Third order equivalent equation of lattice Boltzmann scheme

François Dubois □
Numerical Analysis and Partial Differential Equations
Department of Mathematics, University Paris Sud
Bat. 425, F-91405 Orsay Cedex, France.
francois.dubois@math.u-psud.fr
and
Conservatoire National des Arts et Métiers, Paris.
Department of Mathematics and EA3196

03 October 2008

Abstract
We recall the origin of lattice Boltzmann scheme and detail the version due to D'Humières (1992). We present a formal analysis of this lattice Boltzmann scheme in terms of a single numerical infinitesimal parameter. We derive third order equivalent partial differential equation of this scheme. Both situations of single conservation law and fluid flow with mass and momentum conservations are detailed. We apply our analysis to so-called D1Q3 and D2Q9 lattice Boltzmann schemes in one and two space dimensions.

key words: lattice Boltzmann, Taylor formula, thermics, acoustics.

AMS classification: 65Q05, 76N15, 82C20.

□ Published (doi: 10.3934/ dcds.2009.23.221) in *Discrete and Continuous Dynamical Systems*, volume 23, numbers 1 & 2, January and February 2009, special issue dedicated to Ta-Tsien Li on the Occasion of his 70th Birthday, p. 221 - 248.

1) From cellular automata to lattice Boltzmann scheme

• The idea of studying the evolution of a population on a discrete lattice $\mathcal{L}$ can be attributed to Von Neumann (1953) and Ulam (1962). Nevertheless, this idea became very popular with the so-called "Conway's game of life" described by Gardner (1970). Recall that with this kind of automata, each node x of the lattice ($x \in \mathcal{L}^0$ when we denote by $\mathcal{L}^0$ the set of vertices of lattice $\mathcal{L}$) can be occupied or can be unoccupied. The population at discrete time t on lattice $\mathcal{L}$ is a function $\mathcal{L}^0 \ni x \longmapsto f(x, t) \in \{0, 1\}$. We have $f(x, t) = 0$ if the vertex $x \in \mathcal{L}^0$ is unoccupied at time t and $f(x, t) = 1$ if it is occupied. The evolution $f(\bullet, t) \longrightarrow f(\bullet, t+1)$ defines the rules of the game. We do not enter into the details of game of life in this contribution.

• Independently of these cellular automata, the Boltzmann equation proposes to determine a distribution of particles $\mathbb{R}^3 \times \mathbb{R}^3 \times [0, +\infty[\ni (x, v, t) \longmapsto f(x, v, t) \in [0, +\infty[$ satisfying a continuous evolution typically as

$$\frac{\partial f}{\partial t} + v \bullet \nabla_x f = Q(f) \,. \tag{1.1}$$

The left hand side of equation (1.1) is the advection equation with velocity v and the right hand side is defined by the so-called collision operator $Q(\bullet)$. This operator is local in space and mixes the $f(x, v, t)$ for $v \in \mathbb{R}^3$. Technically speaking, for a given velocity v, $Qf(x, v, t)$ is a functional of all the $f(x, w, t)$ for **all** $w \in \mathbb{R}^3$ with **fixed** space x and time t. It is classical (see *e.g.* the book of Chapman and Cooling, 1939) that the so-called equilibrium distribution $f^{\rm eq}$ that is defined by $Q(f^{\rm eq}) = 0$ is a Maxwellian distribution.

• Due to the difficulties to handle equation (1.1), two important ideas for simplifying the dynamics have been proposed. The first one with Bhatnagar, Gross and Krook ("BGK", 1954), consists in a linearization around the equilibrium distribution $f^{\rm eq}$ and in replacing the collision operator by a linear development around $f^{\rm eq}$:

$$Q^{BGK}(f) = S \bullet (f - f^{\rm eq}) \,, \tag{1.2}$$

where S is the linearized collision operator at the equilibrium:

$$S = {\rm d}Q(f^{\rm eq}) \,. \tag{1.3}$$

On the other hand with Carleman (1957) and Broadwell (1964), one reduces the space of velocities $\mathbb{R}^3$ into a discrete set $\mathcal{V}$. Following this approach, the Boltzmann equation (1.1) is replaced by a system of partial differential equations. This methodology of studying Boltzmann equation with discrete velocities has been developed by Cabannes (1975) and Gatignol (1975).

• In their pioneering work, Hardy, Pomeau and De Pazzis ("HPP", 1973) made the link between cellular automata and Boltzmann equation: they proposed to use a cellular automaton to solve a discrete version of Boltzmann equation. At vertex x, a particle of discrete velocity $v \in \mathcal{V}$ can be present. The discrete velocities v and the time step Δt are chosen in such a way that if $x \in \mathcal{L}^0$, $x + \Delta t\, v$ is necessarily an other vertex of the lattice. In other words,

$$x \in \mathcal{L}^0 \quad \text{and} \quad v \in \mathcal{V} \implies x + \Delta t\, v \in \mathcal{L}^0 \,. \tag{1.4}$$

At discrete time t, the state of the lattice is a function of the type $\mathcal{L}^0 \ni x \longmapsto f(x,\, t) \in \{0\} \cup \mathcal{V}$. If $f(x,\, t) = 0$, there is no particle at position x and time t and when $f(x,\, t) = v_j$ (with $v_j \in \mathcal{V}$), there is one particle of velocity v_j. In their original work, HPP proposed to use a two-dimensional square lattice with four velocities (a D2Q4 automaton in the technical jargon of lattice Boltzmann community) and proposed rules of collision to determine a discrete collision operator $Q(f)$. The fundamental point is that these discrete collisions satisfy locally conservation of mass and momentum, as the physical collisions at the microscopic level. It is possible to introduce density $\rho(x,\, t)$ and momentum $q(x,\, t)$ as mean values of (respectively) $|f(y,\, t)|$ and $|f(y,\, t)|\; f(y,\, t)$ for y in a block of sufficient number of vertices around the vertex x. A remarkable result of cellular automata is that classical conservation laws can be formally derived as the size of the blocks tends towards infinity:

$$\frac{\partial \rho}{\partial t} + \text{div} q \,=\, 0\,, \qquad \frac{\partial q}{\partial t} + \text{div}\,\big(P(\rho,\, q)\big) \,=\, 0\,. \tag{1.5}$$

• With the next generation of cellular automata proposed by Frisch, Hasslacher and Pomeau ("FHP", 1986) a two-dimensional triangular lattice (D2Q6) was introduced and pressure tensor $P(\bullet,\, \bullet)$ of relation (1.5) becomes compatible with isotropy of the equations of hydrodynamics. The extension to three space dimensions ("FCHC", D3Q24 on a four-dimensional lattice in space-time) was proposed by D'Humières, Lallemand and Frisch (1986). The cellular automata suffer of a too important noise and of the fact that the hydrodynamic transport coefficients are strongly imposed by the discrete algorithm.

• The new idea, proposed by Mac Namara and Zanetti (1988), is to fit closer to the original Boltzmann equation and to replace the discrete values $f(x,\, t)$ of cellular automata by a distribution of particle f_j parametrized by discrete velocities $v_j \in \mathcal{V}$, $0 \leq j \leq J$. In the following, we will denote by $J+1$ the number of discrete velocities : $J = \sharp\mathcal{V} - 1$, in order to label with number "0" the null velocity. At discrete time t, the state of lattice $\mathcal{L}$ is now a field of the form

$$\mathcal{L}^0 \ni x \longmapsto f_j(x,\, t) \in \mathbb{R}, \qquad 0 \leq j \leq J\,, \quad v_j \in \mathcal{V} \tag{1.6}$$

and the question is to define the iteration $f_\bullet(\bullet,\, t) \longrightarrow f_\bullet(\bullet,\, t+\Delta t)$ in order to "mimic" the evolution of particle distribution f through the Boltzmann equation (1.1). Then Higuera, Succi and Benzi (1989) proposed to use a BGK approximation of the type (1.2) for the collision operator and Qian, D'Humières and Lallemand (1992) introduced a polynomial equilibrium distribution $f^{\rm eq}$. Due to all these modifications, the cellular automata have been replaced by the so-called Lattice Boltzmann Equation ("LBE"). We prefer the denomination of "lattice Boltzmann scheme" to emphasize that the result of all this work is a numerical method. Such a scheme contains classically two steps: *(i)* a relaxation step where distribution f at vertex x is locally modified into a new distribution f^* and *(ii)* an advection step (the advection equation obtained by neglecting $Q(f)$ in right hand side of equation (1.1)), based on method of characteristic as an **exact** time integration operator (due to (1.4)). Then the scheme can finally be written as:

$$(1.7) \qquad f_j(x,\, t+\Delta t) \,=\, f_j^*(x - v_j\, \Delta t,\, t)\,, \qquad v_j \in \mathcal{V}\,, \quad x \in \mathcal{L}^0\,.$$

We refer to Lallemand and Luo (2000) or to our lecture notes (2007) for detailed explanation of this approach.

• In what follows, we present in the second section the lattice Boltzmann scheme we are studying. We propose to call it Lattice Boltzmann "DDH" scheme in honor of his inventor (D. D'Humières, 1992) instead of the expression "multiple relaxation times" often used as in D'Humières *at al* (2002). In order to analyse this algorithm, the community of lattice Boltzmann schemes intensively use Chapman-Enskog expansions that are not very natural in our opinion in the framework of a completely discretized scheme. We refer for this approach to D'Humières (1992) and to the new point of view proposed by Junk and Rheinländer (2007). We prefer to use the method of equivalent partial differential equation proposed by Lerat and Peyret (1974) and Warming and Hyett (1974) to put in evidence formally the conservation equations that are present under the lattice Boltzmann scheme. The section 3 is devoted to technical lemmas and in section 4, we extend to third order the second order development that we have published in ESAIM (2007) and after the second ICMMES conference (2008). We propose to apply previous ideas to advective thermics in section 5 and diffusive acoustics in section 6.

2) Lattice Boltzmann DDH scheme

• We consider in this contribution a lattice $\mathcal{L}$ included in d-dimensional space $\mathbb{R}^d$ and a discrete velocity set $\mathcal{V}$ composed by $q \equiv J+1$ elements in such a way that $\mathcal{L}$ is invariant by translation. On one hand, set $\mathcal{V}$ does not depend on vertex $x \in \mathcal{L}^0$ and on the other hand the relation (1.4) holds.

In order to define a "DdQq" lattice Boltzmann scheme, two steps have to be defined: relaxation step and advection step. The relaxation step $f \longmapsto f^*$ is local in space and *a priori* nonlinear. The advection step (1.7) couples linearly a vertex x with its neighbors $x + v_j \, \Delta t$ for $0 \leq j \leq J$. All difficulties are concentrated in the relaxation step that we precise now.

• We recall that $f_j(x,\, t)$ is the number of particles at position x and discrete time t with discrete velocity v_j of components v_j^α. We denote by $f(x,\, t)$ the vector of components $f_j(x,\, t)$, $j = 0, \ldots, J$. We construct in this section a matrix M in order to transform linearly the vector f into a so-called vector of momenta. These momenta can be conserved or not. First we introduce two candidates for possible conservation: total sum of particle distribution (or momentum of order zero) ρ

$$\rho(x,\, t) \,\equiv\, \sum_{j=0}^{J} f_j(x,\, t) \,\equiv\, m_0(x,\, t) \tag{2.1}$$

and momentum of first order q_α with $1 \leq \alpha \leq d$:

$$q_\alpha(x,\, t) \,\equiv\, \sum_{j=0}^{J} v_j^\alpha \, f_j(x,\, t) \,\equiv\, m_\alpha(x,\, t). \tag{2.2}$$

We set $M_{0j} \equiv 1$ and $M_{\alpha j} \equiv v_j^\alpha$ for $1 \leq \alpha \leq d$. We suppose that we have completed the matrix M into $(M_{k\,j})_{0 \leq j,\, k \leq J}$ in such a way that M is **invertible**. From particle distribution $f \in \mathbb{R}^q$ at vertex x and time t, D'Humières (1992) introduces the vector of momenta $m \in \mathbb{R}^q$ defined by

$$m_k \,=\, \sum_{j=0}^{J} M_{kj} \, f_j \,, \qquad 0 \leq k \leq J \,. \tag{2.3}$$

• The first N momenta are supposed to be at equilibrium. In this contribution, we restrict ourselves to the case $N = 1$ (only one conservation law!) and to the case $N = d + 1$, *i.e.* we suppose conservation of mass and momentum. For $0 \leq i \leq N - 1$, we have conservation of momentum number i during the relaxation process. The $i^{\rm o}$ momentum after relaxation, denoted by m_i^* is equal to m_i and by definition coincides with the equilibrium value $m_i^{\rm eq}$ also denoted by W_i:

$$m_i^* = m_i \equiv m_i^{\rm eq} \equiv W_i \,, \qquad 0 \leq i \leq N - 1 \,. \tag{2.4}$$

We construct with the above hypothesis a **conserved vector** $W \in \mathbb{R}^N$. For $k \geq N$, the momentum m_k is **not** at thermodynamical equilibrium. It relaxes towards an equilibrium value $m_k^{\rm eq}$ which is a **given** nonlinear function ψ_k of vector W of conserved variables:

(2.5) $\qquad m_k^{\rm eq} \equiv \psi_k(W)\,, \qquad k \geq N.$

We suppose with D'Humières that the collision operator $f \longmapsto f^*$ is **diagonal** in the basis of m_k. This property express that the vectors m_k are eigenvectors of some approximation of the linearized collision operator S introduced in relations (1.2) and (1.3). In consequence strong physical constraints are imposed on matrix M. Due to this hypothesis, the value of m_k^* after collision is given according to

(2.6) $\qquad m_k^* = (1 - s_k)\, m_k + s_k\, m_k^{\rm eq}\,, \qquad k \geq N\,, \qquad s_k > 0.$

Remark that $s_k < 0$ is excluded because it corresponds to a repulsion by $m_k^{\rm eq}$ and $s_k = 0$ refers to equilibrium, considered by convention for the other indices. It is classical (see *e.g.* Lallemand and Luo, 2000) that $s_k \leq 2$ for stability of forward Euler scheme (2.6). After relaxation, distribution f^* is re-constructed thanks to elementary linear algebra:

(2.7) $$f_j^* \,=\, \sum_{\ell=0}^{J} M_{j\ell}^{-1}\, m_\ell^*\,, \qquad 0 \leq j \leq J\,.$$

3) Tensor of momentum-velocity

• Following our previous contributions (2007, 2008), we introduce the so-called "tensor of momentum-velocity" Λ_{kp}^ℓ according to

(3.1) $$\Lambda_{kp}^\ell \equiv \sum_{j=0}^{J} M_{kj}\, M_{pj}\, (M^{-1})_{j\ell}\,, \qquad 0 \leq k,\, p,\, \ell \leq J\,.$$

We introduce in this contribution its two "little brothers" Z_{kpq}^ℓ and Ξ_{kpqr}^ℓ defined according to

(3.2) $$Z_{kpq}^\ell \equiv \sum_{j=0}^{J} M_{kj}\, M_{pj}\, M_{qj}\, (M^{-1})_{j\ell}\,, \qquad 0 \leq k,\, p,\, q,\, \ell \leq J\,,$$

(3.3) $$\Xi_{kpqr}^\ell \equiv \sum_{j=0}^{J} M_{kj}\, M_{pj}\, M_{qj}\, M_{rj}\, (M^{-1})_{j\ell}\,, \qquad 0 \leq k,\, p,\, q,\, r,\, \ell \leq J\,.$$

Due to the hypothesis $M_{0j} \equiv 1$, we have the following elementary properties:

(3.4) $\qquad \Lambda_{0p}^\ell \,=\, \delta_p^\ell\,, \qquad 0 \leq p,\, \ell \leq J\,,$

(3.5) $\qquad Z_{0pq}^\ell \,=\, \Lambda_{pq}^\ell\,, \qquad 0 \leq p,\, q,\, \ell \leq J\,,$

(3.6) $\qquad \Xi_{0pqr}^\ell \,=\, Z_{pqr}^\ell\,, \qquad 0 \leq p,\, q,\, r,\, \ell \leq J\,.$

We have also the not so intuitive following property.

