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05 septembre 2007 *

Keywords: Chapman-Enskog expansion, Taylor formula
AMS (MSC2010) classification: 76M28.

Abstract

We show that when we formulate the lattice Boltzmann equation with a small time step Δt and an associated space scale Δx, a Taylor expansion joined with the so-called equivalent equation methodology leads to establish macroscopic fluid equations as a formal limit. We recover the Euler equations of gas dynamics at the first order and the compressible Navier-Stokes equations at the second order.

1) Discrete geometry

• We denote by d the dimension of space and by $\mathcal{L}$ a regular d-dimensional lattice. Such a lattice is composed by a set $\mathcal{L}^0$ of nodes or vertices and a set $\mathcal{L}^1$ of links or edges between two vertices. From a practical point of view, given a vertex x, there exists a set $V(x)$ of neighbouring nodes, including the node x itself. We consider here that the lattice $\mathcal{L}$ is parametrized by a space step $\Delta x > 0$. For the fundamental example called D2Q9 (see *e.g.* Lallemand and Luo, 2000), the set $V(x)$ is given with the help of the family of vectors $(e_j)_{0 \leq j \leq J}$ defined by $J = 8$,

$$(e_j) = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\} \tag{1.1}$$

and the vicinity

$$V(x) = \{ x + \Delta x \, e_j, \ 0 \leq j \leq J \} . \tag{1.2}$$

* Contribution published in *Computers & Mathematics with Applications*, volume 55, pages 1441-1449, 2008, doi https://doi.org/10.1016/j.camwa.2007.08.003. Edition 07 June 2018.

• In the general case, we still suppose that the equation (1.2) holds but we do not make any precise definition concerning the integer J and the nondimensionalized vectors $(e_j)_{0 \leq j \leq J}$. Nevertheless if x is a node of the lattice ($x \in \mathcal{L}^0$), then $y^j = x + \Delta x \; e_j$ is an other node of the lattice, *i.e.* $y^j \in \mathcal{L}^0$.

2) Lattice Boltzmann framework

• We introduce a time step $\Delta t > 0$ and we suppose that the celerity λ defined according to

$$\lambda = \frac{\Delta x}{\Delta t} \tag{2.1}$$

remains fixed. Then we introduce a local velocity v_j in such a way that

$$\Delta t \; v_j = \Delta x \; e_j \, , \quad 0 \leq j \leq J \, . \tag{2.2}$$

In this d-dimensional framework we will denote by $v_j^\alpha \, (1 \leq \alpha \leq d)$ the Cartesian components of velocities v_j. Recall that if x is a node of the lattice, the point $x + \Delta t \; v_j$ is also a node of the lattice:

$$x \in \mathcal{L}^0 \implies x + \Delta t \; v_j \in \mathcal{L}^0 \, , \quad \forall j = 0, \ldots J. \tag{2.3}$$

• According to D'Humières (1992), the lattice Boltzmann scheme describes the dynamics of the density $f^j(x, \, t)$ of particles of velocity v_j at the node x and for the discrete time t. We introduce the $d+1$ scalar "conservative variables" $W(x, \, t)$ composed by the density ρ and the momentum q. Note that it is also possible to take into account the conservation of the total energy (see D'Humières's article for example). We have

$$\rho(x, \, t) = \sum_{j=0}^{J} f^j(x, \, t) \equiv W^0(x, \, t) \tag{2.4}$$

$$q^\alpha(x, \, t) = \sum_{j=0}^{J} v_j^\alpha \, f^j(x, \, t) \equiv W^\alpha(x, \, t) \, , \quad 1 \leq \alpha \leq d \, , \tag{2.5}$$

and

$$W(x, \, t) = \big(\rho(x, \, t), \, q^1(x, \, t), \, \cdots \, , \, q^d(x, \, t) \big) \, . \tag{2.6}$$

When a state W is given in space $\mathbb{R}^{d+1}$, a Gaussian (or any other choice) equilibrium distribution of particles is defined according to

$$f_{\rm eq}^j = G^j(W) \, , \quad 0 \leq j \leq J \tag{2.7}$$

in such a way that

$$\sum_{j=0}^{J} G^j(W) \equiv W^0 \, , \quad \sum_{j=0}^{J} v_j^\alpha \, G^j(W) \equiv W^\alpha \, , \quad 1 \leq \alpha \leq d \, . \tag{2.8}$$

