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Note:
Alternative Discretization Schemes in Lattice Boltzmann Methods

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Recently several authors investigate the ability of the Lattice Boltzmann method to simulate various complex flow problems governed by the incompressible Navier–Stokes equation, where the range of applications varies, e.g, from multiphase flows (see for example [3]) to the simulation of granular materials [4]. Some references about the Lattice Boltzmann method deal with some more theoretical investigations, like the strict derivation of the incompressible Navier–Stokes equations based on a formal multiscale expansion, see [2], or the stability properties of the scheme based on a von Neumann linear stability analysis, see [5].

The aim of the present note is to investigate more general discretization schemes for the Lattice Boltzmann method; a topic, which is only shortly discussed in the literature, see, e.g., [1], where the authors remark at the end on the possibility to use an implicit discretization scheme. In particular, we show, how the viscosity of the resulting incompressible Navier–Stokes equations is related with the parameters of a general linear explicit–implicit discretization scheme and how to reformulate the scheme in terms of the standard Lattice Boltzmann method.

The basis of the method is a set of discrete velocities denoted by $\mathbf{v}_i$, $i = 1, \ldots, m$, which defines the admissible velocities of microscopic fluid particles moving along a fixed spatial grid. Moreover, the microscopic density functions $f^i(t, \mathbf{x}_j)$ indicate, how many particles with discrete velocity $\mathbf{v}_i$ are located at time t at the spatial position $\mathbf{x}_j$, $j = 1, \ldots, l$ and one defines macroscopic state variables by weighted sums over the microscopic densities $f^i(t, \mathbf{x}_j)$, i.e.

$$(1) \qquad \rho(t, \mathbf{x}_j) = \sum_{i=1}^{m} f^i(t, \mathbf{x}_j), \quad (\rho\mathbf{u})(t, \mathbf{x}_j) = \sum_{i=1}^{m} \mathbf{v}_i f^i(t, \mathbf{x}_j), \quad \text{etc.}$$

The Lattice Boltzmann method draws its main attraction from the simple dynamic behaviour in terms of the microscopic density functions $f^i(t, \mathbf{x}_j)$, which is given by

$$(2) \qquad f^i(t + \delta_t, \mathbf{x} + \delta_t \mathbf{v}_i) - f^i(t, \mathbf{x}_j) = \frac{1}{\tau}(f^{i,eq}(t, \mathbf{x}_j) - f^i(t, \mathbf{x}_j)),$$

where δ_t denotes the time step in the Lattice Boltzmann approach and τ a dimensionless relaxation parameter related with the viscosity of the incompressible Navier–Stokes equations. The equilibrium functions $f^{i,eq}(t, \mathbf{x}_j)$ are obtained from a Taylor expansion of a local Maxwellian distribution around the zero velocity $\mathbf{u} = 0$, where the special form of the equilibrium functions depends on the underlying discrete velocity model and they are chosen in particular to recover the macroscopic state variables when substituting in (1) the density functions f^i by $f^{i,eq}$.

Example 1 *A commonly used discrete velocity model is the 9–velocity model on the two–dimensional square lattice, such that* $\mathbf{v}_1 = (0,0)$, $\mathbf{v}_i = c(\cos(i-2)\pi/2, \sin(i-2)\pi/2)$, $i = 2, \ldots, 5$ *and* $\mathbf{v}_i = c\sqrt{2}(\cos[(i-6)\pi/2 + \pi/4], \sin[(i-6)\pi/2 + \pi/4])$, $i = 6, \ldots, 9$, *where the equilibrium functions* $f^{i,eq}$ *are given by*

$$f^{i,eq} = w_i \rho \left[1 + \left(3 \frac{\mathbf{v}_i \cdot \mathbf{u}}{c^2} + \frac{9}{2} \frac{(\mathbf{v}_i \cdot \mathbf{u})^2}{c^4} - \frac{3}{2} \frac{\mathbf{u} \cdot \mathbf{u}}{c^2} \right) \right]$$

and $w_1 = 4/9$, $w_{2,\ldots,5} = 1/9$ *and* $w_{6,\ldots,9} = 1/36$. *The parameter* c *in the definition of the discrete velocity model given above is related first with the grid size* δ_x *and the time step* δ_t *by* $c = \delta_x/\delta_t$, *but even defines the sound speed* c_s *of the fluid flow by* $c_s = c/\sqrt{3}$.