Proposition 1. Algebraic property.
The tensors Λ, Z and Ξ satisfy the two following relations:

$$\sum_r \Lambda_{kp}^r \, \Lambda_{rq}^\ell \;=\; Z_{kpq}^\ell \,, \qquad 0 \leq k,\, p,\, q,\, \ell \leq J \,. \tag{3.7}$$

$$\sum_{s,t} \Lambda_{kp}^s \, \Lambda_{sq}^t \, \Lambda_{tr}^\ell \;=\; \Xi_{kpqr}^\ell \,, \qquad 0 \leq k,\, p,\, q,\, r,\, \ell \leq J \,. \tag{3.8}$$

Proof of Proposition 1.
We replace the tensor Λ in left hand side of relation (3.7) by its definition (3.1):

$$\begin{aligned}\sum_r \Lambda_{kp}^r \, \Lambda_{rq}^\ell \;&=\sum_{r,j,\nu} M_{kj}\, M_{pj}\, M_{jr}^{-1}\, M_{r\nu}\, M_{q\nu}\, M_{\nu\ell}^{-1} \\ &= \sum_{j,\nu} M_{kj}\, M_{pj}\, \delta_{j\nu}\, M_{q\nu}\, M_{\nu\ell}^{-1} \\ &= \sum_j M_{kj}\, M_{pj}\, M_{qj}\, M_{j\ell}^{-1} \quad = \quad Z_{kpq}^\ell \qquad \text{due to definition (3.2).}\end{aligned}$$

We use a similar methodology for left hand side of (3.8):

$$\begin{aligned}\sum_{s,t} \Lambda_{kp}^s \, \Lambda_{sq}^t \, \Lambda_{tr}^\ell \;&= \sum_{s,t,j,\nu,\mu} M_{kj}\, M_{pj}\, M_{js}^{-1}\, M_{s\nu}\, M_{q\nu}\, M_{\nu t}^{-1}\, M_{t\mu}\, M_{r\mu}\, M_{\mu\ell}^{-1} \\ &= \sum_{j,\nu\mu} M_{kj}\, M_{pj}\, \delta_{j\nu}\, M_{q\nu}\, \delta_{\nu\mu}\, M_{r\mu}\, M_{\mu\ell}^{-1} \\ &= \sum_j M_{kj}\, M_{pj}\, M_{qj}\, M_{rj}\, M_{j\ell}^{-1} \quad = \quad \Xi_{kpqr}^\ell\end{aligned}$$

using simply definition (3.3). □

4) Equivalent equations of Lattice Boltzmann DDH scheme

• We adopt the Einstein convention of implicit summation of repeted indices. Recall that roman letters have to be summed over integer indices from 0 to J whereas greak letters refer to the dimension and are summed from 1 to d. We consider a lattice Boltzman DDH scheme defined by number N of conserved quantities, an invertible matrix M and linear transformation (2.3) between particle distribution f and momenta m, equilibrium functions

$$\mathbb{R}^N \ni W \longmapsto \psi_k(W) \in \mathbb{R} \,, \qquad k \geq N \,, \tag{4.1}$$

that define the equilibrium momenta $m_k^{\rm eq}$ according to (2.5), the discrete relaxation step (2.4)-(2.6) and the final advective step (1.7). In what follows, we fix the geometrical and topological structure of lattice $\mathcal{L}$, we fix the matrix M and the equilibrium function $\psi_k(\bullet)$, and last but not least, we suppose that parameters s_k for $k \geq N$ have a fixed value. Then the whole lattice Boltzmann scheme depends on a 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 and Peyret (1974) and Warming and Hyett (1974). This approach is based on the assumption, that a sufficiently smooth function exists which satisfies the difference equation at the grid points. The idea of the calculus is to suppose that all the data are sufficiently regular and to expand all the variables with Taylor formula. We have the following general framework:

Proposition 2. General development at third order of accuracy.
With the lattice Boltzmann precised previously, we have the following formal development:

$$(4.2) \quad \left\{ \begin{aligned} & m^k \,+\, \Delta t \; \partial_t m^k \,+\, \frac{1}{2}\,\Delta t^2 \; \partial_t^2 m^k \,+\, \frac{1}{6}\,\Delta t^3 \; \partial_t^3 m^k \,+\, \mathrm{O}(\Delta t^4) \,= \\ & \quad = \, m_k^* \,-\, \Delta t \, \Lambda_{k\alpha}^{\ell} \, \partial_\alpha m_\ell^* \,+\, \frac{\Delta t^2}{2} \, Z_{k\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta m_\ell^* \\ & \qquad \qquad -\, \frac{\Delta t^3}{6} \, \Xi_{k\alpha\beta\gamma}^{\ell} \, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^* \,+\, \mathrm{O}(\Delta t^4) \,, \qquad 0 \leq k \leq J \,. \end{aligned} \right.$$

Proof of Proposition 2.
We apply matrix M (relation (2.3)) to the scheme (1.7) and obtain in this way:

$$\begin{aligned} m_k(t + \Delta t) \, &= \, \sum_j M_{kj} \, f_j^*(x - v_j \Delta t) \, = \, \sum_{j\ell} M_{kj} \, M_{j\ell}^{-1} \, m_\ell^*(x - v_j \Delta t) \\ &= \sum_{j\ell} M_{kj} \, M_{j\ell}^{-1} \Big[m_\ell^* \,-\, \Delta t \, v_j^\alpha \, \partial_\alpha m_\ell^* \,+\, \frac{\Delta t^2}{2} \, v_j^\alpha \, v_j^\beta \, \partial_\alpha \partial_\beta m_\ell^* \\ & \qquad \qquad -\, \frac{\Delta t^3}{6} \, v_j^\alpha \, v_j^\beta \, v_j^\gamma \, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^* \,+\, \mathrm{O}(\Delta t^4) \Big] \\ &= \sum_{j\ell} M_{kj} \, M_{j\ell}^{-1} \Big[m_\ell^* \,-\, \Delta t \, M_{\alpha j} \, \partial_\alpha m_\ell^* \,+\, \frac{\Delta t^2}{2} \, M_{\alpha j} \, M_{\beta j} \, \partial_\alpha \partial_\beta m_\ell^* \\ & \qquad \qquad -\, \frac{\Delta t^3}{6} \, M_{\alpha j} \, M_{\beta j} \, M_{\gamma j} \, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^* \,+\, \mathrm{O}(\Delta t^4) \Big] \end{aligned}$$

$$= m_k^* - \Delta t\, \Lambda_{k\alpha}^\ell\, \partial_\alpha m_\ell^* + \frac{\Delta t^2}{2}\, Z_{k\alpha\beta}^\ell\, \partial_\alpha \partial_\beta m_\ell^* - \frac{\Delta t^3}{6}\, \Xi_{k\alpha\beta\gamma}^\ell\, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^* + \mathrm{O}(\Delta t^4)$$

and the result comes from a classical Taylor expansion of left hand side of relation (1.7). □

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

$$f_j(x,\, t) = f_j^{\mathrm{eq}}(x,\, t) + \mathrm{O}(\Delta t) = f_j^*(x,\, t) + \mathrm{O}(\Delta t)\,, \quad 0 \le j \le J\,, \tag{4.3}$$

$$m_k(x,\, t) = m_k^{\mathrm{eq}}(x,\, t) + \mathrm{O}(\Delta t) = m_k^*(x,\, t) + \mathrm{O}(\Delta t)\,, \quad 0 \le k \le J\,. \tag{4.4}$$

Proof of Proposition 3.
The relation (4.4) is clear for $k < N$ due to (2.4). If $k \ge N$, we apply the relation (4.2) by restricting ourselves to order zero and we get:

$$m_k = m_k^* + \mathrm{O}(\Delta t)\,, \quad k \ge N\,. \tag{4.5}$$

The relation (4.5) joined with (2.6) clearly implies (4.4). Then (4.3) is a consequence of (4.4) by applying the fixed matrix M^{-1}. □

• We split now our study into two cases to take into account the number N of conservation laws. We begin by the (simpler ?) case $N = 1$ and we will refer to it as the "thermal problem" even if we still denote by ρ the associated conservative variable, instead of total energy in a correct physically speaking way. Then the first momentum q_α is not at equilibrium and we denote by q_α^{eq} its equilibrium value. It is a (*a priori* nonlinear) fonction of the only conservative variable ρ defined in (2.1). When $N = d + 1$, we have an equilibrium for first momentum q and we have simply $q_\alpha^{\mathrm{eq}} \equiv q_\alpha$.

Proposition 4. First order expansion of mass conservation law.
With the lattice Boltzmann scheme previously defined, we have the conservation of mass at first order:

$$\partial_t \rho + \partial_\alpha q_\alpha^{\mathrm{eq}} = \mathrm{O}(\Delta t)\,. \tag{4.6}$$

When $N = d + 1$, $q_\alpha^{\mathrm{eq}} = q_\alpha$ in relation (4.6).

Proof of Proposition 4.
We have from the relation (4.2) at the order one applied with $k = 0$:

$$\rho + \Delta t\, \partial_t \rho + \mathrm{O}(\Delta t^2) = \rho - \Delta t\, \Lambda_{0\alpha}^\ell\, \partial_\alpha m_\ell^* + \mathrm{O}(\Delta t^2)$$

and due to (3.4) and (4.4),

$$\Lambda_{0\alpha}^{\ell} \, \partial_\alpha m_\ell^* \,=\, \delta_\alpha^\ell \, \partial_\alpha m_\ell^{\rm eq} \,+\, {\rm O}(\Delta t) \,=\, \partial_\alpha q_\alpha^{\rm eq} \,+\, {\rm O}(\Delta t) \,.$$

The relation (4.6) is established. □

Proposition 5. Nonequilibrium momenta at first order.

For $k \geq N$, we introduce the so-called "defect of conservation" according to

(4.7) $$\theta_k \equiv \partial_t m_k^{\rm eq} \,+\, \Lambda_{k\alpha}^{\ell} \, \partial_\alpha m_\ell^{\rm eq} \,, \qquad k \geq N$$

and the viscosity coefficient

(4.8) $$\sigma_k \equiv \frac{1}{s_k} - \frac{1}{2} \,, \qquad k \geq N$$

that defines a number σ_k which is positive due to stability condition $s_k \leq 2$. We have the following first order expansion of nonconservative momenta m_k and associated momentum m_k^* after relaxation step:

(4.9) $$m_k \,=\, m_k^{\rm eq} \,-\, \Delta t \left(\frac{1}{2} + \sigma_k \right) \theta_k \,+\, {\rm O}(\Delta t^2) \,, \qquad k \geq N$$

(4.10) $$m_k^* \,=\, m_k^{\rm eq} \,+\, \Delta t \left(\frac{1}{2} - \sigma_k \right) \theta_k \,+\, {\rm O}(\Delta t^2) \,, \qquad k \geq N \,.$$

Proof of Proposition 5.

We consider relation (4.2) up to first order accuracy with the hypothesis that $k \geq N$ *i.e.* $m_k \neq m_k^*$:

$$m_k \,+\, \Delta t \, \partial_t m_k \,+\, {\rm O}(\Delta t^2) \,=\, m_k^* \,-\, \Delta t \, \Lambda_{k\alpha}^{\ell} \, \partial_\alpha m_\ell^* \,+\, {\rm O}(\Delta t^2) \,.$$

Then we use definition (2.6) of momentum m_k^* after relaxation:

$$s_k \, (m_k - m_k^{\rm eq}) \,=\, m_k \,-\, m_k^* \,=\, -\Delta t \Big(\partial_t m_k^{\rm eq} \,+\, \Lambda_{k\alpha}^{\ell} \, \partial_\alpha m_\ell^{\rm eq} \Big) \,+\, {\rm O}(\Delta t^2)$$

and obtain the intermediate relation (see also our contribution, 2007)

$$m_k \,=\, m_k^{\rm eq} \,-\, \frac{\Delta t}{s_k} \theta_k \,+\, {\rm O}(\Delta t^2) \,.$$

Then relation (4.9) is an elementary consequence of (4.8). After relaxation we use again relation (2.6) and obtain

$$m_k^* \,=\, (1 - s_k) \, m_k \,+\, s_k \, m_k^{\rm eq} \,=\, m_k^{\rm eq} \,+\, \Delta t \left(1 - \frac{1}{s_k} \right) \theta_k \,+\, {\rm O}(\Delta t^2) \,.$$

Thus relation (4.10) is a direct consequence of previous relation and (4.8). □

• The viscosity coefficient $\sigma_k \equiv \frac{1}{s_k} - \frac{1}{2}$ has been introduced by Hénon (1987) in the context of cellular automata. It has been re-discovered and explicited for lattice Boltzmann scheme by D'Humières (1992).