• Following D'Humières (1992), we introduce the "moment vector" m according to

$$m^k = \sum_{j=0}^{J} M_j^k \; f^j \, , \quad 0 \leq k \leq J \, . \tag{2.9}$$

For $0 \leq i \leq d$, the moments m^i are **identical** to the conservative variables:

(2.10) $\quad m^0 \equiv \rho\,, \quad m^\alpha \equiv q^\alpha\,, \quad 1 \leq \alpha \leq d\,.$

In other words, the matrix M satisfies

(2.11) $\quad M_j^0 \equiv 1\,, \quad M_j^\alpha \equiv v_j^\alpha\,, \quad 0 \leq j \leq J\,, \quad 1 \leq \alpha \leq d\,.$

We assume that vectors $(e_j)_{0\leq j\leq J}$ are chosen such that the $(d+1)\times(J+1)$ matrix $(M_{k\,j})_{0\leq k\leq d,\,0\leq j\leq J}$ is of full rank. With this hypothesis, the conservative moments W introduced in relation (2.6) are independent variables.

• When a particle distribution f is given, the moments are evaluated according to (2.9). The matrix M is supposed to be invertible and the inverse relation takes the form:

(2.12) $\quad f^j = \sum_{k=0}^{J} (M^{-1})_k^j\; m^k\,, \quad 0 \leq j \leq J\,.$

When $f_{\rm eq}^j$ is determined according to the relation (2.7), the associated equilibrium moments $m_{\rm eq}^k$ are given simply according to (2.9), *i.e.* in this case

(2.13) $\quad m_{\rm eq}^k = \sum_{j=0}^{J} M_j^k\; f_{\rm eq}^j\,, \quad 0 \leq k \leq J\,.$

We remark also that by construction (relation (2.8)), we have

(2.14) $\quad m_{\rm eq}^i = m^i = W^i\,, \quad 0 \leq i \leq d\,.$

3) Collision step

• The collision step is local in space and is naturally defined in the space of moments. If $m^k(x,\,t)$ denotes the value of the $k^{\rm th}$ component of the moment vector m at position x and time t, the same component $m_*^k(x,\,t)$ of the moment **after** the collision is trivial by construction for the conservative variables:

(3.1) $\quad m_*^i(x,\,t) = m^i(x,\,t)\,, \quad 0 \leq i \leq d\,.$

For the non-conservative components of the moment vector, we **fix** the ratio s_k $(k \geq d+1)$ between the time step Δt and the relaxation time τ_k of an underlying process:

(3.2) $\quad s_k = \dfrac{\Delta t}{\tau_k}\,, \quad d+1 \leq k \leq J\,.$

• Then $m_*^k(x,\,t)$ after the collision is defined according to

(3.3) $\quad m_*^k(x,\,t) = (1-s_k)\,m^k(x,\,t) + s_k\,m_{\rm eq}^k\,, \quad d+1 \leq k \leq J\,.$

Proposition 1. Explicit Euler scheme.
The numerical scheme (3.3) is exactly the explicit Euler scheme relative to the continuous in time relaxation equation

(3.4) $\quad \dfrac{\rm d}{{\rm d}t}\big(m^k - m_{\rm eq}^k\big) + \dfrac{1}{\tau_k}\big(m^k - m_{\rm eq}^k\big) = 0\,, \quad d+1 \leq k \leq J\,.$

Proof of Proposition 1.
Following *e.g.* Strang (1986), we know that the explicit Euler scheme for the evolution (3.4) takes the form

$$\frac{1}{\Delta t}\Big[\big(m^k - m^k_{\rm eq}\big)(t+\Delta t) - \big(m^k - m^k_{\rm eq}\big)(t)\Big] \, + \, \frac{1}{\tau_k}\big(m^k - m^k_{\rm eq}\big)(t) \, = \, 0 \, . \tag{3.5}$$

We have by construction the relation (3.1), that is $m^i(t+\Delta t) = m^i(t)$ for $0 \leq i \leq d$ with these notations. Then $W(t+\Delta t) = W(t)$ and, due to the relation (2.7), $f^j_{\rm eq}(t+\Delta t) = f^j_{\rm eq}(t)$ after the collision step for all the components j of the particle distribution. Due to (2.13), we deduce that $m^k_{\rm eq}(t+\Delta t) = m^k_{\rm eq}(t)$ for all $k \leq J$. Thus the expression (3.5) takes the simpler form

$$\frac{1}{\Delta t}\big[m^k(t+\Delta t) - m^k(t)\big] \, + \, \frac{1}{\tau_k}\big(m^k - m^k_{\rm eq}\big)(t) \, = \, 0 \, , \tag{3.6}$$

which is exactly (3.3), except the change of notations: $m^k(t+\Delta t)$ is replaced by m^k_*. □

