta t} &= \left[\frac{\Delta t D_{l,t} \mathrm{e}^{-\Delta t D_{l,t}}}{(1 - \mathrm{e}^{-\Delta t D_{l,t}})} - 1\right] \\ &= -\frac{\Delta t D_{l,t}}{2}\left(1 - \frac{\Delta t D_{l,t}}{6} + \frac{(\Delta t D_{l,t})^3}{360} - \frac{(\Delta t D_{l,t})^5}{15120} + O((\Delta t D_{l,t})^7)\right). \end{aligned}$$

The relevant point is that the above operator can be rewritten in terms of *a lattice operator* performing an inverse shift in space and time: $S_{l,\Delta t} = (\mathrm{e}^{-\Delta t D_{l,t}} - 1)$. It is easy to realize that its action on any field, say ϕ, defined on the lattice gives back

$$S_{l,\Delta t}\phi(\boldsymbol{x}, t) = \phi(\boldsymbol{x} - \Delta t \boldsymbol{c}_l, t - \Delta t).$$

The action of the operator $\mathscr{L}_{l,\Delta t}$ can be recast as follows:

$$\mathscr{L}_{l,\Delta t} = -\frac{\Delta t}{2}\left(1 + \frac{1}{6} S_{l,\Delta t} - \frac{1}{12} S_{l,\Delta t}^2 + \frac{19}{360} S_{l,\Delta t}^3 - \frac{3}{80} S_{l,\Delta t}^4 + O\left(S_{l,\Delta t}^5\right)\right).$$

This shows that it is possible to rewrite the final dynamics, exactly to all orders in Δt, by retaining *only* shift operators on the lattice:

$$D_{l,t}\left(f_l + \frac{1}{\tau}\mathscr{L}_{l,\Delta t}\left(f_l - f_l^{(0)}\right)\right) = -\frac{1}{\tau}\left(f_l - f_l^{(0)}\right). \tag{3.2}$$

We can then average this equation in velocity space and look at the equations for the first three-order momenta, so as to recover the hydrodynamic evolution for density,

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momentum and total energy (1.8). Simple calculations show that the left-hand side set of macroscopic equations (1.8) is obtained by means of the following definitions of macroscopic hydrodynamic (H) fields (scalars, vectors and second-order tensors):

$$\rho u_i^{(H)} = \sum_l c_l^i f_l + \frac{1}{\tau}\left(\sum_l c_l^i \mathscr{L}_{l,\Delta t}\left[f_l - f_l^{(0)}\right]\right),$$

$$P_{ij}^{(H)} = \sum_l c_l^i c_l^j f_l + \frac{1}{\tau}\left(\sum_l c_l^i c_l^j \mathscr{L}_{l,\Delta t}\left[f_l - f_l^{(0)}\right]\right),$$

$$\mathscr{K}^{(H)} = \left(\frac{D}{2}\rho\theta^{(H)} + \frac{1}{2}\rho(u^{(H)})^2\right) = \frac{1}{2}\sum_l c_l^2 f_l + \frac{1}{\tau}\left(\frac{1}{2}\sum_l c_l^2 \mathscr{L}_{l,\Delta t}\left[f_l - f_l^{(0)}\right]\right),$$

$$q_i^{(H)} = \frac{1}{2}\sum_l c_l^2 c_l^i f_l + \frac{1}{\tau}\left(\frac{1}{2}\sum_l c_l^2 c_l^i \mathscr{L}_{l,\Delta t}\left[f_l - f_l^{(0)}\right]\right).$$

In order to capture the correct right-hand side of (1.8) as well, we must choose the fields entering the shifted equilibrium, $f^{(0)}$, in (1.5), $\bar{\boldsymbol{u}}^{(L)} = \boldsymbol{u}^{(L)} + \Delta\boldsymbol{u}$, $\bar{\theta}^{(L)} = \theta^{(L)} + \Delta\theta$, in the following form:

$$\Delta\boldsymbol{u} = \tau\boldsymbol{g},$$

$$\Delta\theta = \frac{2\tau}{\rho D}\left(\rho g_i\left(u_i^{(H)} - u_i^{(L)}\right) - \frac{\tau\rho g^2}{2}\right).$$

