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LATTICE BOLTZMANN SCHEMES

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CONTENTS

CHAPTER 1

INTRODUCTION : FROM GAS AUTOMATA TO LATTICE BOLTZMANN SCHEMES

We propose an elementary introduction [1] to the lattice Boltzmann scheme. We recall the physical (Boltzmann equation) and algorithmic (cellular automata) origins of this numerical method. For a one-dimensional example, we present in detail the two characteristic steps of the algorithm: the nonlinear collision step, local in space and the linear propagation phase with the neighbouring vertices, explicit in time. We then propose a generic Taylor-type development with the so-called equivalent partial differential equation. We obtain in this way formally a Chapman-Enskog development where the small parameter is the discretization step of the scheme. At order zero, the lattice Boltzmann scheme satisfies a local thermodynamical equilibrium. At first order, it satisfies the Euler equations of gas dynamics and at second order the Navier-Stokes equations. Then we detail the classical case of the nine velocities model on a square lattice.

1.1 INTRODUCTION

- **Thermodynamics of Gases**

At the end of the nineteenth century, work on the kinetic theory of gases Maxwell [104] and Boltzmann [12] have clarified the velocity distribution law of a gas at thermodynamic equilibrium. In this approach, we consider that at point x and time t coexists a continuum of possible speeds for the gas molecules. More precisely, in a box located at point x with a small volume $\mathrm{d}x$ and for a velocity v defined with a precision of $\mathrm{d}v$ the mass of gas $\mathrm{d}m$ is equal to

$$\mathrm{d}m = f_0(v)\,\mathrm{d}x\,\mathrm{d}v\,. \tag{1.1}$$

The Maxwell-Boltzmann distribution specifies the function f_0; it is parameterized by the density ρ, the average speed u of the gas and a parameter β. This parameter is just connected to the temperature T, at the mass μ of a unitary molecule and at the now so-called "Boltzmann constant" k *via* the classical relationship

$$\beta = \frac{\mu}{kT}\,. \tag{1.2}$$

The speeds of distribution law is written in the case of three-dimensional space:

$$f_0(v) = \rho \left(\frac{\beta}{2\pi}\right)^{3/2} \exp\Big(-\frac{\beta}{2}\,|v-u|^2\Big). \tag{1.3}$$

Elementary evaluations of Gaussian integrals (see *e.g.* the section 1.4) show that

$$\rho = \int_{\mathbb{R}^3} f_0(v)\,\mathrm{d}v \tag{1.4}$$

[1] This chapter is the english translation of a part of the reference [42].

$$\rho\, u = \int_{\mathbb{R}^3} v\, f_0(v)\, \mathrm{d}v \tag{1.5}$$

and the specific total energy E gas also satisfies the relationship

$$\rho\, E = \int_{\mathbb{R}^3} \frac{1}{2}\, |v|^2\, f_0(v)\, \mathrm{d}v\,. \tag{1.6}$$

The previous distribution corresponds to the ideal case of an equilibrium, *a priori* independent of space and time. In the case where a dynamic evolution takes place, the velocity distribution f is a function of space x, time x and v velocities; it follows the Boltzmann equation [12]

$$\frac{\partial f}{\partial t} + v{\bullet}\nabla_x f = Q(f)\,, \quad x \in \mathbb{R}^3\,, \quad v \in \mathbb{R}^3\,, \qquad t > 0\,. \tag{1.7}$$

In this equation, the left term $\partial_t + v{\bullet}\nabla$ corresponds to a free transportation at the velocity v, then the term line $Q(f)$ describes the collisions within the gas. In the most classic for a diluted gas, is taken into account "two-point" collisions and $Q(f)$ is a quadratic function of the distribution $Q(f)$.