• The defect of conservation θ_k has a natural interpretation in terms of Chapman-Enskog expansion. Consider Δt as an infinitesimal parameter classically denoted as ϵ (see *e.g.* D'Humières (1992) and introduce the associated Chapman-Enskog expansion for the discrete particle distribution f_j :

(4.11) $$f_j \,=\, f_j^{\rm eq} \,+\, \Delta t \; f_j^1 \,+\, {\rm O}(\Delta t^2) \,.$$

In terms of moments m_k, we have after the linear mapping (2.3):

(4.12) $$m_k \,=\, m_k^{\rm eq} \,+\, \Delta t \; m_k^1 \,+\, {\rm O}(\Delta t^2) \,.$$

If the moment of label k is at equilibrium ($k < N$), we have from relation (2.4) $m_k \equiv m_k^{\rm eq}$ and in consequence

(4.13) $$m_k^1 \,\equiv\, 0 \,, \qquad k < N \,.$$

If moment m_k is not at thermodynamical equilibrium, expansions (4.12) and (4.9) are necessarily identical and it comes taking into account (4.8)

(4.14) $$m_k^1 \,=\, -\frac{1}{s_k} \, \theta_k \,, \qquad k \geq N \,.$$

The defects of conservation $(\theta_k)_{k\geq N}$ naturally define the first order term in Chapman Enskog development of lattice Boltzmann scheme parametrized by the time step Δt.

Proposition 6. Second order expansion of mass conservation law.
With the lattice Boltzmann scheme previously defined, we have the conservation of mass at second order:

(4.15) $$\partial_t \rho \,+\, \partial_\alpha q_\alpha^{\rm eq} \,-\, \Delta t \, \sigma_\alpha \, \partial_\alpha \theta_\alpha \,=\, {\rm O}(\Delta t^2) \,.$$

When $N = d+1$, relation (4.15) is equivalent to

(4.16) $$\partial_t \rho \,+\, \partial_\alpha q_\alpha \,=\, {\rm O}(\Delta t^2) \,.$$

Proof of Proposition 6.

• We first evaluate second order time derivative of density as a function of space derivatives. We differentiate relation (4.6) relatively to time and relation (4.7) with $k = \alpha$ relatively to space. We obtain

$${\rm O}(\Delta t) \,=\, \partial_t^2 \rho \,+\, \partial_\alpha \partial_t q_\alpha^{\rm eq} \,=\, \partial_t^2 \rho \,+\, \partial_\alpha \left(\theta_\alpha \,-\, \Lambda_{\alpha\beta}^\ell \, \partial_\beta m_\ell^{\rm eq} \right)$$

and we deduce the intermediate lemma:

(4.17) $$\partial_t^2 \rho \,+\, \partial_\alpha \theta_\alpha \,-\, \Lambda_{\alpha\beta}^\ell \, \partial_\alpha \partial_\beta m_\ell^{\rm eq} \,=\, {\rm O}(\Delta t) \,.$$

• We now apply relation (4.2) up to second order accuracy with $i = 0$:

$$\rho + \Delta t \, \partial_t \rho + \frac{\Delta t^2}{2} \, \partial_t^2 \rho + {\rm O}(\Delta t^3) \,=\, \rho - \Delta t \, \partial_\alpha q_\alpha^* + \frac{\Delta t^2}{2} \, Z_{0\alpha\beta}^\ell \, \partial_\alpha \partial_\beta m_\ell^* + {\rm O}(\Delta t^3).$$

We have according to (4.10) with $k = \alpha$:

$$q_\alpha^* \,=\, q_\alpha^{\rm eq} \,+\, \Delta t \left(\frac{1}{2} - \sigma_\alpha\right) \theta_\alpha \,+\, {\rm O}(\Delta t^2)$$

and we use relation (3.5) to simplify the expression of $Z_{0\alpha\beta}^\ell$. It comes

$$Z_{0\alpha\beta}^\ell \, \partial_\alpha \partial_\beta m_\ell^* \,=\, \Lambda_{\alpha\beta}^\ell \, \partial_\alpha \partial_\beta m_\ell^{\rm eq} \,+\, {\rm O}(\Delta t) \,.$$

We inject also relation (4.17) for second time derivative of density up to first order. We deduce:

$$\partial_t \rho \,+\, \frac{\Delta t}{2} \left(\Lambda_{\alpha\beta}^\ell \, \partial_\alpha \partial_\beta m_\ell^{\rm eq} \,-\, \partial_\alpha \theta_\alpha \right) \,+\, {\rm O}(\Delta t^2) \,=$$
$$= \, -\partial_\alpha \Big[q_\alpha^{\rm eq} \,+\, \Delta t \left(\frac{1}{2} - \sigma_\alpha\right) \theta_\alpha \Big] \,+\, \frac{\Delta t}{2} \, \Lambda_{\alpha\beta}^\ell \, \partial_\alpha \partial_\beta m_\ell^{\rm eq} \,+\, {\rm O}(\Delta t^2)$$

and relation (4.15) is a simple consequence of the previous equation and relation (3.7). When momenta q_α are at equilibrium ($N = d+1$), the "defect of conservation" θ_α is of order ${\rm O}(\Delta t)$ and the term $\Delta t \, \sigma_\alpha \, \partial_\alpha \theta_\alpha$ inside equation (4.15) is of order ${\rm O}(\Delta t^2)$. Thus relation (4.16) is proven and the proposition is established. □

Proposition 7. Nonequilibrium momenta at second order.
We can be more specific about relations (4.9) and (4.10) up to second order accuracy for non-conserved momenta, *i.e.* $k \geq N$:

(4.18) $$m_k \,=\, m_k^{\rm eq} - \Delta t \, (\tfrac{1}{2} + \sigma_k) \left[\theta_k - \Delta t \left(\sigma_k \, \partial_t \theta_k + \sigma_\ell \, \Lambda_{k\alpha}^\ell \, \partial_\alpha \theta_\ell \right) \right] + {\rm O}(\Delta t^3)$$

(4.19) $$m_k^* \,=\, m_k^{\rm eq} + \Delta t \, (\tfrac{1}{2} - \sigma_k) \left[\theta_k - \Delta t \left(\sigma_k \, \partial_t \theta_k + \sigma_\ell \, \Lambda_{k\alpha}^\ell \, \partial_\alpha \theta_\ell \right) \right] + {\rm O}(\Delta t^3) \,.$$

Proof of Proposition 7.
We consider relation (4.2) up to second order accuracy:

$$m_k \,+\, \Delta t \, \partial_t m_k \,+\, \frac{\Delta t^2}{2} \, \partial_t^2 m_k \,+\, {\rm O}(\Delta t^3) \,=$$
$$= \, m_k^* \,-\, \Delta t \, \Lambda_{k\alpha}^\ell \, \partial_\alpha m_\ell^* \,+\, \frac{\Delta t^2}{2} \, Z_{k\alpha\beta}^\ell \, \partial_\alpha \partial_\beta m_\ell^* \,+\, {\rm O}(\Delta t^3) \,.$$

We transform the expression $\partial_t^2 m_k$ by deriving in time the expression (4.7). It comes

$$\partial_t^2 m_k^{\rm eq} \,=\, \partial_t \big(\theta_k - \Lambda_{k\alpha}^p \, \partial_\alpha m_p^{\rm eq} \big) \,=\, \partial_t \theta_k \,-\, \Lambda_{k\alpha}^p \, \partial_\alpha \big(\theta_p - \Lambda_{p\beta}^\ell \, \partial_\beta m_\ell^{\rm eq} \big)$$

with implicit summation over repeted indices. Then from relaxation definition (2.6), we obtain

$$s_k \, (m_k - m_k^{\rm eq}) \,=\, m_k \,-\, m_k^* \,=\, -\Delta t \, \partial_t \left[m_k^{\rm eq} \,-\, \Delta t \left(\frac{1}{2} + \sigma_k \right) \theta_k \right]$$

$$
\begin{aligned}
& - \frac{\Delta t^2}{2} \Big(\partial_t \theta_k \,-\, \Lambda_{k\alpha}^{\ell} \, \partial_\alpha \theta_\ell \,+\, \Lambda_{k\alpha}^{p} \, \Lambda_{p\beta}^{\ell} \, \partial_\alpha \partial_\beta m_\ell^{\rm eq} \Big) \\
& - \Delta t \, \Lambda_{k\alpha}^{\ell} \, \partial_\alpha \Big[m_\ell^{\rm eq} \,+\, \Delta t \Big(\frac{1}{2} - \sigma_\ell \Big) \, \theta_\ell \Big] \,+\, \frac{\Delta t^2}{2} \, Z_{k\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta m_\ell^{\rm eq} \,+\, {\rm O}(\Delta t^3) \\
& = \, -\Delta t \, \theta_k \,+\, \Delta t^2 \, \sigma_k \, \partial_t \theta_k \,+\, \Delta t^2 \, \sigma_\ell \, \Lambda_{k\alpha}^{\ell} \, \partial_\alpha \theta_\ell \,+\, {\rm O}(\Delta t^3)
\end{aligned}
$$

by taking into account relations (4.7) and (3.7). Then relation (4.18) is a direct consequence of above expression and of first order development (4.9). The expresion (4.19) of momentum of order k after relaxation step follows from analogous considerations. □

Proposition 8. Third order mass conservation for thermal problem. When only one conservation is present ($N = 1$), conservation of mass (4.15) admits the following expression up to third order accuracy:

$$
(4.20) \qquad \left\{ \begin{aligned}
& \partial_t \rho \,+\, \partial_\alpha q_\alpha^{\rm eq} \,-\, \Delta t \, \sigma_\alpha \, \partial_\alpha \theta_\alpha \,+\, \Delta t^2 \, \Big[\Big(\sigma_\alpha^2 - \frac{1}{6} \Big) \, \partial_\alpha \partial_t \theta_\alpha \,+ \\
& \qquad \qquad + \Big(\sigma_\alpha \, \sigma_\ell - \frac{1}{12} \Big) \, \Lambda_{\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta \theta_\ell \Big] \,=\, {\rm O}(\Delta t^3) \, .
\end{aligned} \right.
$$

Proof of Proposition 8.

• We first establish a second order accurate expression to second order time derivative $\partial_t^2 \rho$ and a first order expression for third order time derivative $\partial_t^3 \rho$. We have by derivation of (4.15) relatively to time:

$$
\partial_t^2 \rho \,+\, \partial_\alpha \partial_t q_\alpha^{\rm eq} \,-\, \Delta t \, \sigma_\alpha \, \partial_\alpha \partial_t \theta_\alpha \,=\, {\rm O}(\Delta t^2) \, .
$$

Then by inserting inside the previous expression derivation towards space of relation (4.7):

$$
\partial_t^2 \rho \,+\, \partial_\alpha \Big(\theta_\alpha - \Lambda_{\alpha\beta}^{\ell} \, \partial_\beta m_\ell^{\rm eq} \Big) \,-\, \Delta t \, \sigma_\alpha \, \partial_\alpha \partial_t \theta_\alpha \,=\, {\rm O}(\Delta t^2)
$$

we obtain

$$
(4.21) \qquad \partial_t^2 \rho \,+\, \partial_\alpha \theta_\alpha \,-\, \Lambda_{\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta m_\ell^{\rm eq} \,-\, \Delta t \, \sigma_\alpha \, \partial_\alpha \partial_t \theta_\alpha \,=\, {\rm O}(\Delta t^2) \, .
$$

We now derive relatively to time relation (4.21) and neglect the last term:

$$
\partial_t^3 \rho \,+\, \partial_\alpha \partial_t \theta_\alpha \,-\, \Lambda_{\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta \, \Big(\theta_\ell - \Lambda_{\ell\gamma}^{p} \, \partial_\gamma m_p^{\rm eq} \Big) \,=\, {\rm O}(\Delta t)
$$

and we have established an expression of third order time derivative of density:

$$
(4.22) \qquad \partial_t^3 \rho \,+\, \partial_\alpha \partial_t \theta_\alpha \,-\, \Lambda_{\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta \, \theta_\ell \,+\, \Lambda_{\alpha\beta}^{p} \, \Lambda_{p\gamma}^{\ell} \, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^{\rm eq} \,=\, {\rm O}(\Delta t) \, .
$$

• We consider now the expression (4.2) up to third order in the particular case $i = 0$:

$$
\rho \,+\, \Delta t \, \partial_t \rho \,+\, \frac{\Delta t^2}{2} \, \partial_t^2 \rho \,+\, \frac{\Delta t^3}{6} \, \partial_t^3 \rho \,+\, {\rm O}(\Delta t^4) \,=
$$

$$= \rho - \Delta t \, \partial_\alpha q^*_\alpha + \frac{\Delta t^2}{2} \, Z^\ell_{0\alpha\beta} \, \partial_\alpha \partial_\beta m^*_\ell - \frac{\Delta t^3}{6} \, \Xi^\ell_{0\alpha\beta\gamma} \, \partial_\alpha \partial_\beta \partial_\gamma m^*_\ell + \mathrm{O}(\Delta t^4) \, .$$

We insert in left hand side the previous expressions (4.21) and (4.22) for high order time derivatives and in right hand side the momentum q^*_α with the help of (4.10). We take also into account remarks (3.5) and (3.6). We obtain:

$$\partial_t \rho + \frac{\Delta t}{2} \Big(- \partial_\alpha \theta_\alpha + \Lambda^\ell_{\alpha\beta} \, \partial_\alpha \partial_\beta m^{\mathrm{eq}}_\ell + \Delta t \, \sigma_\alpha \, \partial_\alpha \partial_t \theta_\alpha \Big)$$
$$+ \frac{\Delta t^2}{6} \Big(- \partial_\alpha \partial_t \theta_\alpha + \Lambda^\ell_{\alpha\beta} \, \partial_\alpha \partial_\beta \, \theta_\ell - \Lambda^p_{\alpha\beta} \, \Lambda^\ell_{p\gamma} \, \partial_\alpha \partial_\beta \partial_\gamma m^{\mathrm{eq}}_\ell \Big)$$
$$+ \partial_\alpha \Big[q^{\mathrm{eq}}_\alpha + \Delta t \Big(\frac{1}{2} - \sigma_\alpha \Big) \big[\theta_\alpha - \Delta t \, \big(\sigma_\alpha \, \partial_t \theta_\alpha + \sigma_\ell \, \Lambda^\ell_{\alpha\beta} \, \partial_\beta \theta_\ell \big) \big] \Big]$$
$$- \frac{\Delta t}{2} \, \Lambda^\ell_{\alpha\beta} \, \partial_\alpha \partial_\beta \Big[m^{\mathrm{eq}}_\ell + \Delta t \Big(\frac{1}{2} - \sigma_\ell \Big) \theta_\ell \Big] + \frac{\Delta t^2}{6} \, Z^\ell_{\alpha\beta\gamma} \, \partial_\alpha \partial_\beta \partial_\gamma m^{\mathrm{eq}}_\ell = \mathrm{O}(\Delta t^3) \, .$$

We simplify the above expression by taking into account relation (3.8). We obtain:

$$\partial_t \rho + \partial_\alpha q^{\mathrm{eq}}_\alpha - \Delta t \, \sigma_\alpha \, \partial_\alpha \theta_\alpha + \Delta t^2 \Big[\partial_\alpha \partial_t \theta_\alpha \Big(\frac{\sigma_\alpha}{2} - \frac{1}{6} - \sigma_\alpha \Big(\frac{1}{2} - \sigma_\alpha \Big) \Big) +$$
$$+ \Lambda^\ell_{\alpha\beta} \, \partial_\alpha \partial_\beta \theta_\ell \Big(\frac{1}{6} - \sigma_\ell \Big(\frac{1}{2} - \sigma_\alpha \Big) - \frac{1}{2} \Big(\frac{1}{2} - \sigma_\ell \Big) \Big) \Big] = \mathrm{O}(\Delta t^3)$$

and relation (4.20) is now a consequence of elementary algebra. □

• We focus now on the case of mass conservation and d momentum conservations ($N = d + 1$). Of course Proposition 3 is still valid and we have equilibrium at order zero (relations (4.3) and (4.4)).