Let us notice that the above expression for the temperature shift is implicit; i.e. it is given in terms of the hydrodynamical velocity $u_i^{(H)}$ which depends itself on the equilibrium. One may get a closed expression only via a Taylor expansion in Δt. For example, to first order in the expansion of $\mathscr{L}_{l,\Delta t}$, we have simply $\mathscr{L}_{l,\Delta t} = -\Delta t/2$, corresponding to the following temperature shift:

$$\bar{\theta}^{(L)} = \theta^{(L)} + \frac{\tau(\Delta t - \tau)g^2}{D}.$$

Consequently, the hydrodynamical velocity and temperature become

$$\boldsymbol{u}^{(H)} = \boldsymbol{u}^{(L)} + \frac{\Delta t}{2}\boldsymbol{g},$$

$$\theta^{(H)} = \theta^{(L)} + \frac{(\Delta t)^2 g^2}{4D},$$

where the hydrodynamic velocity is nothing but the pre- and post-collisional average, while the non-trivial correction in Δt to the temperature fields is a new result, as anticipated in the introduction. These kinds of discrete corrections have been known for the transport coefficients and the amplitude of fluctuations. The correction to the velocity was first described in Ginzbourg & Adler (1994) and noted empirically in Ladd (1994) at about the same time. The new result is that in thermal lattice Boltzmann models, a similar correction applies to the temperature as well.

Let us anticipate here that the usual Chapman–Enskog analysis of the model (3.2), limited to the second order in the perturbative expansion, leads to the expected expression for the viscous stress and for the heat flux, which are respectively given by $\eta(\partial_i u_j^{(H)} + \partial_j u_i^{(H)}) - (\eta/c_v)(\partial_k u_k^{(H)})\delta_{ij}$ and $k\partial_i\theta^{(H)}$, with viscosity and thermal conductivity, $\eta = \theta^{(H)}\rho(\tau - \Delta t/2)$, $k = c_p\theta^{(H)}\rho\,(\tau - \Delta t/2)$. In the previous expression we have also used the ideal gas values for specific heats, $c_v = D/2$ and $c_p = D/2 + 1$. Details of the whole calculation will be reported elsewhere.

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4. Numerical tests

We now proceed to the implementation of a test case of the above procedure, where the need for the temperature shift appears in full. The most important instance in which total energy conservation is crucial is the case of a gas (fluid) departing from ideal conditions, as a result of an internal, self-consistent, potential. In this case, the thermo-hydrodynamical equations must conserve the total energy, given by the sum of the total kinetic energy plus the potential energy. Typical relaxation experiments will then show a non-trivial exchange between the kinetic and potential energy components, until a dynamical or static equilibrium is finally attained.

We specialize the discussion to a simple, and yet non-trivial, case in which the interparticle force is purely repulsive:

$$\boldsymbol{F} = \rho \boldsymbol{g}(\boldsymbol{x}, t) = \mathscr{G}\rho(\boldsymbol{x}, t) \sum_l w_l \rho(\boldsymbol{x} + \boldsymbol{c}_l \Delta t, t) \boldsymbol{c}_l \approx -\nabla P_b^{(int)}, \quad P_b^{(int)}(\rho) = -\frac{1}{2}\mathscr{G}\rho^2 \tag{4.1}$$

with w_l a suitable set of weights which enforce the right symmetries on the lattice (Shan & Chen 1993). Repulsion is imposed by choosing a negative coupling constant $\mathscr{G} \leqslant 0$. This case allows full control of the non-ideal part of the equation of state. Indeed, the bulk pressure provides the usual ideal-gas contribution $P_b^{(id)} = \rho\theta$ plus the non-ideal one, given by the Taylor expansion of the forcing term in (4.1), $P_b^{(tot)} = P_b^{(id)} + P_b^{(int)}$. The system also has internal potential energy $E_V = -(1/2)\mathscr{G}\rho^2$, where we have neglected possible contributions coming from strong density gradients. The transport equation for this intermolecular potential energy (Snider 1995; He & Doolen 2001) reads

$$\partial_t E_V + \partial_k \left(u_k^{(H)} E_V\right) = -\left(\partial_j u_j^{(H)}\right) P_b^{(int)}, \tag{4.2}$$

as can be readily derived from the density evolution in (1.4). By summing to the total kinetic energy evolution, we obtain the total energy balance

$$\partial_t (E_V + \mathscr{K}^{(H)}) = -\partial_j \left(u_j^{(H)} P_b^{(int)}\right) - \frac{1}{2}\partial_i q_i^{(H)} - \partial_k \left(u_k^{(H)} E_V\right), \tag{4.3}$$

whose divergence-like structure on the right-hand side ensures total energy conservation.