• We remark also that the classical stability condition for the explicit Euler scheme (see again *e.g.* the book of Strang) takes the form

$$0 \leq \Delta t \leq 2\,\tau_k \, . \tag{3.7}$$

We will suppose in the following that

$$0 \, < \, s_k \, \leq \, 2 \, , \quad d+1 \leq k \leq J \, . \tag{3.8}$$

to put in evidence that the moments m^k are **not** conserved for index k greater than $d+1$. We remark also that for the physically relevant Boltzmann equation, the relaxation times τ_k have a physical sense. With the lattice Boltzmann scheme itself, these physical constants are no longer correctly approximated whereas the **ratios** $s_k = \frac{\Delta t}{\tau_k}$ are supposed to be fixed in all what follows. Despite the usual "LBE" denomination, a lattice Boltzmann scheme is not a numerical method to approach the Boltzmann equation !

• The particle distribution f^j_* after the collision step follows the relation (2.12). We have precisely after the collision step

$$f^j_* \, = \, \sum_{k=0}^{J} (M^{-1})^j_k \; m^k_* \, , \quad 0 \leq j \leq J \, . \tag{3.9}$$

4) Advection step

• The avection step of the lattice Boltzmann scheme claims that after the collision step, the particles having velocity v_j at position x go in one time step Δt to the $j^{\rm th}$ neighbouring vertex. Thus the particle density $f^j(x + v_j\,\Delta t,\, t+\Delta t)$ at the new time step in the neighbouring vertex is equal to the previous particle density $f^j_*(x,\, t)$ at the position x after the collision:

$$f^j(x + v_j\,\Delta t,\, t+\Delta t) \, = \, f^j_*(x,\, t) \, . \tag{4.1}$$

We re-write this relation in term of the "arrival" node $x + v_j\,\Delta t$. We set $\widetilde{x} = x + v_j\,\Delta t$, then we have $x = \widetilde{x} - v_j\,\Delta t$ and going back to the notation x, we write the relation (4.1) in the equivalent manner

$$f^j(x,\, t+\Delta t) \;=\; f^j_*(x - v_j\,\Delta t,\, t)\,, \quad 0 \le j \le J\,, \quad x \in \mathcal{L}^0\,. \tag{4.2}$$

Proposition 2. Upwind scheme for the advection equation.
The scheme (4.2) for the advection step of the lattice Boltzmann method is nothing else that the explicit upwind scheme for the advection equation

$$\frac{\partial f^j}{\partial t} \;+\; v_j \bullet \nabla f^j \;=\; 0\,, \quad 0 \le j \le J\,, \tag{4.3}$$

with a so-called Courant-Friedrichs-Lewy number σ_j in the j^{th} direction of the lattice defined by

$$\sigma_j \;\equiv |\, v_j \,|\, \frac{\Delta t}{\Delta x \;|\, e_j \,|} \tag{4.4}$$

equal, due to the definition (2.2), to unity: $\sigma_j = 1$.

Proof of Proposition 2.
When the Courant-Friedrichs-Lewy number σ_j is equal to unity, it is classical (see *e.g.* Strang, 1986) that the upwind scheme is exact for the advection equation. □

5) Equivalent equation at zero order

• The lattice Boltzmann scheme is defined by the relations (2.4) to (2.9), (3.3) and (4.2). It is parametrized by the lattice step Δx, the matrix M linking the particle distribution f and the moment vector m, the choice of the conservative moments, the nonlinear equilibrium function $G(\bullet)$, the time step Δt and the ratios s_k between the time step and the collision time constants for nonequilibrium moments. In what follows, we fix the geometrical and topological structure of the lattice $\mathcal{L}$, we fix the matrix M and the equilibrium function $G(\bullet)$, we fix also the ratio λ defined in (2.1) and last but not least, we suppose that the parameters s_k for $k \ge d+1$ have a fixed value. Then the whole lattice Boltzmann scheme depends on the single parameter Δt.