Proposition 9. First order expansion of momentum conservation law.
With the lattice Boltzmann scheme previously defined and under the hypothesis $N = d + 1$ of conservation of mass and momentum, we have at first order

$$\partial_t q_\alpha + \Lambda^\ell_{\alpha\beta} \, \partial_\beta m^{\mathrm{eq}}_\ell = \mathrm{O}(\Delta t) \qquad 1 \leq \alpha \leq d \, . \tag{4.23}$$

Proof of Proposition 9.
We detail relation (4.2) at order one for $k = \alpha$. It comes

$$q_\alpha + \Delta t \, \partial_t q_\alpha + \mathrm{O}(\Delta t^2) = q_\alpha - \Delta t \, \Lambda^\ell_{\alpha\beta} \, \partial_\beta m^*_\ell + \mathrm{O}(\Delta t^2)$$

and conclusion (4.23) comes directly from (4.4). □

• We recall that, according to Proposition 6, conservation of mass can be written as (4.16) at second order of accuracy. Moreover, expression of nonequilibrium momenta at first order are still given according to relations (4.9) and (4.10). We can precise now the conservation of momentum up to second order.

Proposition 10. Second order expansion for momentum.
With the lattice Boltzmann scheme previously defined and under the hypothesis $N = d+1$ of conservation of mass and momentum, we have the following conservation of momentum at second order

$$\partial_t q_\alpha \,+\, \Lambda^\ell_{\alpha\beta}\, \partial_\beta m_\ell^{\rm eq} \,-\, \sigma_\ell \,\Delta t\, \Lambda^\ell_{\alpha\beta}\, \partial_\beta \theta_\ell = {\rm O}(\Delta t^2)\,, \qquad 1 \leq \alpha \leq d\,. \tag{4.24}$$

Proof of Proposition 10.

• We first precise second order time derivative of conserved variables. We have by derivation of (4.16) relatively to time and of (4.23) relatively to space:

$$\partial_t^2 \rho \,=\, \Lambda^\ell_{\alpha\beta}\, \partial_\alpha \partial_\beta \rho \,+\, {\rm O}(\Delta t)\,. \tag{4.25}$$

In an analogous way, we differentiate (4.23) relatively to time and replace $\partial_t m_\ell^{\rm eq}$ by expression obtained from definition (4.7):

$$\partial_t^2 q_\alpha \,+\, \Lambda^\ell_{\alpha\beta}\, \partial_\beta \left(\theta_\ell \,-\, \Lambda^p_{\ell\gamma}\, \partial_\gamma m_p^{\rm eq}\right) \,=\, {\rm O}(\Delta t)\,.$$

Then

$$\partial_t^2 q_\alpha \,=\, -\Lambda^\ell_{\alpha\beta}\, \partial_\beta \theta_\ell \,+\, \Lambda^p_{\alpha\beta}\, \Lambda^\ell_{p\gamma}\, \partial_\beta \partial_\gamma m_\ell^{\rm eq} \,+\, {\rm O}(\Delta t)\,. \tag{4.26}$$

• We consider now relation (4.2) with $k = \alpha$ up to second order accuracy:

$$q_\alpha \,+\, \Delta t\, \partial_t q_\alpha \,+\, \frac{\Delta t^2}{2}\, \partial_t^2 q_\alpha \,+\, {\rm O}(\Delta t^3) \,=$$

$$= q_\alpha \,-\, \Delta t\, \Lambda^\ell_{\alpha\beta}\, \partial_\beta m_\ell^* \,+\, \frac{\Delta t^2}{2}\, Z^\ell_{\alpha\beta\gamma}\, \partial_\beta \partial_\gamma m_\ell^* \,+\, {\rm O}(\Delta t^3)\,.$$

We substitute in the right hand side the expression (4.10) of momenta after relaxation:

$$\partial_t q_\alpha \,+\, \frac{\Delta t}{2} \Big(-\Lambda^\ell_{\alpha\beta}\, \partial_\beta \theta_\ell \,+\, \Lambda^p_{\alpha\beta}\, \Lambda^p_{p\gamma}\, \partial_\beta \partial_\gamma m_\ell^{\rm eq} \Big)$$

$$+ \Lambda^\ell_{\alpha\beta}\, \partial_\beta \Big[m_\ell^{\rm eq} \,+\, \Delta t \left(\frac{1}{2} - \sigma_\ell \right) \theta_\ell \Big] \,-\, \frac{\Delta t}{2}\, Z^\ell_{\alpha\beta\gamma}\, \partial_\beta \partial_\gamma m_\ell^{\rm eq} \,=\, {\rm O}(\Delta t^2)$$

and relation (4.24) is a direct consequence of identity (3.7). □

Proposition 11. Third order equivalent equations for fluid model.
When $N = d+1$ conservation laws are present, second order conservation of mass (4.16) and momentum (4.24) admit the following expressions up to third order accuracy:

$$\partial_t \rho + \sum_\alpha \partial_\alpha q_\alpha - \frac{\Delta t^2}{12} \sum_{\alpha\,\beta\,\ell} \Lambda^\ell_{\alpha\beta}\, \partial_\alpha \partial_\beta \theta_\ell \,=\, \mathrm{O}(\Delta t^3) \tag{4.27}$$

$$\left\{ \begin{aligned} & \partial_t q_\alpha \,+\, \sum_{\beta\,\ell} \Lambda^\ell_{\alpha\beta}\, \partial_\beta m^{\mathrm{eq}}_\ell - \sum_{\beta\,\ell} \sigma_\ell\, \Delta t\, \Lambda^\ell_{\alpha\beta}\, \partial_\beta \theta_\ell \\ & \qquad + \Delta t^2 \Big[\sum_{\beta\,\ell} \Big(\sigma_\ell^2 - \frac{1}{6} \Big) \Lambda^\ell_{\alpha\beta}\, \partial_t \partial_\beta \theta_\ell \\ & \qquad + \sum_{\beta\,\gamma\,p\,\ell} \Big(\sigma_\ell\, \sigma_p \,-\, \frac{1}{12} \Big) \Lambda^p_{\alpha\beta}\, \Lambda^\ell_{p\gamma}\, \partial_\beta \partial_\gamma \theta_\ell \Big] \,=\, \mathrm{O}(\Delta t^3)\,, \\ & \qquad\qquad\qquad\qquad\qquad\qquad 1 \leq \alpha \leq d\,. \end{aligned} \right. \tag{4.28}$$

Proof of Proposition 11.

• First, the nonconserved momenta still admit the developments (4.18) and (4.19) as previously. Second, we precise second order and third order time derivative of conserved variables. From (4.16) and (4.24), we have

$$\partial_t^2 \rho \,=\, \Lambda^\ell_{\alpha\beta}\, \partial_\alpha \partial_\beta m^{\mathrm{eq}}_\ell \,-\, \sigma_\ell\, \Delta t\, \Lambda^\ell_{\alpha\beta}\, \partial_\alpha \partial_\beta \theta_\ell \,+\, \mathrm{O}(\Delta t^2) \tag{4.29}$$

$$\partial_t^3 \rho \,=\, \Lambda^\ell_{\alpha\beta}\, \partial_\alpha \partial_\beta \theta_\ell \,-\, \Lambda^p_{\alpha\beta}\, \Lambda^\ell_{p\gamma}\, \partial_\alpha \partial_\beta \partial_\gamma m^{\mathrm{eq}}_\ell \,+\, \mathrm{O}(\Delta t) \tag{4.30}$$

$$\left\{ \begin{aligned} \partial_t^2 q_\alpha \,=\, & -\Lambda^\ell_{\alpha\beta}\, \partial_\beta \theta_\ell \,+\, \Lambda^p_{\alpha\beta}\, \Lambda^\ell_{p\gamma}\, \partial_\beta \partial_\gamma m^{\mathrm{eq}}_\ell \,+ \\ & \qquad + \sigma_\ell\, \Delta t\, \Lambda^\ell_{\alpha\beta}\, \partial_t \partial_\beta \theta_\ell \,+\, \mathrm{O}(\Delta t^2) \end{aligned} \right. \tag{4.31}$$

$$\left\{ \begin{aligned} \partial_t^3 q_\alpha \,=\, & -\Lambda^\ell_{\alpha\beta}\, \partial_t \partial_\beta \theta_\ell \,+\, \Lambda^p_{\alpha\beta}\, \Lambda^\ell_{p\gamma}\, \partial_\beta \partial_\gamma \theta_\ell \\ & \qquad - \Lambda^p_{\alpha\beta}\, \Lambda^q_{p\gamma}\, \Lambda^\ell_{q\zeta}\, \partial_\beta \partial_\gamma \partial_\zeta m^{\mathrm{eq}}_\ell \,+\, \mathrm{O}(\Delta t)\,. \end{aligned} \right. \tag{4.32}$$

• We look for development (4.2) when $i = 0$:

$$\begin{aligned} & \rho \,+\, \Delta t\, \partial_t \rho \,+\, \frac{\Delta t^2}{2}\, \partial_t^2 \rho \,+\, \frac{\Delta t^3}{6}\, \partial_t^3 \rho \,+\, \mathrm{O}(\Delta t^4) \,= \\ & \qquad = \, \rho - \Delta t\, \partial_\alpha q^*_\alpha + \frac{\Delta t^2}{2}\, Z^\ell_{0\alpha\beta}\, \partial_\alpha \partial_\beta m^*_\ell - \frac{\Delta t^3}{6}\, \Xi^\ell_{0\alpha\beta\gamma}\, \partial_\alpha \partial_\beta \partial_\gamma m^*_\ell + \mathrm{O}(\Delta t^4)\,. \end{aligned}$$

We replace $\partial_t^2 \rho$ and $\partial_t^3 \rho$ by their values (4.29) and (4.30) obtained from previous Taylor expansions, we use relations (3.5) and (3.6) and introduce development (4.19) for nonconserved momenta. We get

$$\begin{aligned} & \partial_t \rho \,+\, \frac{\Delta t}{2} \Big(\Lambda^\ell_{\alpha\beta}\, \partial_\alpha \partial_\beta m^{\mathrm{eq}}_\ell \,-\, \sigma_\ell\, \Delta t\, \Lambda^\ell_{\alpha\beta}\, \partial_\alpha \partial_\beta \theta_\ell \Big) \\ & \qquad + \frac{\Delta t^2}{6} \Big(\Lambda^\ell_{\alpha\beta}\, \partial_\alpha \partial_\beta \theta_\ell \,-\, \Lambda^p_{\alpha\beta}\, \Lambda^\ell_{p\gamma}\, \partial_\alpha \partial_\beta \partial_\gamma m^{\mathrm{eq}}_\ell \Big) \,+\, \partial_\alpha q_\alpha \end{aligned}$$

$$- \frac{\Delta t}{2} \, \Lambda^\ell_{\alpha\beta} \, \partial_\beta \partial_\gamma \left[m_\ell^{\rm eq} \, + \, \Delta t \left(\frac{1}{2} - \sigma_\ell \right) \theta_\ell \right] \, + \, \frac{\Delta t^2}{6} \, Z^\ell_{\alpha\beta\gamma} \, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^{\rm eq} \, = \, {\rm O}(\Delta t^3) \, .$$

First order terms vanish and we have a simplification due to (3.7). Coefficient of $\Lambda^\ell_{\alpha\beta} \, \partial_\alpha \partial_\beta \theta_\ell \, \Delta t^2$ is equal to $-\frac{\sigma_\ell}{2} + \frac{1}{6} + \frac{1}{2}\big(\sigma_\ell - \frac{1}{2}\big) = -\frac{1}{12}$ and relation (4.27) is established.