In order to construct alternative discretization schemes for the Lattice Boltzmann method it is useful to investigate a continuous model, i.e. continuous in space and time, which is related to the standard method given by (2).
An appropriate model, which can be related to the scheme, is a discrete velocity model for the Boltzmann equation written in the form

$$\text{(3)} \qquad \partial_t f^i + \frac{1}{\varepsilon} \mathbf{n}_i \nabla f^i = \frac{1}{\varepsilon^2} \frac{f^{i,eq} - f^i}{\tau_1}, \qquad f^i = f^i(t, \mathbf{x})$$

where $f^i = f^i(t, \mathbf{x})$ and $\mathbf{n}_i$ denote the scaled velocities $\mathbf{n}_i = \mathbf{v}_i/c$, $i = 1, \ldots, m$. Here, we already applied the diffusion scaling $x \to \varepsilon x$ and $t \to \varepsilon^2 t$ in order to recover in the limit $\varepsilon \to 0$ the incompressible Navier–Stokes equations. The equilibrium functions $f^{i,eq}$ in (3) are assumed to have the same structure as in the ususal Lattice Boltzmann method.
Using the method of characteristics, Eq. (3) may be written in integral form as

$$\begin{aligned} f^i(t + \delta_t, \mathbf{x} + \frac{\delta_t}{\varepsilon} \mathbf{n}_i) &= \exp\Big(- \frac{\delta_t}{\tau_1 \varepsilon^2} \Big) f^i(t, \mathbf{x}) \\ &\quad + \frac{1}{\tau_1 \varepsilon^2} \int_t^{t+\delta_t} \exp\Big(\frac{s - t - \delta_t}{\tau_1 \varepsilon^2} \Big) f^{i,eq}(s, \mathbf{x} + \frac{s}{\varepsilon} \mathbf{n}_i) \, \mathrm{d}s \end{aligned}$$

If $\delta_t \ll 1$, one may use the approximation

$$\text{(4)} \qquad f^{i,eq}(t + \delta, \mathbf{x} + \frac{\delta}{\varepsilon} \mathbf{n}_i) \approx f^{i,eq}(t, \mathbf{x})$$

for $\delta \in [0, \delta_t]$, such that

$$\text{(5)} \qquad f^i(t + \delta_t, \mathbf{x} + \frac{\delta_t}{\varepsilon} \mathbf{n}_i) = \exp\Big(- \frac{\delta_t}{\tau_1 \varepsilon^2} \Big) f^i(t, \mathbf{x}) + \Big(1 - \exp\Big(- \frac{\delta_t}{\tau_1 \varepsilon^2} \Big) \Big) f^{i,eq}(t, \mathbf{x}),$$

which is already quite close to the standard scheme (2).
Hence, if we introduce the discretization $\delta_x/\delta_t = 1/\varepsilon = c$ and $\delta_t = k\varepsilon^2 = k\left(\frac{\delta_x}{\delta_t}\right)^2$, such that $\delta_x = k\varepsilon$, Eq. (5) reads

$$\begin{aligned} f^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) &= \exp\Big(-\frac{1}{\tau_2}\Big) f^i(t, \mathbf{x}_j) \\ &+ \frac{1}{\delta_t \tau_2} \int_t^{t+\delta_t} \exp\Big(\frac{s-t-\delta_t}{\tau_2 \delta_t}\Big) f^{i,eq}(s, \mathbf{x} + s\mathbf{v}_i)\, \mathrm{d}s \end{aligned}$$

with $\tau_2 = \tau_1/k$.
With the same approximation in the integral as given above, we have

$$f^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) = \exp\Big(-\frac{1}{\tau_2}\Big) f^i(t, \mathbf{x}_j) + \Big(1 - \exp\Big(-\frac{1}{\tau_2}\Big)\Big) f^{i,eq}(t, \mathbf{x}_j) \tag{6}$$