Let us stress that the reconstruction of a total divergence is only possible thanks to the superposition of the contribution $(\partial_j u_j^{(H)}) P_b^{(int)}$, stemming from the evolution of the potential energy, plus the contribution $u_j^{(H)}(\partial_j P_b^{(int)})$, coming from the right-hand side of the total kinetic energy in (1.8). Here, we fully appreciate the importance of the temperature shift, in order to recover the correct total energy dynamics. Using fully periodic boundary conditions, the shifted lattice Boltzmann formulation is therefore expected to provide conservation of the total energy from the hydrodynamical point of view.

To ensure a sufficiently accurate recovery of the thermal transport phenomenon, we employ a two-dimensional 37-speed lattice Boltzmann model, corresponding to a ninth-order accurate Gauss–Hermite quadrature. In conjunction, a fourth-order Hermite expansion of the Maxwellian is used as an equilibrium distribution (Shan *et al.* 2006; Nie *et al.* 2008). A simulation is performed on a $L_x \times L_y = 10 \times 100$ grid, with a small perturbation of a single sinusoidal wave in the temperature field $\theta^{(H)}(x, y, t = 0) = 1.0 + \epsilon \sin(2\pi y/L_y)$ $(\epsilon = 0.01)$. The initial density field is constant. The difference of the total energy $\int((E_V + \mathscr{K}^{(H)}))(t)\mathrm{d}x\mathrm{d}y$ with respect to its initial

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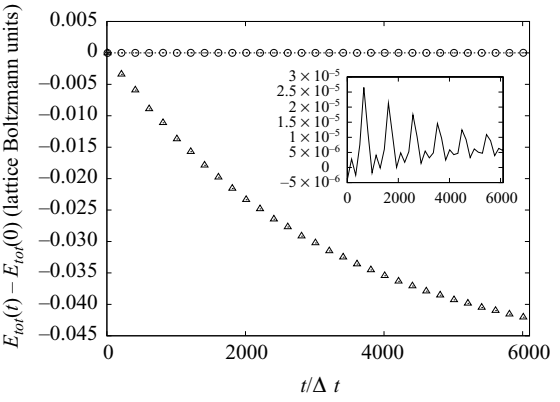


FIGURE 1. Variations of total energy for a non-ideal system with an initial sinusoidal wave in the temperature field $\theta^{(H)}(x, y, t=0) = 1.0 + \epsilon \sin(2\pi y/L_y)$ with $\epsilon = 0.01$ and smooth hydrodynamical velocity fields. The lattice Boltzmann parameters in (4.1) and (1.5) are such that $\tau/\Delta t = 0.6$, $\mathscr{G} = -3.0$. Two simulations are carried out. The first simulation is only with shifted momentum (△). The second one is with shifted momentum and temperature (○), enlarged in the inset.

value is monitored in figure 1. This figure clearly shows that the lattice Boltzmann formulation without shifted temperature is not able to sustain satisfactory energy conservation. On the other hand, upon shifting the temperature field, the correct energy balance is recovered. The energy conservation is still not exact within machine precision (see inset of figure 1), due to the fact that our expression for the total energy is given in terms of a continuum description of the non-ideal forcing term (4.1). In order to further improve the accuracy of energy conservation, a discrete version of the internal potential energy, E_V, thermodynamically consistent on the lattice needs to be developed.

In figure 2 we show another test: the density and temperature profile of our model for the case of an ideal gas between two parallel walls under the action of a constant gravity force. The numerical results, with and without thermal shift in the equilibrium, are compared with the exact analytical hydrodynamical solution $\rho(y) = \rho_0 \mathrm{e}^{-gy}$ ($T = 1$ and $\rho_0 = \text{const.}$). Figure 2 shows that only the case in which the equilibriums is shifted recovers the correct hydrodynamical manifold.