- We explicit relation (4.2) when $k = \alpha$:

$$q_\alpha \, + \, \Delta t \, \partial_t q_\alpha \, + \, \frac{\Delta t^2}{2} \, \partial_t^2 q_\alpha \, + \, \frac{\Delta t^3}{6} \, \partial_t^3 q_\alpha \, + \, {\rm O}(\Delta t^4) \, =$$
$$= q_\alpha - \Delta t \, \Lambda^\ell_{\alpha\beta} \, \partial_\beta m_\ell^* + \frac{\Delta t^2}{2} \, Z^\ell_{\alpha\beta\gamma} \, \partial_\beta \partial_\gamma m_\ell^* - \frac{\Delta t^3}{6} \, \Xi^\ell_{\alpha\beta\gamma\zeta} \, \partial_\beta \partial_\gamma \partial_\zeta m_\ell^* + {\rm O}(\Delta t^4).$$

We insert the expressions (4.31), (4.32) and (4.19) of $\partial_t^2 q_\alpha$, $\partial_t^3 q_\alpha$ and m_ℓ^* respectively inside the previous relation and we divide by Δt. We have

$$\partial_t q_\alpha \, + \, \frac{\Delta t}{2} \Big(- \Lambda^\ell_{\alpha\beta} \, \partial_\beta \theta_\ell \, + \, \Lambda^p_{\alpha\beta} \, \Lambda^\ell_{p\gamma} \, \partial_\beta \partial_\gamma m_\ell^{\rm eq} \, + \, \sigma_\ell \, \Delta t \, \Lambda^\ell_{\alpha\beta} \, \partial_t \partial_\beta \theta_\ell \Big)$$
$$+ \frac{\Delta t^2}{6} \Big(- \Lambda^\ell_{\alpha\beta} \, \partial_t \partial_\beta \theta_\ell \, + \, \Lambda^p_{\alpha\beta} \, \Lambda^\ell_{p\gamma} \, \partial_\beta \partial_\gamma \theta_\ell \, - \, \Lambda^p_{\alpha\beta} \, \Lambda^q_{p\gamma} \, \Lambda^\ell_{q\zeta} \, \partial_\beta \partial_\gamma \partial_\zeta m_\ell^{\rm eq} \Big)$$
$$+ \Lambda^\ell_{\alpha\beta} \, \partial_\beta \left[m_\ell^{\rm eq} \, + \, \Delta t \left(\frac{1}{2} - \sigma_\ell \right) \left[\theta_\ell \, - \, \Delta t \left(\sigma_\ell \, \partial_t \theta_\ell \, + \, \sigma_p \, \Lambda^p_{\ell\gamma} \, \partial_\gamma \theta_p \right) \right] \right]$$
$$- \frac{\Delta t}{2} \, Z^\ell_{\alpha\beta\gamma} \, \partial_\beta \partial_\gamma \left[m_\ell^{\rm eq} + \Delta t \left(\frac{1}{2} - \sigma_\ell \right) \theta_\ell \right] + \frac{\Delta t^2}{6} \, \Xi^\ell_{\alpha\beta\gamma\zeta} \, \partial_\beta \partial_\gamma \partial_\zeta m_\ell^{\rm eq} = {\rm O}(\Delta t^3).$$

We replace $Z^\ell_{\alpha\beta\gamma}$ and $\Xi^\ell_{\alpha\beta\gamma\zeta}$ by their values obtained from relations (3.7) and (3.8) and four terms are droped out by this way. The coefficient of $\Lambda^\ell_{\alpha\beta} \, \partial_t \partial_\beta \theta_\ell \, \Delta t^2$ is equal to $\frac{\sigma_\ell}{2} - \frac{1}{6} + \sigma_\ell \left(\sigma_\ell - \frac{1}{2} \right) = \sigma_\ell^2 - \frac{1}{6}$ and the coefficient of $\Lambda^p_{\alpha\beta} \, \Lambda^\ell_{p\gamma} \, \partial_\beta \partial_\gamma \theta_\ell \, \Delta t^2$ is simply: $\frac{1}{6} + \sigma_\ell \left(\sigma_p - \frac{1}{2} \right) + \frac{1}{2} \left(\sigma_\ell - \frac{1}{2} \right) = \sigma_\ell \, \sigma_p - \frac{1}{12}$. Then relation (4.28) is proven. □

- If we compare third order mass conservation (4.20) for a single conservation law and third order momentum conservation (4.28) for fluid flow, we observe analogous coefficients of the type $\sigma_\ell^2 - \frac{1}{6}$ and $\sigma_\ell \, \sigma_p - \frac{1}{12}$ related to the terms $\partial_t \partial_\beta \theta_\ell$ and $\partial_\beta \partial_\gamma \theta_\ell$ respectively. Relation (4.28) contains one more factor of the type "Λ" than relation (4.20). Nevertheless, a structure is clearly appearing!

5) Application to advective thermics

- We begin this application with the very simple one-dimensional model D1Q3 illustrated on Figure 1.

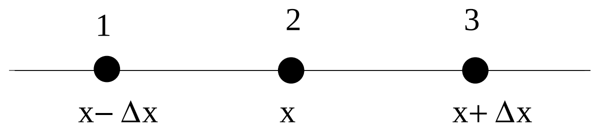

Figure 1. Neighboring nodes for D1Q3 lattice Boltzmann scheme.

In order to compare time step Δt and space step Δx, we introduce a velocity scale λ according to

$$\lambda \equiv \frac{\Delta x}{\Delta t} \,. \tag{5.1}$$

A vertex x is connected with itself and with its two neighbors $x - \Delta x$ and $x + \Delta x$. Three families of particles exist in this model: $f_0(x,\, t)$ with null velocity, $f_-(x,\, t)$ with velocity $-\lambda$ and $f_+(x,\, t)$ with velocity $+\lambda$. Density ρ is defined from the f's with the help of relation (2.1). There is only one component of momentum:

$$q \equiv -\lambda \, f_- \,+\, \lambda \, f_+ \,. \tag{5.2}$$

We choose internal energy according to

$$\epsilon \equiv \frac{\lambda^2}{2} \big(f_- \,+\, f_+ \big) \tag{5.3}$$

as the third momentum. In consequence, matrix M takes the form

$$M \,=\, \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \frac{\lambda^2}{2} & 0 & \frac{\lambda^2}{2} \end{pmatrix} \,. \tag{5.4}$$

It is therefore easy to explicit the tensor of mementum-velocity Λ defined at relation (3.1). We have for D1Q3 model

$$\Lambda^0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \, \Lambda^1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & \frac{\lambda^2}{2} \\ 0 & \frac{\lambda^2}{2} & 0 \end{pmatrix} , \, \Lambda^2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & \frac{\lambda^2}{2} \end{pmatrix} . \tag{5.5}$$

• The application of lattice Boltzmann framework for thermal problem has been intensively studied and we refer *e.g.* to the contributions of Chen, Ohashi and Akiyama (1994), Shan (1997), Chen-Doolen (1998) and Ginzburg (2005). In our particular case, the two last momenta q and ϵ are not conserved. We introduce a velocity $V \equiv v \, \lambda$ and a coefficient parameter ζ in order to precise equilibrium values. We restrict here to a linear case and these two equilibrium values are proportional to the only conservative variable (density):

$$q^{\rm eq} \,=\, v\,\lambda\,\rho\,, \qquad \epsilon^{\rm eq} \,=\, \zeta\,\frac{\lambda^2}{2}\,\rho\,. \tag{5.6}$$

Due to equilibrium values (5.6), defects of conservation θ introduced in (4.7) take the simple algebraic form

$$\theta_1 \,\equiv\, v\,\lambda\,\frac{\partial\rho}{\partial t} + \zeta\,\lambda^2\,\frac{\partial\rho}{\partial x}\,, \qquad \theta_2 \,\equiv\, \frac{\lambda^2}{2}\Big(\zeta\,\frac{\partial\rho}{\partial t} + v\,\lambda\,\frac{\partial\rho}{\partial x}\Big)\,. \tag{5.7}$$

We have also the relaxation parameters s_1, s_2 and the associated viscosity coefficients σ_1, σ_2 defined from the previous ones according to relation (4.8). Then relations (2.4) and (2.6) can be summarized in a single matricial relation. The momenta after relaxation satisfy

$$m^* \,=\, J_0 \bullet m\,, \tag{5.8}$$

with

$$J_0 \,=\, \begin{pmatrix} 1 & 0 & 0 \\ s_1\,v\,\lambda & 1-s_1 & 0 \\ \zeta\,s_2\,\frac{\lambda^2}{2} & 0 & 1-s_2 \end{pmatrix}\,. \tag{5.9}$$

Proposition 12. Third order equivalent equation for advective thermal D1Q3 lattice Boltzmann scheme.
With notations explicited previously, the D1Q3 scheme defined by (1.7), (2.3), (5.8) and (5.9) satisfy the following partial equivalent equation

$$\left\{ \begin{aligned} & \frac{\partial\rho}{\partial t} + v\,\lambda\,\frac{\partial\rho}{\partial x} - \sigma_1\,\Delta t\,\lambda^2\,(\zeta-v^2)\,\frac{\partial^2\rho}{\partial x^2} \\ & \qquad - \Delta t^2\,v\,\lambda^3\,\Big[2\,\Big(\sigma_1^2-\frac{1}{12}\Big)\,(\zeta-v^2) \\ & \qquad\qquad + \Big(\frac{1}{12}-\sigma_1\,\sigma_2\Big)\,(1-\zeta)\Big]\,\frac{\partial^3\rho}{\partial x^3} \,=\, {\rm O}(\Delta t^3)\,. \end{aligned} \right. \tag{5.10}$$

Proof of Proposition 12.
Due to (5.6) and (4.6), we write the equivalent equation at order one:

$$\frac{\partial\rho}{\partial t} + v\,\lambda\,\frac{\partial\rho}{\partial x} \,=\, {\rm O}(\Delta t)$$

and we report this expression to precise defects of equilibrium:

$$\theta_1 \,=\, (\zeta-v^2)\,\lambda^2\,\frac{\partial\rho}{\partial x} + {\rm O}(\Delta t)\,, \qquad \theta_2 \,=\, \frac{\lambda^3}{2}\,v\,(1-\zeta)\,\frac{\partial\rho}{\partial x} + {\rm O}(\Delta t)\,. \tag{5.11}$$

We replace expression (5.11) of θ_1 inside relation (4.15) and obtain mass conservation at second order:

$$\frac{\partial\rho}{\partial t} + v\,\lambda\,\frac{\partial\rho}{\partial x} - \sigma_1\,\Delta t\,\lambda^2\,(\zeta-v^2)\,\frac{\partial^2\rho}{\partial x^2} \,=\, {\rm O}(\Delta t^2)\,.$$

This expression for $\frac{\partial \rho}{\partial t}$ allows us to precise θ_1 defined in (5.7):

$$\theta_1 \,=\, (\zeta - v^2)\, \lambda^2 \, \frac{\partial \rho}{\partial x} \,+\, \sigma_1 \, \Delta t \, \lambda^2 \, (\zeta - v^2) \, \frac{\partial^2 \rho}{\partial x^2} \,+\, {\rm O}(\Delta t^2) \,. \qquad (5.12)$$

We use relation (5.11) for complementary third order terms of relation (4.20). Then conservation law at third order takes the form:

$$\frac{\partial \rho}{\partial t} + v \, \lambda \, \frac{\partial \rho}{\partial x} - \sigma_1 \, \Delta t \, \frac{\partial}{\partial x} \Big[(\zeta - v^2) \, \lambda^2 \, \frac{\partial \rho}{\partial x} + \sigma_1 \, \Delta t \, \lambda^2 \, (\zeta - v^2) \, \frac{\partial^2 \rho}{\partial x^2} \Big]$$
$$+ \Delta t^2 \, \bigg[\Big(\sigma_1^2 - \frac{1}{6} \Big) \, (-v \, \lambda) \, \lambda^2 \, (\zeta - v^2) \, \frac{\partial^3 \rho}{\partial x^3}$$
$$+ \Big(\sigma_1 \, \sigma_2 - \frac{1}{12} \Big) \, v \, \lambda^3 \, (1 - \zeta) \, \frac{\partial^2}{\partial x^2} \Big(\frac{\partial \rho}{\partial x} \Big) \bigg] \,=\, {\rm O}(\Delta t^3)$$

and relation (5.10) is a consequence of factorization of $\Delta t^2 \, v \, \lambda^3$ in the previous expression. □

• We consider now the lattice Boltzmann scheme for a two-dimensional application, with the so-called D2Q9 scheme. The vicinity of a node x in lattice $\mathcal{L}$ is represented on Figure 2. It is composed by x itself and the eight nodes around x following the axis and the diagonals of a square lattice.

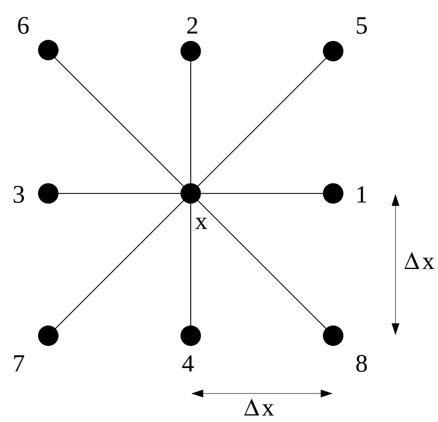

Figure 2. Neighboring nodes for the D2Q9 lattice Boltzmann scheme

The moments m satisfy relation (2.3) with a 9×9 matrix M classically (see Lallemand and Luo, 2000) given by the relation

$$
(5.13) \qquad M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & +1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix} .
$$

It is easy to evaluate the tensor of momentum-velocity Λ and we have explicited it at the Annex. We have in particular the following two by two blocs that correspond to the usefull data for relations (4.20), (4.27) and (4.28):

$$
(5.14) \qquad \begin{cases} \Lambda^0_{\alpha\beta} = \dfrac{2}{3}\,\lambda^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \ \Lambda^1_{\alpha\beta} = \Lambda^2_{\alpha\beta} = 0 \,, \ \Lambda^3_{\alpha\beta} = \dfrac{1}{6}\,\lambda^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \\ \Lambda^4_{\alpha\beta} = \Lambda^5_{\alpha\beta} = \Lambda^6_{\alpha\beta} = 0 \,, \ \Lambda^7_{\alpha\beta} = \dfrac{1}{2}\,\lambda^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \\ \Lambda^8_{\alpha\beta} = \lambda^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad\qquad 1 \leq \alpha, \, \beta \leq 2 \,. \end{cases}
$$

The equilibrium momenta are linear functions of the only conserved variable ρ. It is classical (see Lallemand and Luo, 2000) to observe that by a rotation of the coordinates, m^1 and m^2 are two components of a vector, m^3 and m^4 are two scalars, m^5 and m^6 are also two components of a vector (the momentum of order 3, defined from $\sum_j \, |v_j|^2 \; v_j \; f_j$, *id est* heat flux for fluid applications) and m^7 and m^8 are partial cordinates of a tensor of order two. We intoduce u and v as adimensionalized components of a given velocity and we set

$$
(5.15) \qquad q_x^{\rm eq} \,=\, u \, \lambda \, \rho \,, \quad q_y^{\rm eq} \,=\, v \, \lambda \, \rho \,.
$$

Due to the vectorial nature of m^5 and m^6, we complete this equilibrium distribution in setting *a priori*

$$
(5.16) \qquad m_5^{\rm eq} \,=\, a_5 \, u \, \rho \,, \qquad m_6^{\rm eq} \,=\, a_6 \, v \, \rho \,.
$$

We complete this equilibrium distribution in a very simple manner:

$$
(5.17) \qquad m_3^{\rm eq} \,=\, a_3 \, \rho \,, \quad m_4^{\rm eq} \,=\, a_4 \, \rho \,, \quad m_7^{\rm eq} \,=\, a_7 \, \rho \,, \qquad m_8^{\rm eq} \,=\, a_8 \, \rho \,.
$$