Finally, substituting $\exp(-1/\tau_2) = \frac{\tau-1}{\tau}$, Eq. (6) can be written as

$$f^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) - f^i(t, \mathbf{x}_j) = \frac{1}{\tau}\Big(f^{i,eq}(t, \mathbf{x}_j) - f^i(t, \mathbf{x}_j)\Big), \tag{7}$$

which exactly coincides with the standard Lattice Boltzmann method given by (2).
Thus, we derived the standard Lattice Boltzmann method by discretizing the discrete velocity model for the Boltzmann equation formulated in (3) applying the approximation (4) in the integral representation of (3).
Here, one has to be a bit more precies, because this only holds as long as the parameter τ in (7) fulfills the restriction $\tau \geq 1$, because $\exp(-1/\tau_2) \geq 0$ for $\tau_2 \in [0, \infty)$ and passing from (6) to (7) without any further approximation exactly yields the restriction $\tau \geq 1$.
As a consequence, the minimal viscosity for the scheme defined by (7) is reached in the limit $\tau \to 1$, where

$$\nu = \frac{1}{6}\frac{\delta_x^2}{\delta_t} = \frac{1}{6}k$$

In particular, with $k = 1$, i.e. $\delta_x^2 = \delta_t$, the viscosity is bounded from below by $1/6$, which would restrict the Lattice Boltzmann method to the simulation of flows at moderate Reynolds numbers.
To cover higher Reynolds number, one may choose the parameter k as $\min\{6\nu, 1\}$; but, because the ratio δ_x/δ_t should remain large enough to neglect the higher order terms to solve the incompressible Navier–Stokes equations and $\delta_x/\delta_t = k/\delta_x$, one has to choose sufficiently small grids, which leads to an enormous computational effort at high Reynolds numbers.
It is well-known, that in practice one uses a different approach, namely to extend the range of the relaxation parameter τ to values less than 1, in order to cover the whole range of possible viscosities. This method may be seen as a so–called over–relaxation, but it is even obvious that the value $\tau = 1/2$ yields a stability bound of the method for uniform flows, due to the vanishing viscosity, see, e.g., [5].
The derivation of the Lattice Boltzmann method from discrete velocity models suggests to investigate more general discretizations written in the form

$$f^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) = c_1 f^i(t, \mathbf{x}_j) + c_2 f^{i,eq}(t, \mathbf{x}_j) + c_3 f^{i,eq}(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i), \tag{8}$$

with $\sum c_i = 1$.

Example 2

a) the standard scheme is recovered using $c_1 = 1 - 1/\tau$, $c_2 = 1/\tau$ and $c_3 = 0$,

b) if we use the approximation

$$f^{i,eq}(t+\delta, \mathbf{x} + \frac{\delta}{\varepsilon}\mathbf{n}_i) \approx f^{i,eq}(t+\delta_t, \mathbf{x} + \frac{\delta_t}{\varepsilon}\mathbf{n}_i)$$

for the integral term, we obtain the implicit scheme

$$f^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) = \Big(1 - \frac{1}{\tau}\Big) f^i(t, \mathbf{x}_j) + \frac{1}{\tau} f^{i,eq}(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i),$$

such that $c_1 = 1 - 1/\tau$, $c_2 = 0$ and $c_3 = 1/\tau$,

c) a higher order approximation is given by the trapezoidal rule

$$f^{i,eq}(t+\delta, \mathbf{x} + \frac{\delta}{\varepsilon}\mathbf{n}_i) \approx \frac{1}{2}\Big(f^{i,eq}(t, \mathbf{x}) + f^{i,eq}(t+\delta_t, \mathbf{x} + \frac{\delta_t}{\varepsilon}\mathbf{n}_i)\Big)$$

which yields an explicit–implicit scheme with $c_1 = 1 - 1/\tau$ and $c_2 = c_3 = 1/(2\tau)$.