• We explore now formally what are the partial differential equations associated with the Boltzmann numerical scheme, following the so-called "equivalent equation method" introduced and developed by Lerat-Peyret (1974) and Warming-Hyett (1974). This approach is based on the assumption, that a sufficiently smooth function exists which satisfies the difference equation at the grid points. This assumption gives formal responses to put in evidence partial differential equations that minimimize the truncation errors of the numerical scheme. Nevertheless, we note here that this method of analysis fails to predict initial layers and boundary effects properly, as discussed by Griffiths and Sanz-Serna (1986) or Chang (1990). The idea of the calculus is to suppose that all the data are sufficiently regular and to expand all the variables with the Taylor formula.

Proposition 3. Taylor expansion at zero order.
With the lattice Boltzmann defined previously, we have

$$f^j(x,\,t) \,=\, f^j_{\rm eq}(x,\,t) \,+\, {\rm O}(\Delta t)\,, \quad 0 \leq j \leq J\,, \tag{5.1}$$

$$f^j_*(x,\,t) \,=\, f^j_{\rm eq}(x,\,t) \,+\, {\rm O}(\Delta t)\,, \quad 0 \leq j \leq J\,, \tag{5.2}$$

with $f^j_{\rm eq}$ defined from the conservative variables W according to the relation (2.7).

Proof of Proposition 3.
The key point is to expand the relation (4.2) relative to the infinitesimal Δt. We have on one hand

$$f^j(x,\,t+\Delta t) \,=\, f^j(x,\,t) \,+\, {\rm O}(\Delta t) \tag{5.3}$$

and on the other hand

$$f^j_*(x - v_j\,\Delta t,\,t) \,=\, f^j_*(x,\,t) \,+\, {\rm O}(\Delta t) \tag{5.4}$$

Then $\displaystyle m^k_*(x,\,t) \,=\, \sum_{j=0}^{J} M^k_j\, f^j_*(x,\,t) \,=\, m^k(x,\,t) \,+\, {\rm O}(\Delta t)$ and

$$m^k_*(x,\,t) \,-\, m^k(x,\,t) \,=\, {\rm O}(\Delta t)\,. \tag{5.5}$$

But, due to (3.3), we have

$$m^k_*(x,\,t) \,-\, m^k(x,\,t) \,=\, -s_k\,\big(m^k(x,\,t) - m^k_{\rm eq}(x,\,t)\big)\,. \tag{5.6}$$

From (5.5) and (5.6) we deduce, due to the fact that $s_k \neq 0$ when $k \geq d+1$:

$$m^k(x,\,t) \,=\, m^k_{\rm eq}(x,\,t) + {\rm O}(\Delta t)\,, \quad k \geq d+1\,. \tag{5.7}$$

We insert (5.7) into (5.5) and we deduce

$$m^k_*(x,\,t) \,=\, m^k_{\rm eq}(x,\,t) + {\rm O}(\Delta t)\,, \quad k \geq d+1\,. \tag{5.8}$$

Taking into account the relations (2.14) and (3.1) on one hand and (2.12) and (3.9) on the other hand, we deduce (5.1) and (5.2) from (5.7) and (5.8). □

6) Taylor expansion at first order

• We expand now the relation (4.2) one step further with respect to the time step Δt. We introduce the second order moment

$$F^{\alpha\,\beta} \,\equiv\, \sum_{j=0}^{J} \,v^\alpha_j\; v^\beta_j\; f^j_{\rm eq}\,, \quad 1 \leq \alpha,\,\beta \leq d\,. \tag{6.1}$$

We denote in the following ∂_t instead of $\frac{\partial}{\partial t}$ and ∂_β in place of $\frac{\partial}{\partial x_\beta}$. Then we have the following result at the first order.

Proposition 4. Euler equations of gas dynamics.
With the lattice Boltzmann scheme previously defined, we have the conservation of mass and momentum at the first order:

$$\partial_t \rho \,+\, \sum_{\beta=1}^{d} \partial_\beta\, q^\beta \;=\; {\rm O}(\Delta t) \tag{6.2}$$

$$\partial_t q^\alpha \,+\, \sum_{\beta=1}^{d} \partial_\beta \, F^{\alpha\,\beta} \;=\; \mathrm{O}(\Delta t)\,. \tag{6.3}$$