The momenta m^* after equilibrium satisfy the relation (5.8) with matrix J_0 that takes into account the *a priori* vectorial structure of equilibrium momenta thus in particular $s_1 = s_2$ and $s_5 = s_6$, and is given by the relation:

$$
(5.18) \quad J_0 = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
u\,\lambda\,s_1 & 1{-}s_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
v\,\lambda\,s_1 & 0 & 1{-}s_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
a_3\,s_3 & 0 & 0 & 1{-}s_3 & 0 & 0 & 0 & 0 & 0 \\
a_4\,s_4 & 0 & 0 & 0 & 1{-}s_4 & 0 & 0 & 0 & 0 \\
a_5\,u\,s_5 & 0 & 0 & 0 & 0 & 1{-}s_5 & 0 & 0 & 0 \\
a_6\,v\,s_5 & 0 & 0 & 0 & 0 & 0 & 1{-}s_5 & 0 & 0 \\
a_7\,s_7 & 0 & 0 & 0 & 0 & 0 & 0 & 1{-}s_7 & 0 \\
a_8\,s_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1{-}s_8
\end{pmatrix} .
$$

We have the first following property:

Proposition 13. Second order scheme for D2Q9 advective thermal lattice Boltzmann scheme.
With notations explicited previously, the D2Q9 scheme defined by (1.7), (2.3), (5.8) and (5.18) is equivalent to the following advective thermal model

$$
(5.19) \qquad \frac{\partial \rho}{\partial t} + \lambda \left(u \, \frac{\partial \rho}{\partial x} + v \, \frac{\partial \rho}{\partial y} \right) - \lambda^2 \, \xi \, \sigma_1 \, \Delta t \left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right) = \mathrm{O}(\Delta t)^2
$$

if and only if the coefficients a_3, a_7 and a_8 satisfy the relations

$$
(5.20) \qquad a_3 = 3\,(u^2+v^2) - 4 + 6\,\xi \,, \quad a_7 = u^2 - v^2 \,, \quad a_8 = u\,v \,.
$$

Proof of Proposition 13.
From Proposition 4, the relation (5.19) is true at order one, due to the particular choice of conservated momenta (5.15), (5.16) and (5.17). We apply now Proposition 6 (relation (4.15)). We just have to evaluate the defects of conservation θ_1 and θ_2. Due to the relations (4.7) and (5.14), the only equilibrium momenta that contribute to θ_1 and θ_2 have labels 0, 3, 7 and 8. It comes

$$
\theta_1 = u\,\lambda \, \frac{\partial \rho}{\partial t} + \frac{2}{3} \lambda^2 \, \frac{\partial \rho}{\partial x} + \frac{\lambda^2}{6} \, \frac{\partial (a_3\,\rho)}{\partial x} + \frac{\lambda^2}{2} \, \frac{\partial (a_7\,\rho)}{\partial x} + \lambda^2 \, \frac{\partial (a_8\,\rho)}{\partial y} + \mathrm{O}(\Delta t)^2
$$

and taking into account relation (5.19) at order one:

$$
(5.21) \qquad \theta_1 = \left(\frac{2}{3} + \frac{a_3}{6} + \frac{a_7}{2} - u^2 \right) \lambda^2 \, \frac{\partial \rho}{\partial x} + \left(a_8 - u\,v \right) \lambda^2 \, \frac{\partial \rho}{\partial y} + \mathrm{O}(\Delta t)^2 \,.
$$

In a similar way,

$$
\theta_2 = v\,\lambda \, \frac{\partial \rho}{\partial t} + \frac{2}{3} \lambda^2 \, \frac{\partial \rho}{\partial y} + \frac{\lambda^2}{6} \, \frac{\partial (a_3\,\rho)}{\partial y} - \frac{\lambda^2}{2} \, \frac{\partial (a_7\,\rho)}{\partial y} + \lambda^2 \, \frac{\partial (a_8\,\rho)}{\partial x} + \mathrm{O}(\Delta t)^2
$$

and

$$\theta_2 = \Big(a_8 - u\,v\Big)\,\lambda^2\,\frac{\partial\rho}{\partial x} + \Big(\frac{a_3}{6} - \frac{a_7}{2} + \frac{2}{3} - v^2\Big)\,\lambda^2\,\frac{\partial\rho}{\partial y} + \mathrm{O}(\Delta t)^2\,. \tag{5.22}$$

Then due to relation (4.15),

$$\sigma_\alpha\,\Delta t\,\partial_\alpha\sigma_\alpha \equiv \sigma_1\,\Delta t\,\frac{\partial\theta_1}{\partial x} + \sigma_2\,\Delta t\,\frac{\partial\theta_2}{\partial y} = \lambda^2\,\xi\,\sigma_1\,\Delta t\left(\frac{\partial^2\rho}{\partial x^2} + \frac{\partial^2\rho}{\partial y^2}\right) + \mathrm{O}(\Delta t)^2$$

for an arbitrary field $\rho(\bullet,\,\bullet)$ if and only if $a_8 - u\,v = 0$ and a_3 and a_7 are solution of the following linear system:

$$\frac{a_3}{6} + \frac{a_7}{2} = \xi - \frac{2}{3} + u^2\,, \qquad \frac{a_3}{6} - \frac{a_7}{2} = \xi - \frac{2}{3} + v^2\,.$$

From the previous lines, the explicitation of a_3 and a_7 with (5.20) is clear and the proposition is established. $\square$

- The expression (5.18) for coefficients a_7 and a_8 shows clearly the natural tensorial structure of momenta m_7 and m_8. Under a rotation of space of angle $+\frac{\pi}{2}$, m_7 exchange sign and components and m_8 exchange the coordinates, as observed in (5.18). For development of the algebraic consequences of representations of lattice symmetry group for the conception of lattice Boltzmann scheme, we refer to Lallemnd-Luo (2003) and Rubinstein (2006). We precise now the equivalent equation of the Boltzmann scheme at order three.

Proposition 14. Third order scheme for D2Q9 advective thermal lattice Boltzmann scheme.

With previous notations and hypotheses, the D2Q9 Boltzmann scheme defined by (1.7), (2.3), (5.8) and (5.18) is equivalent at third order to the following partial differential equation

$$
(5.23)\quad \left\{ \begin{array}{l}
\dfrac{\partial \rho}{\partial t} + \lambda \left(u \, \dfrac{\partial \rho}{\partial x} + v \, \dfrac{\partial \rho}{\partial y} \right) - \lambda^2 \, \xi \, \sigma_1 \, \Delta t \left(\dfrac{\partial^2 \rho}{\partial x^2} + \dfrac{\partial^2 \rho}{\partial y^2} \right) \\
\qquad - \lambda^3 \, \Delta t^2 \Big\{ \dfrac{1}{6} \Big(2 \, \sigma_1^2 - \dfrac{1}{6} \Big) \, \xi \, \Big(u \, \dfrac{\partial}{\partial x} + v \, \dfrac{\partial}{\partial y} \Big) \, (\Delta \rho) \\
\qquad + \dfrac{1}{6} \Big(\sigma_1 \, \sigma_3 - \dfrac{1}{12} \Big) \Big[\Big(3 \, (u^2 + v^2) + (6 \, \xi - 5) - a_5 \Big) \, u \, \dfrac{\partial}{\partial x} \\
\qquad \qquad \qquad + \Big(3 \, (u^2 + v^2) + (6 \, \xi - 5) - a_6 \Big) \, v \, \dfrac{\partial}{\partial y} \Big] \, (\Delta \rho) \\
\qquad + \dfrac{1}{6} \Big(\sigma_1 \, \sigma_7 - \dfrac{1}{12} \Big) \Big[\Big(3 \, (u^2 - v^2) - 1 + a_5 \Big) \, u \, \dfrac{\partial}{\partial x} \\
\qquad \qquad \qquad + \Big(3 \, (u^2 - v^2) + 1 - a_6 \Big) \, v \, \dfrac{\partial}{\partial y} \Big] \Big(\dfrac{\partial^2 \rho}{\partial x^2} - \dfrac{\partial^2 \rho}{\partial y^2} \Big) \\
\qquad + \dfrac{2}{3} \Big(\sigma_1 \, \sigma_8 - \dfrac{1}{12} \Big) \Big[(3 u^2 - 2 - a_6) \, v \, \dfrac{\partial}{\partial x} \\
\qquad \qquad \qquad + (3 v^2 - 2 - a_5) \, u \, \dfrac{\partial}{\partial y} \Big] \, \dfrac{\partial^2 \rho}{\partial x \partial y} \Big\} = \mathrm{O}(\Delta t)^3 \,.
\end{array} \right.
$$

Proof of Proposition 14.
We complete the relation (5.19) by the two extra terms present in relation (4.20) and we take into account an expansion of defect of conservation θ_1 and θ_2 at order 2. On one side, from (4.21), (5.21) and (5.22), taking into account the equation (5.19), we have easily

$$
(5.24)\quad \left\{ \begin{array}{l}
\sigma_1 \, \Delta t \, \dfrac{\partial \theta_1}{\partial x} + \sigma_2 \, \Delta t \, \dfrac{\partial \theta_2}{\partial y} = \lambda^2 \, \xi \, \sigma_1 \, \Delta t \left(\dfrac{\partial^2 \rho}{\partial x^2} + \dfrac{\partial^2 \rho}{\partial y^2} \right) \\
\qquad \qquad + \sigma_1^2 \, \Delta t^2 \, \lambda^3 \, \xi \, \Big(u \, \dfrac{\partial}{\partial x} + v \, \dfrac{\partial}{\partial y} \Big) \, (\Delta \rho) + \mathrm{O}(\Delta t)^3 \,.
\end{array} \right.
$$

On the other side,

$$
\Delta t^2 \Big(\sigma_\alpha^2 - \frac{1}{6} \Big) \, \partial_\alpha \, \partial_t \, \theta_\alpha = \Delta t^2 \Big(\sigma_1^2 - \frac{1}{6} \Big) \Big[\frac{\partial^2 \theta_1}{\partial x \partial t} + \frac{\partial^2 \theta_2}{\partial y \partial t} \Big] =
$$

$$
= \Delta t^2 \Big(\sigma_1^2 - \frac{1}{6} \Big) \, \xi \, \lambda^2 \, \Delta \Big(\frac{\partial \rho}{\partial t} \Big) + \mathrm{O}(\Delta t)^3
$$

$$
= -\Delta t^2 \Big(\sigma_1^2 - \frac{1}{6} \Big) \, \xi \, \lambda^3 \, \Big(u \, \frac{\partial}{\partial x} + v \, \frac{\partial}{\partial y} \Big) \, (\Delta \rho) + \mathrm{O}(\Delta t)^3
$$

and due to (5.24), the first four terms in (4.20) expand as the first two lines of (5.23) at third order of accuracy. The other lines correspond to the fifth term $\big(\sigma_\alpha \, \sigma_\ell - \frac{1}{12} \big) \, \Lambda^\ell_{\alpha\beta} \, \partial_\alpha \partial_\beta \theta_\ell$ of relation (4.20). We remark that due to (5.14) the only terms that have to be taken into account concern θ_3, θ_7 and θ_8. After some lines of elementary algebra that use explicitly the Annex, we have from (4.7) and (5.13):

$$(5.25)\quad \left\{ \begin{aligned} \theta_3 \,=\, -\lambda \Big[& \big(3\,(u^2+v^2) \,+\, (6\,\xi-5) - a_5\big)\, u \, \frac{\partial \rho}{\partial x} \\ & + \big(3\,(u^2+v^2) \,+\, (6\,\xi-5) - a_6\big)\, v \, \frac{\partial \rho}{\partial y} \Big] + \mathrm{O}(\Delta t) \end{aligned} \right.$$

$$(5.26)\quad \left\{ \begin{aligned} \theta_7 \,=\, -\frac{\lambda}{3} \Big[& \big(3\,(u^2-v^2) - 1 + a_5\big)\, u \, \frac{\partial \rho}{\partial x} \\ & + \big(3\,(u^2-v^2) + 1 - a_6\big)\, v \, \frac{\partial \rho}{\partial y} \Big] + \mathrm{O}(\Delta t)\,. \end{aligned} \right.$$

$$(5.27)\quad \left\{ \begin{aligned} \theta_8 \,=\, -\frac{\lambda}{3} \Big[& \big(3u^2 - 2 - a_6\big)\, v \, \frac{\partial \rho}{\partial x} \\ & + \big(3\,v^2 - 2 - a_5\big)\, u \, \frac{\partial \rho}{\partial y} \Big] + \mathrm{O}(\Delta t)\,. \end{aligned} \right.$$

The proposition is established. □

6) Application to diffusive acoustics

• We use the D1Q3 lattice Boltzmann scheme presented in the first part of Section 5 for simulating diffusive acoustics. Figure 1 is still valid and momenta are still density (defined in (2.1)), momentum (see (5.2)) and kinetic energy (*c.f.* (5.3)). Then matrix M proposed at relation (5.4) remains valid for this new physical model and in consequence the tensor of momentum-velocity Λ is still given according to the relation (5.5). For acoustics, density (2.1) and momentum (5.2) are in equilibrium. Kinetic energy ϵ admits an equilibrium value ϵ^{eq} given as in (5.6) in order to respect Galilean invariance. We suppose

$$(6.1)\qquad \epsilon^{\mathrm{eq}} \,=\, \zeta \, \frac{\lambda^2}{2} \, \rho \,.$$

The present model is linear and relation (5.8) is still valid but matrix J_0 is no longer given by relation (5.9) and we suppose now

$$(6.2)\qquad J_0 \,=\, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \zeta\, s\, \lambda^2/2 & 0 & 1-s \end{pmatrix} .$$

There is only one nonequilibrium momentum, thus only one relaxation parameter and we set simply $\sigma \equiv \frac{1}{s} - \frac{1}{2}$. There is also only one defect of conservation θ now evaluated according to

$$(6.3)\qquad \theta \equiv \zeta \, \frac{\lambda^2}{2} \, \frac{\partial \rho}{\partial t} \,+\, \frac{\lambda^2}{2} \, \frac{\partial q}{\partial x} \,.$$

Proposition 15. Third order scheme for D1Q3 diffusive acoustics lattice Boltzmann scheme.
With previous notations, the D1Q3 Boltzmann scheme defined by (1.7), (2.3), (5.8) and (6.2) admits the following partial differential equations for conservation of mass and conservation of momentum at third order of accuracy:

$$\frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} - \frac{1}{12}\,(1-\zeta)\,\lambda^2\,\Delta t^2\,\frac{\partial^3 q}{\partial x^3} \;=\; \mathrm{O}(\Delta t^3) \tag{6.4}$$

$$\left\{ \begin{aligned} & \frac{\partial q}{\partial t} + \zeta\,\lambda^2\,\frac{\partial \rho}{\partial x} - \sigma\,\lambda^2\,\Delta t\,(1-\zeta)\,\frac{\partial^2 q}{\partial x^2} \\ & \qquad\qquad - \frac{\lambda^4\,\Delta t^2}{6}\,\zeta\,(1-\zeta)\,(6\sigma^2-1)\,\frac{\partial^3 \rho}{\partial x^3} \;=\; \mathrm{O}(\Delta t^3)\,. \end{aligned} \right. \tag{6.5}$$

Proof of Proposition 15.