5. Conclusions and perspectives

Before concluding, let us discuss further the physical meaning of the shifted Boltzmann equation (1.2). It is easy to realize that it can also be rewritten as

$$\frac{\partial f(\boldsymbol{x}, \boldsymbol{\xi}, t)}{\partial t} + \boldsymbol{\xi} \cdot \nabla f(\boldsymbol{x}, \boldsymbol{\xi}, t) = -\frac{1}{\tau}\left(f(\boldsymbol{x}, \boldsymbol{\xi}, t) - \mathrm{e}^{-\tau \boldsymbol{g}\cdot\nabla_\xi - \tau^2 \frac{g^2}{2D}\nabla_\xi\cdot\nabla_\xi} f^{(0)}(\boldsymbol{\xi}; \rho, \theta, \boldsymbol{u})\right).$$

Upon Taylor expanding the terms on the right-hand side corresponding to the shift in the momentum, $-\mathrm{e}^{-\tau \boldsymbol{g}\cdot\nabla_\xi} f^{(0)}$, up to the second order in τ, we obtain

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\nabla f = -\frac{1}{\tau}\left(f - f^{(0)}\right) - \boldsymbol{g}\cdot\nabla_\xi f^{(0)} + \frac{\tau}{2}\boldsymbol{g}\boldsymbol{g} : \nabla_\xi\nabla_\xi f^{(0)}. \tag{5.1}$$

It is simple to check that, as for the isothermal dynamics of density and momentum, the shifted equilibrium Boltzmann equation (1.2) is equivalent to (5.1). A stabilizing diffusion term in velocity space stands therefore out.

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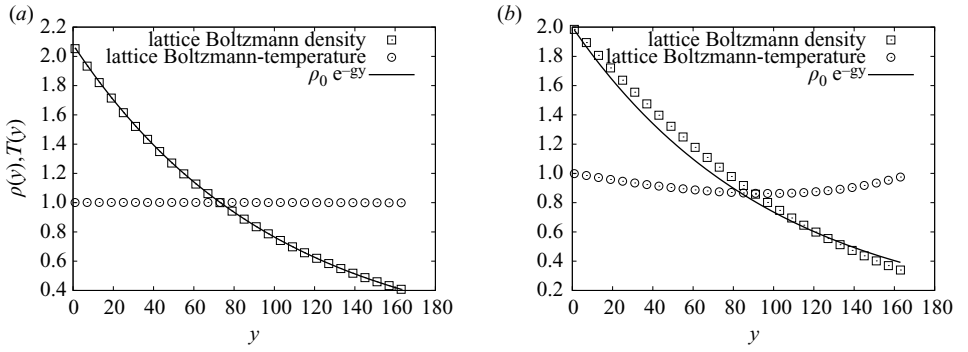


FIGURE 2. The static hydrodynamic behaviour of an ideal gas between two parallel walls at the same temperature ($T=1$) and under the action of a constant gravity force g. The hydrodynamic equations predict a constant temperature with an exponentially decreasing density. Two formulations have been compared: (a) with shifted momentum and temperature and (b) with shifted momentum only. The hydrodynamic limit is correctly approached only in the first case. The whole density is conserved and equal in both simulations. Simulations are performed on an $L_x \times L_y = 10 \times 165$ grid points. Diffuse boundary conditions for the lattice Boltzmann populations are introduced at the walls (Ansumali & Karlin 2002), and gravity is acting along the negative y-direction.

It is also noted that, as a first order of approximation, this kind of diffusion term can be thought as deriving from standard BGK dynamics, with the equilibrium distribution $f^{(0)}(\boldsymbol{x}, \boldsymbol{\xi}, t)$ replaced by a smoothed version, resulting from coarse-graining in velocity space, filtering fluctuations up to $\delta \boldsymbol{v}' < \boldsymbol{g}\tau$. Considering the Taylor expansion of the temperature shift operator, $-\mathrm{e}^{-\tau^2(g^2/2D)\nabla_\xi \cdot \nabla_\xi} f^{(0)}$, we obtain, up to τ^2, an extra term proportional to