The first observation concerning the generalized scheme (8) is that the viscosity of the resulting fluid model is independent of the two parameters c_2 and c_3

Theorem 3 *The viscosity ν of the scheme (8) is given by*

$$\nu = \frac{1}{6}\frac{1+c_1}{1-c_1}\frac{\delta_x^2}{\delta_t} \tag{9}$$

Proof To derive the expression given above we act on the same way as in the usual Lattice Boltzmann method, see, e.g., [2]. First, one applies the Taylor expansions

$$\begin{aligned} f^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) &= f^i(t, \mathbf{x}_j) + \delta_t\Big(\partial_t + \mathbf{v}_i\nabla\Big) f^i(t, \mathbf{x}_j) \\ &\quad + \frac{\delta_t^2}{2}\Big(\partial_t + \mathbf{v}_i\nabla\Big)^2 f^i(t, \mathbf{x}_j) + O(\delta_t^3) \end{aligned} \tag{10}$$

$$\begin{aligned} f^{i,eq}(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) &= f^{i,eq}(t, \mathbf{x}_j) + \delta_t\Big(\partial_t + \mathbf{v}_i\nabla\Big) f^{i,eq}(t, \mathbf{x}_j) \\ &\quad + \frac{\delta_t^2}{2}\Big(\partial_t + \mathbf{v}_i\nabla\Big)^2 f^{i,eq}(t, \mathbf{x}_j) + O(\delta_t^3) \end{aligned} \tag{11}$$

Then we use a multiple scale expansion for the single distribution function $f^i(t, \mathbf{x}_j)$ given by

$$f^i(t, \mathbf{x}_j) = \sum_{k=0}^{\infty} \delta_t^k f_k^i(t_0, t_1, \mathbf{x}_j) \tag{12}$$

with $t_0 = t$ and $t_1 = \delta_t t$, where the single terms f_j^i should fulfill the restrictions

$$\sum_{i=1}^{m} \begin{pmatrix} 1 \\ \mathbf{v}_i \end{pmatrix} f_0^i = \begin{pmatrix} \rho \\ \rho\mathbf{u} \end{pmatrix} \tag{13}$$

$$\sum_{i=1}^{m} \begin{pmatrix} 1 \\ \mathbf{v}_i \end{pmatrix} f_n^i = 0, \quad n \geq 1 \tag{14}$$

which means, that the macroscopic state variables only depend on the zeroth order expansion f_0^i, $i = 1, ..., m$.
Substituting (12)–(14) into (8) and comparing powers in δ_t yields the system of equations

$$(1 - c_1) f_0^i = (c_2 + c_3) f^{i,eq} \tag{15}$$

$$\left(\partial_{t_0} + \mathbf{v}_i \nabla\right) f_0^i - c_3 \left(\partial_{t_0} + \mathbf{v}_i \nabla\right) f^{i,eq} = (c_1 - 1) f_1^i \tag{16}$$

$$\begin{aligned} \partial_{t_1} f_0^i + \left(\partial_{t_0} + \mathbf{v}_i \nabla\right) f_1^i + \frac{1}{2}\left(\partial_{t_0} + \mathbf{v}_i \nabla\right)^2 f_0^i & \\ -c_3 \left(\partial_{t_1} + \frac{1}{2}\left(\partial_{t_0} + \mathbf{v}_i \nabla\right)^2\right) f^{i,eq} = (c_1 - 1) f_2^i & \end{aligned} \tag{17}$$

Because $\sum c_i = 1$, we have from (15) $f_0^i = f^{i,eq}$ and Eq. (16) reads

$$(1 - c_3)\left(\partial_{t_0} + \mathbf{v}_i \nabla\right) f_0^i = (c_1 - 1) f_1^i \tag{18}$$