Proof of Proposition 4.
We expand both sides of relation (4.2) up to first order:
$f^j(x\,,\,t\,+\,\Delta t) \,=\, f^j(x\,,\,t) \,+\, \Delta t\;\partial_t f^j \,+\, \mathrm{O}(\Delta t^2)$
$f^j_*(x\,-\,v_j\,\Delta t\,,\,t) \,=\, f^j_*(x\,,\,t) \,-\, \Delta t\;v_j^\beta\;\partial_\beta f^j_* \,+\, \mathrm{O}(\Delta t^2)\,.$
We take the moment of order k of this identity:

$$m^k(x\,,\,t) \,+\, \Delta t\;\partial_t m^k \,+\, \mathrm{O}(\Delta t^2) \,=\, m^k_*(x\,,\,t) \,-\, \Delta t\;\sum_{j=0}^{J}\; M^k_j\;v_j^\beta\;\partial_\beta f^j_* \,+\, \mathrm{O}(\Delta t^2)$$

and we use the previous Taylor expansions (5.1) (5.2) at the order zero:

$$m^k(x\,,\,t) \,+\, \Delta t\;\partial_t m^k_{\mathrm{eq}} \,=\, m^k_*(x\,,\,t) \,-\, \Delta t\;\sum_{j=0}^{J}\; M^k_j\;v_j^\beta\;\partial_\beta f^j_{\mathrm{eq}} \,+\, \mathrm{O}(\Delta t^2)\,. \tag{6.4}$$

We take $k=0$ inside the relation (6.4). We get (6.2) since $m^0(x\,,\,t)\equiv m^0_*(x\,,\,t)\equiv\rho(x\,,\,t)$. Considering now the particular case $k=\alpha$ with $1\leq\alpha\leq d$, we have also $m^\alpha(x\,,\,t)\equiv m^\alpha_*(x\,,\,t)\equiv q^\alpha(x\,,\,t)$ and the relation (6.3) is a direct consequence of the definition (6.1) and the property (2.11). □

Proposition 5. Technical lemma.
We introduce the "conservation defect" θ^k according to the relation

$$\theta^k(x\,,\,t) \,=\, \partial_t m^k_{\mathrm{eq}} \,+\, \sum_{j=0}^{J}\; M^k_j\;v_j^\beta\;\partial_\beta f^j_{\mathrm{eq}} \,\equiv\, \sum_{j=0}^{J}\; M^k_j\;\left(\,\partial_t f^j_{\mathrm{eq}} \,+\, v_j^\beta\;\partial_\beta f^j_{\mathrm{eq}}\,\right). \tag{6.5}$$

Then we have the following properties:

$$m^k(x\,,\,t) \,=\, m^k_{\mathrm{eq}}(x\,,\,t) \,-\, \frac{\Delta t}{s_k}\;\theta^k \,+\, \mathrm{O}(\Delta t^2)\,,\quad k\geq d+1\,, \tag{6.6}$$

$$m^k_*(x\,,\,t) \,=\, m^k_{\mathrm{eq}}(x\,,\,t) \,-\, \Big(\frac{1}{s_k}\,-\,1\Big)\;\Delta t\;\theta^k \,+\, \mathrm{O}(\Delta t^2)\,,\quad k\geq d+1\,, \tag{6.7}$$

$$\partial_\beta f^j_* \,=\, \partial_\beta f^j_{\mathrm{eq}} \,-\, \Delta t\;\sum_{k=d+1}^{J}\;\Big(\frac{1}{s_k}\,-\,1\Big)\;(M^{-1})^j_k\;\partial_\beta\theta^k \,+\, \mathrm{O}(\Delta t^2)\,. \tag{6.8}$$

Proof of Proposition 5.
We start from the relation (6.4) and we have observed at the previous proposition that

$$\theta^i \,=\, \mathrm{O}(\Delta t)\,,\quad 0\leq i\leq d\,. \tag{6.9}$$

We remark also that from the relation (5.6), we have

$$m^k(x\,,\,t) - m^k_{\mathrm{eq}}(x\,,\,t) \,=\, \frac{1}{s_k}\,\big(m^k(x\,,\,t) \,-\, m^k_*(x\,,\,t)\big)\quad \text{if } k\geq d+1.$$