$$g^2 \Delta_\xi f^{(0)}. \tag{5.2}$$

Such contribution can be interpreted as deriving from a stochastic component in the acceleration field. To illustrate the point, let us start again from the continuum BGK equation (1.1), and let us consider the streaming term in velocity space $(\mathrm{d}\boldsymbol{\xi}/\mathrm{d}t) \cdot \nabla_\xi f$ in which the molecular velocity ξ_i obeys the following Langevin equation:

$$\frac{\mathrm{d}\xi_i}{\mathrm{d}t} = \eta_i,$$

where η_i is a standard delta-correlated Gaussian noise with zero average and the normalization $\langle \eta_i \rangle = 0$, $\langle \eta_i \eta_j \rangle = (1/2)\sigma \delta_{ij}$. We expect the stochastic term to provide a mechanism for producing thermal fluctuations in the fluid. The key ingredient is a correct evaluation of the term $\langle (\mathrm{d}\xi_i/\mathrm{d}t) \nabla_{\xi_i} f \rangle$, where ξ_i is now a stochastic variable and $\langle \ldots \rangle$ stands for an average over possible realizations of the stochastic term. We can apply Novikov's (1964) theorem and approximate $\xi_i \approx (\mathrm{d}\xi_i/\mathrm{d}t)\tau = \eta_i \tau$. This yields

$$\left\langle \frac{\mathrm{d}\xi_i}{\mathrm{d}t} \nabla_{\xi_i} f \right\rangle = \left\langle \frac{\mathrm{d}\xi_i}{\mathrm{d}t} \xi_j \right\rangle \langle \nabla_{\xi_i} \nabla_{\xi_j} f \rangle \approx \tau \langle \eta_i \eta_j \rangle \langle \nabla_{\xi_i} \nabla_{\xi_j} f \rangle$$

which is of the same form of (5.2) for a suitable choice of σ. Let us emphasize that the shifted equilibrium formulation (1.2) is equivalent to the standard BGK formulation (1.1), as far as the macroscopic equations (1.4) and their Chapman–Enskog expansion up to second order are concerned. The diffusive extra terms stemming from the Taylor expansion indicate that although maintaining the same hydrodynamics, the shifted

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equilibrium formulation should nonetheless feature better stability with concern to the global evolution of the probability density, $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$.

Summarizing, we have investigated lattice kinetic equations, incorporating the effects of external/self-consistent force fields via a shift of the local fields in the local equilibria. The mathematical treatment reveals that besides momentum, temperature also receives a self-consistent shift from the force field. The contribution of the temperature shift can also be traced back to a *stochastic* component in the acceleration field, thus pointing to potentially new directions for the formulation of lattice Boltzmann models for non-ideal fluids with thermo-hydrodynamic transport effects (Rowlinson & Widom 1982; Brennen 2005). Work along these lines is in progress, which will hopefully permit to attack a broad class of complex flow problems with thermal effects, such as thermally driven phase transitions, crystal growth, melting and many other non-equilibrium thermo-hydrodynamic transport problems.

Finally, it has been shown that in order to recover the correct thermo-hydrodynamical equations (Boghosian 2008) on the lattice, the macroscopic temperature must acquire new terms, directly related to the lattice spacing. These terms naturally vanish in the continuum limit, thus preserving the consistency of the discrete theory. Many items remain open to future investigation. For instance, it would be interesting to extend the present treatment to more general collision operators, including multi-time relaxation models, which would permit to model fluids at non-unitary Prandtl numbers (Ahlers, Grossmann & Lohse 2009). The establishment of an H-theorem for continuum and discrete kinetic equations with self-consistently shifted equilibria also appears an interesting topic for future research (Succi, Karlin & Chen 2002)

REFERENCES

Ahlers, G., Grossmann, S. & Lohse, D. 2009 Heat transfer and large-scale dynamics in turbulent Rayleigh–Bénard convection. *Rev. Mod. Phys.* **81**, 503–537.

Ansumali, S & Karlin, I. 2002 Kinetic boundary conditions in the lattice Boltzmann method. *Phys. Rev.* E **66**, 026311.

Bathnagar, P.-L., Gross, E. & Krook, M. 1954 A model for collision processes in gases. *Phys. Rev.* **94**, 511–525.

Benzi, R., Succi, S. & Vergassola, M. 1992 The lattice Boltzmann equation: theory and applications. *Phys. Rep.* **222**, 145–197.