A microscopic analysis of molecular collisions shows that the mass, momentum and energy is conserved in every interaction. The effect on the macroscopic scale interest here is that, in particular, the collision kernel $Q(f_0)$ has zero integral when tested against 1, v and $\frac{1}{2}\,|v|^2$:

$$\int_{\mathbb{R}^3} Q(f_0)\Big(1, v, \frac{1}{2}\, |v|^2\Big)^{\mathrm{t}}\, \mathrm{d}v = 0\,. \tag{1.8}$$

When injected this hypothesis in the Boltzmann equation (1.7), the conserved quantities

$$W = (\rho, q \equiv \rho\, u, \varepsilon \equiv \rho E)^{\mathrm{t}} \equiv (W_0, W_\alpha, W_4)^{\mathrm{t}} \tag{1.9}$$

are functions of time and space that satisfy the Euler equations of gas dynamics:

$$\frac{\partial W}{\partial t} + \mathrm{div}\, F(W) = 0\,. \tag{1.10}$$

The tensor F has three spatial components, a scalar (for density), a vector (for the momentum) and a final scalar for energy. We have:

$$\left\{ \begin{array}{lcl} F_{0\alpha} & = & \displaystyle\int_{\mathbb{R}^3} v_\alpha\, f_0(v)\, \mathrm{d}v \\ F_{\alpha\beta} & = & \displaystyle\int_{\mathbb{R}^3} v_\alpha\, v_\beta\, f_0(v)\, \mathrm{d}v \\ F_{4\alpha} & = & \displaystyle\int_{\mathbb{R}^3} \frac{1}{2}\, |v|^2\, v_\alpha\, f_0(v)\, \mathrm{d}v \end{array} \right. \tag{1.11}$$

with the convention of using Greek indices for the spatial parameters: $1 \leqslant \alpha, \beta \leqslant d$.

The situation of perfect thermodynamic equilibrium is only a first approximation. By introducing thermodynamic parameters such as the mean free path between two collisions or average time between collisions, we can consider velocity distributions f "not so far" from the equilibrium. We introduce a "small parameter" ε as:

$$\varepsilon = \frac{\text{mean free path}}{\text{typical macroscopic dimension}} \tag{1.12}$$

and we are looking f in the form of an asymptotic expansion in ε:

$$f(v) = f_0(v) + \varepsilon f_1(v) + \varepsilon^2 f_2(v) + \cdots \tag{1.13}$$

where $f_0(\bullet)$ is the Maxwellian function (1.3). The development of the second order, said Chapman-Enskog (1915) allows to find the Navier-Stokes equations. We refer the reader to the classic book of Chapman and Cowling [26] or the treaty by Diu *et al* [40].

- **Some classical approximations**

One of the difficulties in studying the Boltzmann equation is to link the collision dynamic and obtaining the equilibrium f_0. With the approximation "BGK" of Bhatnagar, Gross and Krook [9] is *a priori* injected as an equilibrium representation $f_0(v)$. The operator of a collision $Q_{BGK}(f)$ models the interaction with a mean field. Then we have:

$$Q_{BGK}(f) = S(f - f_0(v)), \qquad S \simeq \mathrm{d}Q(f_0). \tag{1.14}$$

The effect of collisions is to "back" the distribution f to a reference equilibrium, parameterized by conserved quantities W (see the relations (1.4) to (1.6) and (1.9)).

Another difficulty is the introduction of a "gigantic" parameter space with the space $\mathbb{R}^3$ for all velocities. Models Carleman [24] or [18], then generalized by Renée Gatignol [61], while keeping a continuous space-time, consider only a finite set of possible speeds. The result is a set of coupled partial differential equations whose study is a difficulty in itself.

- **Cellular automata**

Instead of seeking mathematical models, the development of computer modelling tools led to the idea of discrete simulators easy to program. In such an approach, the space, time, velocity, number of molecules present at a given time at a given point are discrete variables. The development of these cellular automata have been three highlights.