• We have the relation (6.4) at first order of accuracy, due to Proposition 4 (relation (4.6)). Conservation of momentum at first order is a consequence of Proposition 9 (relation (4.23)) and of the expression (5.5) of the tensor of momentum-velocity that implies that Λ^2_{11} [make attention that tensor Λ^ℓ_{kp} is labelled from 0 to 2 !] is not null only for $\ell = 2$. Then

$$\frac{\partial q}{\partial t} + 2\,\frac{\partial}{\partial x}\big(\epsilon^{\mathrm{eq}}\big) \;=\; \mathrm{O}(\Delta t)$$

and the relation (6.4) is true at first order.

• Conservation of mass (4.27) implies that no first order term in Δt is present. We deduce an expansion of the defect of conservation θ at second order :

$$\theta \;=\; (1-\zeta)\,\frac{\lambda^2}{2}\,\frac{\partial q}{\partial x} + \mathrm{O}(\Delta t^2)\,. \tag{6.6}$$

Conservation of momentum (4.24) allows to explicit the complementary term $\sigma_\ell\,\Delta t\,\Lambda^\ell_{\alpha\beta}\,\partial_\beta \theta_\ell$. We have

$$\sigma_\ell\,\Delta t\,\Lambda^\ell_{\alpha\beta}\,\partial_\beta \theta_\ell \;=\; \sigma\,\Delta t\,\Lambda^2_{11}\,\frac{\partial \theta}{\partial x} \;=\; \sigma\,(1-\zeta)\,\frac{\lambda^2}{2}\,\Delta t\,\frac{\partial^2 \theta}{\partial x^2} + \mathrm{O}(\Delta t^3)$$

due to relation (4.6). In consequence, relations (6.4) and (6.5) are valid at order two of accuracy and no extra term will come from the above expression when considering one extra order.

• We apply now relations (4.27) and (4.28). To establish mass conservation, we have

$$-\frac{\Delta t^2}{12}\,\Lambda^\ell_{\alpha\beta}\,\partial_\alpha\partial_\beta\theta_\ell \;=\; -\frac{\Delta t^2}{12}\,\Lambda^2_{11}\,\frac{\partial^2\theta}{\partial x^2} \;=\; -\frac{1-\zeta}{12}\,\Delta t^2\,\lambda^2\,\frac{\partial^3 q}{\partial x^3} + \mathrm{O}(\Delta t^3)\,,$$

and this complementary term closes the proof for the first equation. Concerning conservation of momentum, we have on one hand

$$\begin{aligned}\Big(\sigma_\ell^2-\frac{1}{6}\Big)\,\Lambda^\ell_{\alpha\beta}\,\partial_t\partial_\beta\theta_\ell \;&=\; \Big(\sigma^2-\frac{1}{6}\Big)\,\Lambda^2_{11}\,\frac{\partial^2\theta}{\partial x\,\partial t}\\ &=\;\Big(\sigma^2-\frac{1}{6}\Big)\,(1-\zeta)\,\lambda^2\,\frac{\partial^2}{\partial x^2}\Big(\frac{\partial q}{\partial x}\Big)\;+\;\mathrm{O}(\Delta t^2) \qquad \text{due to (6.6)}\\ &=\;-\Big(\sigma^2-\frac{1}{6}\Big)\,(1-\zeta)\,\lambda^4\,\frac{\partial^3 q}{\partial x^3}\;+\;\mathrm{O}(\Delta t^2)\,,\end{aligned}$$

and on the other hand

$$\Big(\sigma_\ell\,\sigma_p\;-\;\frac{1}{12}\Big)\,\Lambda^p_{\alpha\beta}\,\Lambda^\ell_{p\gamma}\,\partial_\beta\partial_\gamma\theta_\ell\;=\;\Big(\sigma^2\;-\;\frac{1}{12}\Big)\,\Lambda^2_{11}\,\Lambda^2_{21}\,\frac{\partial^2\theta}{\partial x^2}\;=\;0\,.$$

The relation (6.5) is completely established and the proposition is proved. □

• We adapt now the D2Q9 Boltzmann scheme presented at second subsection of Section 5 for two-dimensional acoustics. Labelling the degrees of freedom with Figure 2 remains valid and momentum matrix M is still given by relation (5.13). In consequence, the momentum-velocity tensor Λ is still obtained according to relations (5.14). This model conserves mass and the two components of momentum. Then following Lallemand and Luo (2000), relations (5.15) to (5.17) have to be replaced by

$$m_3^{\mathrm{eq}}=-2\rho\,,\;\;m_4^{\mathrm{eq}}=\rho\,,\;\;m_5^{\mathrm{eq}}=-\frac{q_x}{\lambda}\,,\;\;m_6^{\mathrm{eq}}=-\frac{q_6}{\lambda}\,,\;\;m_7^{\mathrm{eq}}=m_8^{\mathrm{eq}}=0 \tag{6.7}$$

and in consequence the matrix J_0 takes the form

$$J_0=\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\ -2\,s_3 & 0 & 0 & 1{-}s_3 & 0 & 0 & 0 & 0 & 0\\ s_4 & 0 & 0 & 0 & 1{-}s_4 & 0 & 0 & 0 & 0\\ 0 & -\frac{s_5}{\lambda} & 0 & 0 & 0 & 1{-}s_5 & 0 & 0 & 0\\ 0 & 0 & -\frac{s_5}{\lambda} & 0 & 0 & 0 & 1{-}s_5 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1{-}s_7 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1{-}s_7 \end{pmatrix}. \tag{6.8}$$

Due to relation (5.14), only three defects of conservation play an active role for determining the equivalent equations. We have now (see details *e.g.* in our ESAIM contribution, 2007)

$$\theta_3\equiv-2\,\frac{\partial\rho}{\partial t}\,,\quad \theta_7\equiv\frac{2}{3}\,\Big(\frac{\partial q_x}{\partial x}\;-\;\frac{\partial q_y}{\partial y}\Big)\,,\quad \theta_8\equiv\frac{1}{3}\,\Big(\frac{\partial q_y}{\partial x}\;+\;\frac{\partial q_x}{\partial y}\Big)\,. \tag{6.9}$$

Proposition 16. Third order scheme for D2Q9 diffusive acoustics lattice Boltzmann scheme.
With previous notations, the D2Q9 Boltzmann scheme defined by (1.7), (2.3), (5.8) and (6.6) admits the following partial differential equations for conservation of mass and momentum at third order of accuracy:

$$\frac{\partial \rho}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} - \frac{1}{18} \lambda^2 \Delta t^2 \Delta\big(\mathrm{div} q\big) = \mathrm{O}(\Delta t^3) , \tag{6.10}$$

$$\left\{ \begin{aligned} & \frac{\partial q_x}{\partial t} + \frac{\lambda^2}{3} \frac{\partial \rho}{\partial x} - \frac{\lambda^2}{3} \Delta t \Big[\sigma_3 \frac{\partial}{\partial x} \mathrm{div} q + \sigma_8 \Delta q_x \Big] \\ & \qquad - \frac{\lambda^4 \Delta t^2}{9} \Big(\sigma_3^2 + \sigma_8^2 - \frac{1}{3} \Big) \frac{\partial}{\partial x} \Delta \rho = \mathrm{O}(\Delta t^3) , \end{aligned} \right. \tag{6.11}$$

$$\left\{ \begin{aligned} & \frac{\partial q_y}{\partial t} + \frac{\lambda^2}{3} \frac{\partial \rho}{\partial y} - \frac{\lambda^2}{3} \Delta t \Big[\sigma_3 \frac{\partial}{\partial y} \mathrm{div} q + \sigma_8 \Delta q_y \Big] \\ & \qquad - \frac{\lambda^4 \Delta t^2}{9} \Big(\sigma_3^2 + \sigma_8^2 - \frac{1}{3} \Big) \frac{\partial}{\partial y} \Delta \rho = \mathrm{O}(\Delta t^3) . \end{aligned} \right. \tag{6.12}$$

Proof of Proposition 16.
• We have to go step by step as in the other examples. Equation of mass (6.10) is valid at first order. Second, due to (4.24) and (5.14),

$$\begin{aligned} \Lambda^\ell_{\alpha\beta} \, \partial_\beta m_\ell^{\mathrm{eq}} &= \Lambda^0_{\alpha\beta} \, \partial_\beta m_0^{\mathrm{eq}} + \Lambda^3_{\alpha\beta} \, \partial_\beta m_3^{\mathrm{eq}} + \Lambda^7_{\alpha\beta} \, \partial_\beta m_7^{\mathrm{eq}} + \Lambda^8_{\alpha\beta} \, \partial_\beta m_8^{\mathrm{eq}} \\ &= \frac{2}{3} \lambda^2 \, \partial_\alpha \rho + \frac{1}{6} \lambda^2 \, \partial_\alpha \big(m_3^{\mathrm{eq}} \big) = \frac{2}{3} \lambda^2 \, \partial_\alpha \rho + \frac{1}{6} \lambda^2 \, (-2) \, \partial_\alpha \rho = \frac{1}{3} \lambda^2 \, \partial_\alpha \rho \end{aligned}$$

and relations (6.11) and (6.12) are established at first order.

• The equation of mass is exact up to second order of accuracy and we evaluate θ_3 as consequence of (6.9) and (6.10) at second order:

$$\theta_3 = 2 \, \mathrm{div} \, q + \mathrm{O}(\Delta t^2) . \tag{6.13}$$

For momentum transfer, we have from (4.24)

$$\sigma_\ell \, \Delta t \, \Lambda^\ell_{\alpha\beta} \, \partial_\beta \theta_\ell = \Delta t \Big[\sigma_3 \, \Lambda^3_{\alpha\beta} \, \partial_\beta \theta_3 + \sigma_7 \, \Lambda^7_{\alpha\beta} \, \partial_\beta \theta_7 + \sigma_7 \, \Lambda^8_{\alpha\beta} \, \partial_\beta \theta_8 \Big] .$$

In particular for $\alpha = 1$ we have

$$\begin{aligned} \sigma_\ell \, \Delta t \, \Lambda^\ell_{1\beta} \, \partial_\beta \theta_\ell &= \lambda^2 \, \Delta t \, \bigg[\frac{\sigma_3}{6} \frac{\partial}{\partial x} \big(2 \, \mathrm{div} \, q \big) + \frac{\sigma_7}{2} \frac{\partial}{\partial x} \Big(\frac{2}{3} \Big(\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} \Big) \Big) \\ & \qquad + \sigma_7 \frac{\partial}{\partial y} \Big(\frac{1}{3} \Big(\frac{\partial q_y}{\partial x} + \frac{\partial q_x}{\partial y} \Big) \Big) \bigg] + \mathrm{O}(\Delta t^3) \\ &= \lambda^2 \, \Delta t \, \Big[\frac{\sigma_3}{3} \frac{\partial}{\partial x} \big(\mathrm{div} \, q \big) + \frac{\sigma_7}{3} \, \Delta q_x \Big] + \mathrm{O}(\Delta t^3) , \end{aligned}$$

and for $\alpha = 2$

$$\sigma_\ell \, \Delta t \, \Lambda^\ell_{2\beta} \, \partial_\beta \theta_\ell \;=\; \lambda^2 \, \Delta t \, \Big[\frac{\sigma_3}{6} \, \frac{\partial}{\partial y} \big(2 \, \mathrm{div} \, q \big) \;-\; \frac{\sigma_7}{2} \, \frac{\partial}{\partial y} \Big(\frac{2}{3} \Big(\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} \Big) \Big) + \sigma_7 \, \frac{\partial}{\partial x} \Big(\frac{1}{3} \Big(\frac{\partial q_y}{\partial x} + \frac{\partial q_x}{\partial y} \Big) \Big) \Big] \;+\; \mathrm{O}(\Delta t^3)$$

$$= \; \lambda^2 \, \Delta t \; \frac{\sigma_3}{3} \, \frac{\partial}{\partial y} \big(\mathrm{div} \, q \big) \;+\; \frac{\sigma_7}{3} \, \Delta q_y \Big] \;+\; \mathrm{O}(\Delta t^3) \, .$$

These expressions prove that momentum conservation (6.11) and (6.12) is established at order two.