Boghosian, B. M. 2008 Exact hydrodynamics of the lattice BGK equation. arXiv:0810.2344v1.

Brennen, C. 2005 *Fundamentals of Multiphase Flow*. Cambridge University Press.

Buick, J. M. & Greated, C. A. 2000 Gravity in a lattice Boltzmann model. *Phys. Rev.* E **61**, 5307–5320

Chen, S. & Doolen, G. 1998 Lattice Boltzmann method for fluid flows. *Annu. Rev. Fluid Mech.* **30**, 329–364.

Ginzbourg, I & Adler, P. M. 1994 Boundary flow condition analysis for the 3-dimensional lattice Boltzmann model. *J. Phys.* II **2**, 191–214.

Gonnella, G., Lamura, A. & Sofonea, V. 2007 Lattice Boltzmann simulation of thermal nonideal fluids. *Phys. Rev.* E **76**, 036703.

Gradshtein, I. S. & Ryzhik, I. M. 2000 *Tables of Integrals and Series*, 6th edn. Academic.

Guo, Z., Zheng, C. & Shi, B. 2002 Discrete lattice effects on the forcing term in the lattice Boltzmann method, *Phys. Rev.* E **65**, 046308.

He, X. & Doolen, G. 2001 Thermodynamic foundations of kinetic theory and lattice Boltzmann models for multiphase Flows. *J. Stat. Phys.* **107**, 309–328.

He, X. & Luo, L. S. 1997 Theory of the lattice Boltzmann method: from the Boltzmann equation to the lattice Boltzmann equation. *Phys. Rev.* E **56** 6811–6817.

Ladd 1994 Numerical simulations of particulate suspensions via a discretized Boltzmann equation. Part 2. Numerical results. *J. Fluid Mech.* **271** 311–339.

https://doi.org/10.1017/S002211200900665X Published online by Cambridge University Press

Li, Q. & Wagner, A. J. 2007 Symmetric free-energy-based multicomponent lattice Boltzmann method. *Phys. Rev.* E **76**, 036701.

Martys, N. S., Shan, X. & Chen, H. 1998 Evaluation of the external force term in the discrete Boltzmann equation. *Phys. Rev.* E **58**, 6865.

Nie, X., Shan, X. & Chen, H. 2008 Thermal lattice Boltzmann model for gases with internal degrees of freedom. *Phys. Rev.* E **77**, 035701(R).

Novikov, E. A. 1964 Functionals and the method of random forces in turbulence theory. *Zh. Exp. Teor. Fiz.* **47**, 1919–1926.

Qi, D. W. 2006 Direct simulations of flexible cylindrical fibres suspensions in finite Reynolds numbers flows. *J. Chem. Phys.* **125**, 114901.

Rowlinson, J. R. & Widom, B. 1982 *Molecular Theory of Capillarity*. Clarendon.

Shan, X. & Chen, H. 1993 Lattice Boltzmann model for simulating flows with multiple phases and components. *Phys. Rev.* E **47**, 1815.

Shan, X. & He, X. 1998 Discretization of the velocity space in the solution of the Boltzmann equation. *Phys. Rev. Lett.* **80**, 65–68.

Shan, X., Yuan, F. & Chen, H. 2006 Kinetic theory representation of hydrodynamics: a way beyond the Navier–Stokes equation. *J. Fluid Mech.* **550**, 413–441.

Snider, R. F. 1995 Conversion between kinetic energy and potential energy in the classical non-local Boltzmann equation. *J. Stat. Phys.* **80**, 1085–1117.

Swift, M. R., Osborn, W. R. & Yeomans, J. M. 1995 Lattice Boltzmann simulation of nonideal fluids. *Phys. Rev. Lett.* **75**, 830–833.

Wolf-Gladrow, D. 2000 *Lattice-Gas Cellular Automata and Lattice Boltzmann Models*. Springer.

Succi, S., Karlin, I. & Chen, H. 2002 *Colloquium*: role of the *H* theorem in lattice Boltzmann hydrodynamic simulations. *Rev. Mod. Phys.* **74**, 1203.

https://doi.org/10.1017/S002211200900665X Published online by Cambridge University Press