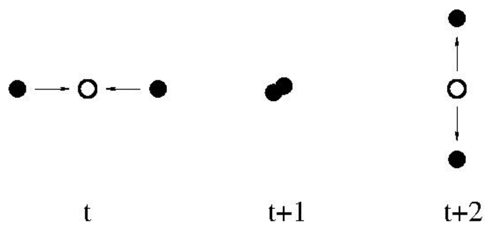

Figure 1.1 – *Frontal collision dynamics in the HPP [73] model.*

The first idea is to use a square two-dimensional lattice. The lattice set of Gaussian integers has a state defined by a binary variable field being 0 or 1. A value of 0 indicates that the site (i,j) is free and the value 1 it is occupied. The discrete evolution of the lattice is described by the discrete velocities linking a vertex (i,j) to its four neighbors $(i \pm 1, j \pm 1)$. With a unity space step and utity time step, the speed range therefore take values in the set $\{e_1, -e_1, e_2, -e_2\}$, with $e_1 = (1,0)$ and $e_2 = (0,1)$. Each particle (or occupied site) is one of four previous proposed velocities. It remains to define collision rules when there is conflict to occupy a site at a new discrete time. Without describing in detail here the model of Hardy, de Pazzis and Pomeau [73], we must build collision rules that respect the conservation of mass, momentum and energy while taking into account a discrete time and space. The Figure 1 describes the dynamics in the event of a frontal collision. We remark that during the intermediate time $t+1$, two discrete particles are present at the same time on the same vertex of the lattice.

A remarkable point in the study of cellular automata is that it is possible (at least formally), to pass to the limit. Taking blocks of larger and larger size allows to define a macroscopic density ρ (ratio of the number of occupied sites towards the number of sample sites) and macroscopic momentum J. We introduce also a “big” time scale compared to the elementary time (equal to 1!) and a “big” spatial scale compared to the lattice step (still equal to 1!) Using these continuous variables, the limits equations take the form

$$\frac{\partial \rho}{\partial t} + \mathrm{div} J = 0 \tag{1.15}$$

$$\frac{\partial J}{\partial t} + \mathrm{div}\, P(\rho, J) = 0 . \tag{1.16}$$

Conservation of mass and momentum are satisfied by cellular automata at the macroscopic limit. As against the pressure tensor P (see also (1.11) is not isotropic.

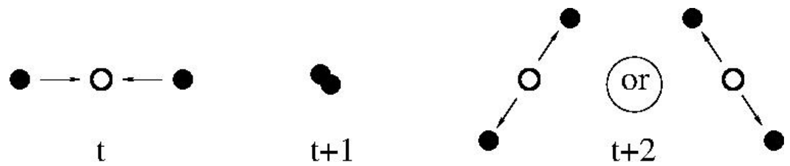

Figure 1.2 – *Frontal collision dynamics in the FHP [59] model.*

To remedy this defect isotropy, Frisch, Hasslacher and Pomeau [59] proposed to use a hexagonal lattice, *i.e.* vertices of the form $a+b\,j$, where $a, b \in \mathbb{Z}$ and $1+j+j^2=0$. The discrete velocity space contains more than in velocity directions and the collision dynamics is also more complex (Figure 2). A random draw is needed to describe the post-collision state after a frontal collision. With this new model, the hydrodynamic limit is isotropic, therefore physically admissible. The extension to three dimensions space was realized soon after by d’Humières, Lallemand and Frisch [84] using a 4-dimensional model with 24 velocities and a face-centered cubic lattice.

Cellular automata however suffer from several shortcomings that have limited their development: intrinsic noise, imposed limit value on the transport coefficients and non-compliance of the Galilean invariance.

- **Lattice Boltzmann equation**

The new idea, proposed by Mac Namara and Zanetti [101], is to keep a discrete lattice but to seek a **continuous** variable f which describes the average population on a given site, with a discrete velocity imposed by the geometry. If we denote space with the letter x, time with the letter t and $(v_j)_{0\leq j\leq q-1}$ the q discrete velocities associated with the lattice, we can write a discrete form of

Boltzmann equation (1.7) by introducing a discrete collision operator. In the approach of Higuera and Jiménez [78] developed afterwards by Higuera, Succi and Benzi [79], an equilibrium distribution $f_j^{\mathrm{eq}}(x,t)$ is introduced and a scattering matrix S_{ij} for the explicitation of the i^{o} component $Q_i(f)$ of the collision operator:

$$Q_i(f) = \sum_{j=0}^{q-1} S_{ij}\left(f_j - f_j^{\mathrm{eq}}\right), \qquad 0 \leqslant i \leqslant q-1. \tag{1.17}$$

The discrete changes between times t et $t+1$ (the physics community has kept automatons the use of a cell no time unit) then takes the form:

$$f_i(x+v_i,\, t+1) = f_i(x,t) + Q_i(f)(x,\, t), \qquad 0 \leqslant i \leqslant q-1. \tag{1.18}$$

where x is a vertex of the lattice.