• The extension to third order of accuracy follow (4.27) and (4.28). Due to relation (4.27),

$$\frac{\Delta t^2}{12} \, \Lambda^\ell_{\alpha\beta} \, \partial_\alpha \partial_\beta \theta_\ell \;=\; \frac{\Delta t^2}{12} \, \Big(\Lambda^3_{\alpha\beta} \partial_\alpha \partial_\beta \theta_3 \,+\, \Lambda^7_{\alpha\beta} \partial_\alpha \partial_\beta \theta_7 \,+\, \Lambda^8_{\alpha\beta} \partial_\alpha \partial_\beta \theta_8 \Big)$$

$$= \; \frac{\lambda^2 \, \Delta t^2}{12} \, \Big[\frac{1}{6} \Delta \big(2 \, \mathrm{div} q \big) \;+\; \frac{1}{2} \big(\partial_x^2 - \partial_y^2 \big) \, \Big(\frac{2}{3} \Big(\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} \Big) \Big) + 2 \, \partial_x \partial_y \Big(\frac{1}{3} \Big(\frac{\partial q_x}{\partial y} + \frac{\partial q_x}{\partial y} \Big) \Big) \Big] \;+\; \mathrm{O}(\Delta t^4)$$

$$= \; \frac{\Delta t^2}{12} \, \Big[\frac{2}{3} \Delta \Big(\frac{\partial q_x}{\partial x} \Big) \;+\; \frac{2}{3} \Delta \Big(\frac{\partial q_y}{\partial y} \Big) \Big] \;+\; \mathrm{O}(\Delta t^4)$$

and the relation (6.10) is completely established. We observe now that by derivation of (6.9) relatively to time and taking into account the relations (6.11) and (6.12) at first order, we have

$$\frac{\partial \theta_3}{\partial t} \;=\; -\frac{2}{3} \lambda^2 \, \Delta \rho \, , \quad \frac{\partial \theta_7}{\partial t} \;=\; -\frac{2}{9} \lambda^2 \, \Big(\frac{\partial^2 \rho}{\partial x^2} - \frac{\partial^2 \rho}{\partial y^2} \Big) \, , \quad \frac{\partial \theta_8}{\partial t} \;=\; -\frac{2}{9} \lambda^2 \; \frac{\partial^2 \rho}{\partial x \, \partial y} \, .$$

We consider one of the last terms of equation (4.28). We have

$$\Big(\sigma_\ell^2 - \frac{1}{6} \Big) \, \Lambda^\ell_{\alpha\beta} \, \partial_t \partial_\beta \theta_\ell \;=\; \Big(\sigma_3^2 - \frac{1}{6} \Big) \, \Lambda^3_{\alpha\beta} \, \partial_\beta \big(\partial_t \theta_3 \big) + \Big(\sigma_7^2 - \frac{1}{6} \Big) \, \Big[\Lambda^7_{\alpha\beta} \, \partial_\beta \big(\partial_t \theta_7 \big) \;+\; \Lambda^8_{\alpha\beta} \, \partial_\beta \big(\partial_t \theta_8 \big) \Big]$$

and for $\alpha = 1$,

$$\Big(\sigma_\ell^2 - \frac{1}{6} \Big) \, \Lambda^\ell_{1\beta} \, \partial_t \partial_\beta \theta_\ell \;=\; \frac{\lambda^2}{6} \, \Big(\sigma_3^2 - \frac{1}{6} \Big) \, \frac{\partial}{\partial x} \Big(- \frac{2}{3} \lambda^2 \, \Delta \rho \Big) + \frac{\lambda^2}{2} \, \Big(\sigma_7^2 - \frac{1}{6} \Big) \, \frac{\partial}{\partial x} \Big(- \frac{2}{9} \lambda^2 \, \Big(\frac{\partial 2 \rho}{\partial x^2} - \frac{\partial 2 \rho}{\partial y^2} \Big) \Big)$$

$$+\lambda^2\left(\sigma_7^2-\frac{1}{6}\right)\frac{\partial}{\partial y}\Big(-\frac{2}{9}\lambda^2\,\frac{\partial 2\rho}{\partial x\,\partial y}\Big)\;+\;\mathrm{O}(\Delta t)$$

$$-\frac{\lambda^4}{9}\left[\left(\sigma_3^2-\frac{1}{6}\right)\frac{\partial}{\partial x}(\Delta\rho)\;+\;\left(\sigma_7^2-\frac{1}{6}\right)\frac{\partial}{\partial x}(\Delta\rho)\right]\;+\;\mathrm{O}(\Delta t)$$

and all the terms of equation (6.11) have been put in evidence. For $\alpha = 2$, we have

$$\begin{aligned}\left(\sigma_\ell^2-\frac{1}{6}\right)\Lambda_{2\beta}^{\ell}\,\partial_t\partial_\beta\theta_\ell \;=\;& \frac{\lambda^2}{6}\left(\sigma_3^2-\frac{1}{6}\right)\frac{\partial}{\partial y}\Big(-\frac{2}{3}\lambda^2\,\Delta\rho\Big)\\ &-\frac{\lambda^2}{2}\left(\sigma_7^2-\frac{1}{6}\right)\frac{\partial}{\partial y}\Big(-\frac{2}{9}\lambda^2\,\Big(\frac{\partial 2\rho}{\partial x^2}-\frac{\partial 2\rho}{\partial y^2}\Big)\Big)\\ &+\lambda^2\left(\sigma_7^2-\frac{1}{6}\right)\frac{\partial}{\partial x}\Big(-\frac{2}{9}\lambda^2\,\frac{\partial 2\rho}{\partial x\,\partial y}\Big)\;+\;\mathrm{O}(\Delta t)\\ =\;&-\frac{\lambda^4}{9}\left[\left(\sigma_3^2-\frac{1}{6}\right)\frac{\partial}{\partial y}(\Delta\rho)\;+\;\left(\sigma_7^2-\frac{1}{6}\right)\frac{\partial}{\partial y}(\Delta\rho)\right]\;+\;\mathrm{O}(\Delta t)\end{aligned}$$

and all the terms of (6.12) have been found. We finally observe that the last term in relation (4.28), *id est* $\sum_{\beta\,\gamma\,p\,\ell}(\sigma_\ell\,\sigma_p\;-\;\frac{1}{12})\,\Lambda_{\alpha\beta}^{p}\,\Lambda_{p\gamma}^{\ell}\,\partial_\beta\partial_\gamma\theta_\ell$ is null due to the particular form of tensor terms Λ_{kp}^{ℓ} detailed in the Annex. The proposition is proved. □

7) Conclusion

• We have proposed a formal development of lattice Bolzmann schemes at third order of accuracy, with a particular emphasis on single conservation law (thermal model) and conservation of mass and momentum. The algebraic calculus has a simple structure due to the efficient role taken by the so-called tensor of momentum-velocity. This development has been applied to classical D1Q3 and D2Q9 schemes for one and two-dimensional Boltzmann schemes. Of course, this study can be applied to three-dimensional schemes without any conceptual difficulty. The next idea is to generalize the determination of equivalent equation of a lattice Boltzmann scheme at an arbitrary order for linear Boltzmann models; this work is in preparation in collaboration with Pierre Lallemand.

8) Acknowledgments

The author thanks Pierre Lallemand for very helpfull discussions all along the elaboration of this contribution.

9) Annex.

Tensor of momentum-velocity for D2Q9 lattice Boltzmann scheme.

• We explicit matrices Λ^{ℓ}_{kp} for all indices α, β and ℓ in the range from 0 to 8. Recall that Λ^{ℓ}_{kp} is defined from matrix M according to (3.1) and for classical D2Q9 scheme, the matrix M follows (5.23). The result is just a tedious exercice of calculus. We obtain

$$\text{(A.0)} \qquad \Lambda^{0}_{kp} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{2}{3}\lambda^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{2}{3}\lambda^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{4}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{4}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{4}{9} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{4}{9} \end{pmatrix},$$

$$\text{(A.1)} \qquad \Lambda^{1}_{kp} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{3} \\ 0 & 1 & 0 & 0 & 0 & 2/\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2/\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 2/\lambda & 2/\lambda & 0 & 0 & -2/(3\lambda) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2/(3\lambda) \\ 0 & \frac{1}{3} & 0 & 0 & 0 & -2/(3\lambda) & 0 & 0 & 0 \\ 0 & 0 & \frac{2}{3} & 0 & 0 & 0 & 2/(3\lambda) & 0 & 0 \end{pmatrix},$$

$$\text{(A.2)} \qquad \Lambda^{2}_{kp} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{3} \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{1}{3} & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 2/\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2/\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2/(3\lambda) \\ 0 & 0 & 0 & 2/\lambda & 2/\lambda & 0 & 0 & 2/(3\lambda) & 0 \\ 0 & 0 & -\frac{1}{3} & 0 & 0 & 0 & 2/(3\lambda) & 0 & 0 \\ 0 & \frac{2}{3} & 0 & 0 & 0 & 2/(3\lambda) & 0 & 0 & 0 \end{pmatrix},$$

$$\text{(A.3)} \qquad \Lambda^3_{kp} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{6}\lambda^2 & 0 & 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{6}\lambda^2 & 0 & 0 & 0 & \frac{1}{3}\lambda & 0 & 0 \\ 1 & 0 & 0 & -1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -2 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{9} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{9} \end{pmatrix} ,$$

$$\text{(A.4)} \qquad \Lambda^4_{kp} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3}\lambda & 0 & 0 \\ 0 & 0 & 0 & 2 & -2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & -\frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{2}{9} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{9} \end{pmatrix} ,$$

$$\text{(A.5)} \qquad \Lambda^5_{kp} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda & \lambda & 0 & 0 & -\frac{1}{3}\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3}\lambda \\ 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & -\frac{1}{3}\lambda & 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 \end{pmatrix} ,$$

$$\text{(A.6)} \qquad \Lambda^6_{kp} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3}\lambda \\ 0 & 0 & 0 & \lambda & \lambda & 0 & 0 & \frac{1}{3}\lambda & 0 \\ 0 & 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 & -\frac{2}{3} & 0 \\ 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & -\frac{2}{3} & 0 & 0 \\ 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \end{pmatrix} ,$$

$$\Lambda^7_{kp} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & \frac{1}{2}\lambda^2 & 0 & 0 & 0 & -\lambda & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2}\lambda^2 & 0 & 0 & 0 & \lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & -\lambda & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & \lambda & 0 & 0 & 0 & -2 & 0 & 0 \\ 1 & 0 & 0 & -1 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{A.7}$$

$$\Lambda^8_{kp} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & \lambda^2 & 0 & 0 & 0 & \lambda & 0 & 0 \\ 0 & \lambda^2 & 0 & 0 & 0 & \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & \lambda & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & \lambda & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{A.8}$$

10) References

P. Bhatnagar, E. Gross, M. Krook, "A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems", *Physical Review*, vol. **94**, p. 511-525, 1954.

J. Broadwell, "Study of a rarefied shear flow by the discrete velocity method", *Journal of Fluid Mechanics*, vol. **19**, p. 401-414, 1964.

H. Cabannes. "Etude de la propagation des ondes dans un gaz à 14 vitesses", *Journal de Mécanique*, vol. **14**, p. 705-744, 1975.

T. Carleman. *Problèmes Mathématiques dans la Théorie Cinétique des Gaz*, Almqvist & Wiksell, Uppsala, 1957.

S. Chapman, T. G. Cooling, *The mathematical theory of non-uniform gases*, Cambridge University Press, 1939.

S. Chen, G.D. Doolen. "Lattice Boltzmann method for fluid flows", *Annual Review of Fluid Mechanics*, vol. **30**, p. 329-364, 1998.

Y. Chen, H. Ohashi, M. Akiyama. "Thermal lattice Bhatnagar-Gross-Krook model without nonlinear deviations in macrodynamic equations", *Physical Review E*, vol.**50**, p. 2776-2783, 1994.

D. D'Humières. "Generalized Lattice-Boltzmann Equations", in *Rarefied Gas Dynamics: Theory and Simulations*, vol. **159** of *AIAA Progress in Astronautics and Astronautics*, p. 450-458, 1992.

D. D'Humières, I. Ginzburg, M. Krafczyk, P. Lallemand, L.S. Luo. "Multiple-relaxation-time lattice Boltzmann models in three dimensions", *Philosophical Transactions of the Royal Society*, London, vol. **360**, p. 437-451, 2002.

D. D'Humières, P. Lallemand, U. Frisch. "Lattice gas models for $3D-$hydrodynamics", *Europhysics Letters*, vol. **2**, n° 4, p. 291-297, 1986.

F. Dubois. "Une introduction au schéma de Boltzmann sur réseau", *ESAIM: Proceedings*, vol. **18**, p. 181-215, 2007.

F. Dubois. "Equivalent partial differential equations of a Boltzmann scheme", *Computers and mathematics with applications*, vol. **55**, p. 1441-1449, 2008.

U. Frisch, B. Hasslacher, Y. Pomeau, "Lattice gas automata for the Navier Stokes equation", *Physical Review Letters*, vol. **56**, n° 14, p. 1505-1508, 1986.

M. Gardner, "The fantastic combinations of John Conway's new solitaire game "life"", *Scientific American*, vol. **223**, p. 120-123, 1970.

R. Gatignol, *Théorie cinétique des gaz à répartition discrète de vitesses*, *Lecture Notes in Physics*, vol. **36**, Springer Verlag, Berlin, 1975.

I. Ginzburg. "Equilibrium-type and link-type lattice Boltzmann models for generic advection and anisotropic-dispersion equation", *Advances in Water resources*, vol. **28**, p. 1171-1195, 2005.

J. Hardy, Y. Pomeau, O. De Pazzis. "Time Evolution of a Two-Dimensional Classical Lattice System", *Physical Review Letters*, vol. **31**, p. 276 - 279, 1973.

M. Hénon. "Viscosity of a Lattice Gas", *Complex Systems*, vol. **1**, p. 763-789, 1987.

F. Higuera, S. Succi, R. Benzi, "Lattice gas dynamics with enhanced collisions", *Europhysics Letters*, vol. **9**, n° 7, p. 663-668, 1989.

M. Junk, M. Rheinländer, "Regular and multiscale expansions of a lattice Boltzmann method, *Proceedings of Computational Fluid Dynamics*, vol. **8**, p. 25-37, 2008.

P. Lallemand, L.-S. Luo. "Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability", *Physical Review E*, vol.**61**, p. 6546-6562, June 2000.

P. Lallemand, L.-S. Luo. "Theory of the lattice Boltzmann method: Acoustic and thermal properties in two and three dimensions", *Physical Review E*, vol.**68**:036706, September 2003.

A. Lerat, R. Peyret, "Noncentered Schemes and Shock Propagation Problems", *Computers and Fluids*, vol. **2**, p. 35-52, 1974.

G. Mc Namara, G. Zanetti, "Use of Boltzmann equation to simulate lattice gas automata", *Physical Review Letters*, vol. **61**, n° 20, p. 2332-2335, 1988.

Y.H. Qian, D. D'Humières, P. Lallemand, "Lattice BGK for Navier-Stokes equation", *Europhysics Letters*, vol. **17**, n° 6, p. 479-484, 1992.

R. Rubinstein. "Symmetry properties of discrete velocity sets", in Third ICMMES Conference, Hampton, Virginia, July 2006.

X. Shan. "Simulation of Rayleigh-Bénard convection using a lattice Boltzmann method", *Physical Review E*, vol. **55**, p. 2780-2788, 1997.

S. Ulam. "On Some Mathematical Problems Connected with Patterns of Growth of Figures", *J. Proc. Symp. Applied Math.* , vol. **14**, p. 215-224, 1962.

J. Von Neumann. "The General and logical theory of automata", *in "Cerebral Mechanisms in behavior: The Hixon symposium"*, originally presented in september 1948, edited by L. A. Jeffress, p. 1-41, New York, John Wiley and Sons, 1951.

R.F. Warming, B.J. Hyett. "The modified equation approach to the stability and accuracy analysis of finite difference methods", *Journal of Computational Physics*, vol. **14**, p. 159-179, 1974.