Hence, multiplying with $(1, \mathbf{v}_i)$ and summation over the discrete velocites gives the standard Euler equations on the time scale t_0, like in the standard Lattice Boltzmann scheme. Together with (18) we may write Eq. (17) as

$$\partial_{t_1} f_0^i + \frac{1 + c_1}{2(1 - c_3)}\left(\partial_{t_0} + \mathbf{v}_i \nabla\right) f_1^i = \frac{c_1 - 1}{1 - c_3} f_2^i$$

and the corresponding macroscopic equations read

$$\begin{aligned} \partial_{t_1} \rho &= 0 \\ \partial_{t_1}(\rho u) + \frac{1 + c_1}{2(1 - c_3)} \operatorname{div} \Pi^{(1)} &= 0 \end{aligned}$$

where

$$\Pi^{(1)} = \sum_{i=1}^{m} \mathbf{v}_i \otimes \mathbf{v}_i f_1^i \tag{19}$$

Substituting (18) into (19) yields finally the standard Lattice Boltzmann approximation for the incompressible Navier–Stokes equations with a visosity exactly given by (9). ■

The second result is, that the generalized scheme can actually be written as the standard Lattice Boltzmann method – applying an appropriate transformation of the single density functions f^i.

Theorem 4 *If the equilibrium functions $f^{i,eq}[\rho, \mathbf{u}]$ are homogeneous of degree one in the density, i.e.*

$$f^{i,eq}[c\rho, \mathbf{u}] = c f^{i,eq}[\rho, \mathbf{u}], \quad c \in I\!R,$$

then the generalized scheme (8) may be written under an appropriate transformation as the standard explicit Lattice Boltzmann scheme (2).

Proof If we define the functions $g^i(t, \mathbf{x}_j)$, $i = 1, \ldots, m$ by

$$g^i(t, \mathbf{x}_j) = c_1 f^i(t - \delta_t, \mathbf{x}_j - \delta_t \mathbf{v}_i) + c_2 f^{i,eq}(t - \delta_t, \mathbf{x}_j - \delta_t \mathbf{v}_i) \tag{20}$$

we can rewrite the scheme (8) in the form

$$f^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) = g^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) + c_3 f^{i,eq}(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) \tag{21}$$

and

$$g^i(t+2\delta_t, \mathbf{x}_j + 2\delta_t \mathbf{v}_i) = c_1 f^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) + c_2 f^{i,eq}(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) \tag{22}$$

Subsituting (21) into (22) yields

$$g^i(t+2\delta_t, \mathbf{x}_j + 2\delta_t \mathbf{v}_i) = c_1 g^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) + (c_1 c_3 + c_2) f^{i,eq}(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) \tag{23}$$

Now, from (21) we have

$$\sum g^i(t, \mathbf{x}_j) = (c_1 + c_2) \sum f^i(t, \mathbf{x}_j)$$

and, because the equilibrium functions are homogeneous of degree one in the density,

$$g^{i,eq}(t, \mathbf{x}_j) = (c_1 + c_2) f^{i,eq}(t, \mathbf{x}_j)$$

Thus, we may rewrite (23) in the form

$$g^i(t+2\delta_t, \mathbf{x}_j + 2\delta_t \mathbf{v}_i) = c_1 g^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) + \frac{c_1 c_3 + c_2}{c_1 + c_2} g^{i,eq}(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) \tag{24}$$

Due to mass conservation, i.e. $\sum c_i = 1$, we have

$$\frac{c_1 c_3 + c_2}{c_1 + c_2} = \frac{c_1(1 - c_1 - c_2) + c_2}{c_1 + c_2} = 1 - c_1$$

and (24) reads

$$g^i(t+2\delta_t, \mathbf{x}_j + 2\delta_t \mathbf{v}_i) = c_1 g^i(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i) + (1 - c_1) g^{i,eq}(t+\delta_t, \mathbf{x}_j + \delta_t \mathbf{v}_i)$$

which is exactly the form of the standard Lattice Boltzmann method given by (2). ■

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