The difficulty of this approach is the determination of the equilibrium distribution f_j^{eq} $(0 \leqslant j \leqslant q-1)$ and the scattering matrix S_{ij}. These parameters include physical invariants and the dynamics of the evolution towards the equilibrium state, following the BGK Ansatz type. Moreover, the Galilean invariance of gas dynamics equations is still in default; pressure law $p(\rho)$ admits the typical form

$$p(\rho) = \xi^2 \rho \left(1 - g(\rho)\, \frac{|u|^2}{\xi^2} + \cdots\right) \tag{1.19}$$

where ρ is the density, ξ the velocity of sound waves, u the gas velocity and $g(\rho)$ a corrective factor of the model, named “of Galileo”.

In the case of several discrete models, Qian, d’Humières and Lallemand [113] propose a polynomial velocity distribution law for the equilibrium distribution f^{eq} and a diagonal relaxation operator S_{ij}. This approach has been enriched by d’Humières [80] proposing that the collision operator is diagonal in linearly transformed variables from the particle distribution f, say “moments”. We detail in following a fundamental example of this lattice Boltzmann method, called “Lattice Boltzmann Equation” of “lattice Boltzmann schemes”.

1.2 A ONE DIMENSIONAL MODEL

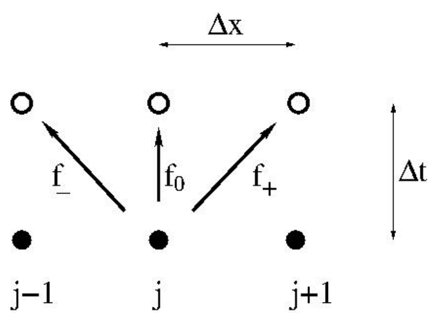

Figure 1.3 – *Free advection for the D1Q3 model.*

- **Introduction**

We consider a one dimensional real lattice $\mathscr{L}$ with elementary space step Δx, and a time step Δt. These two parameters naturally fix a grid velocity λ such that

$$\lambda = \frac{\Delta x}{\Delta t}. \tag{1.20}$$

At vertex $x_j = j\,\Delta x$ for $j \in \mathbb{Z}$ and at the discrete time $t^n = n\,\Delta t$ $(n \in \mathbb{N})$, we consider particle densities $\left(f_0\right)_j^n$, $\left(f_+\right)_j^n$ and $\left(f_-\right)_j^n$. The notation $\left(f_0\right)_j^n$ (respectively $\left(f_+\right)_j^n$, $\left(f_-\right)_j^n$) describes the average number of particles at rest (respectively moving velocity $+\lambda$, $-\lambda$) at time t^n and position x_j (see the Figure 3).

A time step consists of two phases: collision and free transportation. The collision phase is **local** in space. It therefore fails indices j and n to ease writing. Therefore we have the field $f \equiv \left(f_0\,,\, f_+\,,\, f_+\right)$.

- **Moments**

We first introduce a vector of **conserved variables** W composed by the density ρ and the momentum J:

$$\rho \;=\; f_0 + f_+ + f_+ \tag{1.21}$$
$$J \;=\; \lambda\left(f_+ - f_+\right) \tag{1.22}$$

since the zero velocity does not contribute to the momentum. We set now

$$W \equiv (\rho\,,\, J)\,, \qquad \text{conserved variables}. \tag{1.23}$$

A third momentum is introduced in analogy with total energy. We define

$$\varepsilon = \frac{\lambda^2}{2}\left(f_- + f_+\right). \tag{1.24}$$

since the seminal work of d'Humières [80], a set of moments is defined by the variables ρ, J and ε:

$$m \equiv \left(\rho\,,\, J\,,\, \varepsilon\right)^{\mathrm{t}}.$$

The moment representation is connected to the initial distribution f using a matrix M:

$$M = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \lambda & -\lambda \\ 0 & \dfrac{\lambda^2}{2} & \dfrac{\lambda^2}{2} \end{pmatrix}. \tag{1.25}$$

and we have

$$m = M\,f\,. \tag{1.26}$$

The relation $f \longrightarrow m$ defined through (1.21), (1.22) and (1.24) or (1.26) and (1.25) can be inverted without difficulty:

$$f_0 \;=\; \rho - \frac{2}{\lambda^2}\,\varepsilon \tag{1.27}$$
$$f_+ \;=\; \frac{1}{2\,\lambda}\,J + \frac{1}{\lambda^2}\,\varepsilon \tag{1.28}$$
$$f_- \;=\; -\frac{1}{2\,\lambda}\,J + \frac{1}{\lambda^2}\,\varepsilon \tag{1.29}$$

and we deduce

$$M^{-1} = \begin{pmatrix} 1 & 0 & -\dfrac{2}{\lambda^2} \\ 0 & \dfrac{1}{2\lambda} & \dfrac{1}{\lambda^2} \\ 0 & -\dfrac{1}{2\lambda} & \dfrac{1}{\lambda^2} \end{pmatrix}. \tag{1.30}$$

- **Equilibrium and collision**

Then we introduce an equilibrium state. This equilibrium state is fonction **only** of the conserved variables W it is here defined by its equilibrium moments, denoted m^{eq}:

$$m^{\text{eq}} = \Big(\rho^{\text{eq}} \equiv \rho\,, J^{\text{eq}} \equiv J\,, \varepsilon^{\text{eq}} \equiv \psi(W)\Big). \tag{1.31}$$

After using the relations (1.27), (1.28) and (1.29) for the equilibrium momenta (1.31), one defines without difficulty and equilibrium distribution of particles:

$$f^{\text{eq}} = \Phi(W)\,. \tag{1.32}$$

The post-collision state is defined easily through the moments. It is a linear combination of the running state m and the equilibrium state m^{eq}:

$$m^* = \Big(\rho^* \equiv \rho\,, J^* \equiv J\,, \varepsilon^* \equiv \varepsilon + s\big(\varepsilon^{\text{eq}} - \varepsilon\big)\Big). \tag{1.33}$$

Note that during the relaxation, the energy ε relaxes towards the equillibrium value ε^{eq}. Note also that ε^{eq} is only function of the conserved variables W:

$$\varepsilon^* = (1-s)\,\varepsilon + s\,\varepsilon^{\text{eq}}. \tag{1.34}$$

The relaxation parameter s can be interpreted in the following way: during the collision step, we proceed to an explicit Euler scheme in time to integrate an ordinary differential equation associated to the return (for long times) towards the equilibrium value ε^{eq}:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\varepsilon - \varepsilon^{\text{eq}}) + \frac{1}{\tau}\big(\varepsilon - \varepsilon^{\text{eq}}\big) = 0\,. \tag{1.35}$$

When we apply one time step of the explicit Euler scheme to the differential equation (1.35), we obtain

$$\frac{\varepsilon(\Delta t) - \varepsilon(0)}{\Delta t} + \frac{1}{\tau}\,(\varepsilon(0) - \varepsilon^{\text{eq}}) = 0\,.$$

Then with the notation $\varepsilon^* = \varepsilon(\Delta t)$ and $\varepsilon = \varepsilon(0)$, we obtain the relation (1.34), with the condition

$$s = \frac{\Delta t}{\tau}\,. \tag{1.36}$$

The condition (1.36) measures the ratio between the time step Δt and the time constant τ of the relaxation process. It is well known that for a dynamical system of the type (1.35), the **stability** condition can be written as:

$$0 \leqslant s \leqslant 2 \tag{1.37}$$

and this relation has been re-established in the context of lattice gaz automata and lattice Boltzmann scheme.