Then the relation (6.6) is a direct consequence of (6.4) and the definition (6.5). In consequence, the relation (6.7) follows from (6.6) and (6.4). Due to (6.7), (6.9) and (3.9), we have

$$f^j_*(x\,,\,t) \,=\, f^j_{\mathrm{eq}}(x\,,\,t) \,-\, \Delta t\;\sum_{k\geq d+1}\;\Big(\frac{1}{s_k}\,-\,1\Big)\;(M^{-1})^j_k\;\theta^k \,+\, \mathrm{O}(\Delta t^2) \tag{6.10}$$

and the relation (6.8) follows from derivating (6.10) in the direction x_β. $\square$

7) Equivalent equation at second order

- We introduce the tensor $\Lambda_k^{\alpha\,\beta}$ according to

$$\Lambda_k^{\alpha\,\beta} \equiv \sum_{j=0}^{J} v_j^\alpha \; v_j^\beta \; (M^{-1})_k^j \,, \quad 1 \leq \alpha, \, \beta \leq d \,, \quad 0 \leq k \leq J \,. \tag{7.1}$$

We can now establish the major result of our contribution.

Proposition 6. Navier-Stokes equations of gas dynamics.
With the lattice Boltzmann method defined in previous sections and the conservation defect θ^k defined in (6.5), we have the following expansions up to second order accuracy:

$$\partial_t \rho + \sum_{\beta=1}^{d} \partial_\beta \, q^\beta \; = \; \mathrm{O}(\Delta t^2) \tag{7.2}$$

$$\partial_t q^\alpha + \sum_{\beta=1}^{d} \partial_\beta \left(F^{\alpha\,\beta} - \Delta t \sum_{k \geq d+1} \Big(\frac{1}{s_k} - \frac{1}{2} \Big) \Lambda_k^{\alpha\,\beta} \; \theta^k \right) \; = \; \mathrm{O}(\Delta t^2) \,. \tag{7.3}$$

- A consequence of relation (7.3) is the fact that a lattice Boltzmann scheme approximates at second order of accuracy a Navier-Stokes type equation with viscosities μ_k of the form

$$\mu_k \; = \; \Delta t \, \Big(\frac{1}{s_k} - \frac{1}{2} \Big) \,. \tag{7.4}$$

We refer for the details to D. D'Humières (1992), Lallemand and Luo (2000) or to our recent survey (2007). The relations (7.4) are known as the "D'Humières relations". We observe that in practice, the scalar μ_k is imposed by the physics and by the parameter Δt is constrained by the space discretization Δx and the relation (2.1). Then the parameter s_k must be chosen in order to satisfy the D'Humières relations (7.4).

Proof of Proposition 6.
We start again from the identity (4.2). We expand both terms up to second order accuracy:

$$f^j(x \, , \, t + \Delta t) \; = \; f^j(x \, , \, t) \; + \; \Delta t \; \partial_t f^j \; + \; \frac{1}{2} \, \Delta t^2 \; \partial_{tt}^2 f^j \; + \; \mathrm{O}(\Delta t^3)$$

$$f_*^j(x \, - \, v_j \, \Delta t \, , \, t) \; = \; f_*^j(x \, , \, t) \; - \; \Delta t \; v_j^\beta \; \partial_\beta f_*^j \; + \; \frac{1}{2} \, \Delta t^2 \; v_j^\beta \; v_j^\gamma \; \partial_{\beta\gamma}^2 f_*^j \; + \; \mathrm{O}(\Delta t^3) \,.$$

We take the moment of order i $(0 \leq i \leq d)$ of this identity. We obtain:

$$\left\{ \begin{array}{l} m^i(x \, , \, t) \; + \; \Delta t \; \partial_t m^i \; + \; \dfrac{1}{2} \, \Delta t^2 \; \partial_{tt}^2 m^i \; + \; \mathrm{O}(\Delta t^3) \; = \; m_*^i(x \, , \, t) + \\ \qquad - \Delta t \; \displaystyle\sum_{j=0}^{J} \; M_j^i \; v_j^\beta \; \partial_\beta f_*^j \; + \; \frac{1}{2} \, \Delta t^2 \; \sum_{j=0}^{J} \; M_j^i \, v_j^\beta \; v_j^\gamma \; \partial_{\beta\gamma}^2 f_*^j \; + \; \mathrm{O}(\Delta t^3) \,. \end{array} \right. \tag{7.5}$$

We use the microscopic conservation $m_*^i(x \, , \, t) \equiv m^i(x \, , \, t)$ in (7.5) and the previous Taylor expansion at order one, in particular the relation (6.8). We divide by Δt and we deduce:

$$\partial_t m^i \,+\, \frac{1}{2}\,\Delta t\;\partial_{tt}^2 m^i \;=\; -\sum_{j=0}^{J} M_j^i\;v_j^\beta\;\partial_\beta f_{\rm eq}^j \,+$$
$$+\,\Delta t\;\sum_{j=0}^{J}\;\sum_{k\geq d+1} M_j^i\,v_j^\beta\,\Big(\frac{1}{s_k}-1\Big)\,(M^{-1})_k^j\;\partial_\beta\,\theta^k \,+$$
$$+\,\frac{1}{2}\,\Delta t\;\sum_{j=0}^{J}\;M_j^i\;v_j^\beta\,v_j^\gamma\;\partial_{\beta\gamma}^2 f_{\rm eq}^j \,+\, {\rm O}(\Delta t^2)\,.$$

Then

$$(7.6)\qquad \left\{\begin{array}{l} \partial_t m^i \,+\, \displaystyle\sum_{\beta=1}^{d}\sum_{j=0}^{J} M_j^i\;v_j^\beta\;\partial_\beta f_{\rm eq}^j \;= \\ \qquad =\; \Delta t\displaystyle\sum_{\beta=1}^{d}\sum_{j=0}^{J}\sum_{k\geq d+1} M_j^i\;v_j^\beta\,\Big(\frac{1}{s_k}-1\Big)\,(M^{-1})_k^j\;\partial_\beta\theta^k + \\ \qquad\quad +\,\dfrac{\Delta t}{2}\,\Big(-\,\partial_{tt}^2 m^i \;+\; \displaystyle\sum_{\beta=1}^{d}\sum_{j=0}^{J} M_j^i\;v_j^\beta\,v_j^\gamma\;\partial_{\beta\gamma}^2 f_{\rm eq}^j\Big) \,+\, {\rm O}(\Delta t^2)\,. \end{array}\right.$$

• We set $i=0$ in the relation (7.6) and we look for the conservation of mass. Due to the property $M_j^0\equiv 1$, the sum over j in the second line of (7.6) is null since $\sum_{j=0}^{J} v_j^\beta\,(M^{-1})_k^j$ is equal to zero. We have also the following algebraic calculus:

$$\partial_{tt}^2 m^0 \;=\; \partial_{tt}^2\rho \;=\; -\sum_{\beta=1}^{d}\partial_{t\beta}^2\,q^\beta \,+\, {\rm O}(\Delta t) \;=\; -\sum_{\beta=1}^{d}\partial_\beta\,\partial_t\,q^\beta \,+\, {\rm O}(\Delta t) \;=$$
$$=\;\sum_{\beta=1}^{d}\sum_{\gamma=1}^{d}\partial_{\beta\gamma}^2\,F^{\beta\,\gamma} \,+\, {\rm O}(\Delta t) \;=\; \sum_{\beta=1}^{d}\sum_{\gamma=1}^{d}\sum_{j=0}^{J} v_j^\beta\,v_j^\gamma\;\partial_{\beta\gamma}^2 f_{\rm eq}^j \,+\, {\rm O}(\Delta t)$$

and the third line of (7.6) is null up to second order accuracy. Thus the conservation of mass (7.2) up to second order accuracy is established.

• We set $i=\alpha$ with $1\leq\alpha\leq d$ and we look for the conservation of momentum. In this particular case, the relation (7.6) takes the form:

$$(7.7)\qquad \left\{\begin{array}{l} \partial_t q^\alpha \,+\, \displaystyle\sum_{\beta=1}^{d}\sum_{j=0}^{J} v_j^\alpha\;v_j^\beta\;\partial_\beta f_{\rm eq}^j \;= \\ \qquad =\; \Delta t\displaystyle\sum_{k\geq d+1}\Big(\frac{1}{s_k}-1\Big)\sum_{\beta=1}^{d}\Big[\sum_{j=0}^{J} v_j^\alpha\;v_j^\beta\;(M^{-1})_k^j\Big]\,\partial_\beta\theta^k + \\ \qquad\quad +\,\dfrac{\Delta t}{2}\,\Big(-\,\partial_{tt}^2 q^\alpha \;+\; \displaystyle\sum_{\beta=1}^{d}\sum_{j=0}^{J} v_j^\alpha\,v_j^\beta\,v_j^\gamma\;\partial_{\beta\gamma}^2 f_{\rm eq}^j\Big) \,+\, {\rm O}(\Delta t^2)\,. \end{array}\right.$$

We have now to play with some algebra:

$$-\partial_{tt}^2 q^\alpha \; + \sum_{\beta=1}^{d} \sum_{j=0}^{J} \; v_j^\alpha \, v_j^\beta \, v_j^\gamma \; \partial_{\beta\gamma}^2 f_{\rm eq}^j \; =$$

$$= \; \sum_{\beta=1}^{d} \Big(\partial_t \partial_\beta F^{\alpha\,\beta} + \sum_{j=0}^{J} \; v_j^\alpha \; v_j^\beta \, v_j^\gamma \; \partial_{\beta\gamma}^2 f_{\rm eq}^j \Big) \; + \; {\rm O}(\Delta t)$$

$$= \; \sum_{\beta=1}^{d} \partial_\beta \Big(\; \sum_{j=0}^{J} \; v_j^\alpha \; v_j^\beta \, \big(\partial_t f_{\rm eq}^j \; + \; v_j^\gamma \, \partial_\gamma f_{\rm eq}^j \big) \Big) \; + \; {\rm O}(\Delta t)$$

$$= \; \sum_{\beta=1}^{d} \partial_\beta \Big(\; \sum_{j=0}^{J} \; v_j^\alpha \; v_j^\beta \; \sum_{k=0}^{J} (M^{-1})_k^j \, \theta^k \Big) \; + \; {\rm O}(\Delta t)$$

$$= \; \sum_{\beta=1}^{d} \partial_\beta \Big(\; \sum_{k \geq d+1} \Big[\sum_{j=0}^{J} \; v_j^\alpha \; v_j^\beta \; (M^{-1})_k^j \Big] \; \theta^k \; \Big) \; + \; {\rm O}(\Delta t)$$

$$= \; \sum_{\beta=1}^{d} \partial_\beta \Big(\; \sum_{k \geq d+1} \Lambda_k^{\alpha\,\beta} \; \theta^k \; \Big) \; + \; {\rm O}(\Delta t)$$

due to the definition (7.1). We deduce from (6.1), (7.7) and the above calculus:

$$\partial_t q^\alpha \; + \sum_{\beta=1}^{d} \partial_\beta F^{\alpha\,\beta} \; = \; \Delta t \sum_{k \geq d+1} \Big(\frac{1}{s_k} - 1 \Big) \sum_{\beta=1}^{d} \Lambda_k^{\alpha\,\beta} \; \partial_\beta \, \theta^k \, +$$

$$+ \; \frac{\Delta t}{2} \; \sum_{\beta=1}^{d} \partial_\beta \Big(\; \sum_{k \geq d+1} \Lambda_k^{\alpha\,\beta} \; \theta^k \; \Big) \; + \; {\rm O}(\Delta t^2)$$

$$= \; \Delta t \sum_{\beta=1}^{d} \sum_{k \geq d+1} \Big(\frac{1}{s_k} - \frac{1}{2} \Big) \, \Lambda_k^{\alpha\,\beta} \; \partial_\beta \, \theta^k \; + \; {\rm O}(\Delta t^2) \, .$$

and the relation (7.3) is established. □

8) Equivalent equation at second order

• The previous propositions establish that the equivalent partial differential equations of a Boltzmann scheme are given up to second order accuracy by the same result as the formal Chapman-Enskog expansion. We find Euler type equation at the first order (Proposition 4) and Navier-Stokes type equation at the second order (Proposition 6). Note that with the above framework no *a priori* formal two-time multiple scaling is necessary to establish the Navier-Stokes equations from a lattice Boltzmann scheme, as done previously in the contribution of D'Humières. We remark also that a so-called diffusive scaling like $\frac{\Delta t}{\Delta x^2} = $ constant, instead of our condition (2.1) $\frac{\Delta t}{\Delta x} = $ constant, leads to the incompressible Navier-Stokes equations, as proposed by Junk, Klar and Luo (2005). In both cases, we have just to use the Taylor formula for a single infinitesimal parameter.

9) Acknowledgments

The author thanks Li-Shi Luo to his kind invitation to present the scientific work of Orsay's team at ICMMES Conference in July 2005. The author thanks also with a great emphasis Pierre Lallemand for very helpfull discussions all along the elaboration of this contribution. Last but not least, the referees transmitted to the author very good remarks that have been incorporated inside the present edition of the article.

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