We observe that the collision operator C is determined in such a way that the conserved variables are not affected by the collision:

$$f^* = C(f) \quad \text{with} \qquad W^* = W\,. \tag{1.38}$$

Then the post-collision distribution of particles can be explicited thanks to (1.27), (1.28), (1.29) and (1.33):

$$f_0^* \;=\; \rho - \frac{2}{\lambda^2}\,\varepsilon^* \tag{1.39}$$

$$f_+^* \;=\; \frac{1}{2\,\lambda}\,J + \frac{1}{\lambda^2}\,\varepsilon^* \tag{1.40}$$

$$f_-^* \;=\; -\frac{1}{2\,\lambda}\,J + \frac{1}{\lambda^2}\,\varepsilon^* \tag{1.41}$$

This collision step is local in space, nonlinear in general and the determination of an equilibrium state f^{eq} can produce a lot of computation, as in the "entropy" methods developed by Karlin and his team [91]. After this collision step, the right hand side of the Boltzmann equation (1.7) is approached.

- **Free advection**

The second step is the advection A to transform the post-collision state f^* into a new particle distribution at time step $n+1$:

$$f^{n+1} = A{\bullet}f^*\,. \tag{1.42}$$

During the free transport, we solve the advection equation

$$\frac{\partial f}{\partial t} + a\,\frac{\partial f}{\partial x} = 0 \tag{1.43}$$

for three velocities $a \in \{0\,,\,\lambda\,,\,-\lambda\}$. The initial condition is the field $\big(f^*\big)_j^n$ of post-collision density of particles f^* at time t^n and for all grid points x_j. Due to the relation between the space step Δx, the time step Δt and the velocity λ defined in (1.20), the method of characteristics is **exact**. After the advection phase, we obtain (see also the Figure 3):

$$\big(f_0\big)_j^{n+1} \;=\; \big(f_0^*\big)_j^n \tag{1.44}$$

$$\big(f_+\big)_j^{n+1} \;=\; \big(f_+^*\big)_{j-1}^n \tag{1.45}$$

$$\big(f_-\big)_j^{n+1} \;=\; \big(f_0^*\big)_{j+1}^n \tag{1.46}$$

This advection phase is linear, explicit and solves the advection equation (1.43) without any numerical viscosity. It couples a vertex j with its neighbours j and $j \pm 1$.

A global time step of a lattice Boltzmann scheme is composed by a collision step C followed by an advection step A:

$$f^{n+1} = A \bullet C\,(f)\,. \tag{1.47}$$

Of course, we can reverse the order of these two operators A and C. Nevertheless, a practical question is the choice of the discrete sub-time step to measure the physical quantities. Note here that the results can differ if we measure the particle distribution "f" **before** the collision, or if we consider the distribution "f^*" **after** the collision.

- **First synthesis**

A lattice Boltzmann scheme is therefore defined by the following ingredients:

(i) choice of conserved variables W, or "moments at equilibrium" of the particle distribution f

(ii) matrix M making the interface between the representation f with particle density and momenta m

(iii) equilibrium value $\psi_k(W)$ for moments that are not at equilibrium

(iv) ratio s_k between the time step Δt and the time constant τ_k that characterizes the duration of the process of return to equilibrium of the k^{o} moment.

1.3 EQUIVALENT PARTIAL DIFFERENTIAL EQUATIONS

We detail in what follows the so-called D1Q3 model, with one space dimension and three discrete velocities. The energy ε defined in relation (1.24) relaxes to a steady energy $\psi(\rho, q)$ given by:

$$\psi(\rho, J) = \alpha \frac{\lambda^2}{2} \rho \tag{1.48}$$

where $\lambda = \frac{\Delta x}{\Delta t}$ is the fixed numerical reference velocity (see (1.20) and α a srictly positive constant. We consider at a discrete time t^n and a discrete position x_j a field $f = (f_0, f_+, f_-)$. We can move in momentum space, which allows you to write:

$$\begin{cases} \rho_j^n &= \big(f_0 + f_+ + f_-\big)_j^n \\ J_j^n &= \lambda\,(f_+)_j^n - \lambda\,(f_-)_j^n \\ \varepsilon_j^n &= \frac{\lambda^2}{2}\,(f_+)_j^n + \frac{\lambda^2}{2}\,(f_-)_j^n \end{cases} \tag{1.49}$$

given the choice of matrix M detailed in equation (1.25). The collision phase can be expressed very simply in momentum space:

$$\begin{cases} (\rho^*)_j^n &= \rho_j^n \\ (J^*)_j^n &= J_j^n \\ (\varepsilon^*)_j^n &= (1-s)\,\varepsilon_j^n + s(\psi(W))_j^n \end{cases} \tag{1.50}$$

with a fixed $s \in]0,2[$ and $\psi(W)$ given in equation (1.48). The state f^* after the collision at time t^n and position x_j is given with the help of the matrix M^{-1} (see the relation (1.30)):

$$\begin{cases} (f_0^*)_j^n &= \Big(\rho^* - \frac{2}{\lambda^2}\,\varepsilon^*\Big)_j^n \\ (f_+^*)_j^n &= \Big(\frac{1}{2\lambda}\,J^* + \frac{1}{\lambda^2}\,\varepsilon^*\Big)_j^n \\ (f_-^*)_j^n &= \Big(-\frac{1}{2\lambda}\,J^* + \frac{1}{\lambda^2}\,\varepsilon^*\Big)_j^n . \end{cases} \tag{1.51}$$

Taking into account (1.50) we deduce the discrete time iteration of the numerical scheme:

$$\left\{ \begin{array}{rcl} (f_0^*)_j^n & = & \big(\rho - \frac{2}{\lambda^2}\,\varepsilon^*\big)_j^n \\ (f_+^*)_j^n & = & \Big(\frac{1}{2\lambda}\,J + \frac{1}{\lambda^2}\,\varepsilon^*\Big)_j^n \\ (f_-^*)_j^n & = & \Big(-\frac{1}{2\lambda}\,J + \frac{1}{\lambda^2}\,\varepsilon^*\Big)_j^n . \end{array} \right. \tag{1.52}$$

We can use these values to deduce the iteration in momentum space:

$$\rho_j^{n+1} = \rho_j^n - \frac{1}{2\lambda}\,(J_{j+1}^n - J_{j-1}^n) + \frac{1}{\lambda^2}\,(\varepsilon^*_{j+1} - 2\varepsilon^*_j + \varepsilon^*_{j+1})^n \tag{1.53}$$

$$J_j^{n+1} = \frac{1}{2}\,(J_{j+1}^n + J_{j-1}^n) - \frac{1}{\lambda}\,(\varepsilon^*_{j+1} - \varepsilon^*_{j-1})^n \tag{1.54}$$

$$\varepsilon_j^{n+1} = \frac{1}{2}\,(\varepsilon^*_{j+1} + \varepsilon^*_{j-1})^n - \frac{\lambda}{4}\,(J_{j+1}^n - J_{j-1}^n)\,. \tag{1.55}$$

In the pages that follow, we use the method of equivalent equation to construct gradually the partial differential equation "best simulated by the scheme" at a given order of approximation (relative to Δx to fix ideas). It looks formally equivalent to the classical approach proposed by Lerat-Peyret [100] and Warming-Hyett [133] (see also the thesis of Lerat [99]). We initially the

Proposition 1. Equilibrium.

Energy is at equilibrium, with a typically first order error:

$$\varepsilon_j^n = \psi(\rho_j^n) + \mathrm{O}(\Delta x)\,. \tag{1.56}$$

- Proof of Proposition 1.

We derive from (1.55): $\varepsilon_j^{n+1} = \varepsilon_j^* + \mathrm{O}(\Delta x)$, and taking into account (1.34) and Taylor's formula in time:

$$\varepsilon_j^n + \mathrm{O}(\Delta t) = (1-s)\,\varepsilon_j^n + s\,\psi(\rho_j^n) + \mathrm{O}(\Delta x)$$

which we immediately deduce (1.56) after subtracting ε_j^n then division by s, assumed **nonzero**. □

Proposition 2. Fluid model

At the first order almost, density and momentum are solutions of the acoustic system

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = \mathrm{O}(\Delta x) \tag{1.57}$$

$$\frac{\partial J}{\partial t} + \frac{\partial p}{\partial x} = \mathrm{O}(\Delta x) \tag{1.58}$$

in relation to a pressure law $p(\rho)$ given by

$$p(\rho) = c_0^2\,\rho\,, \qquad c_0 = \lambda\,\sqrt{\alpha}\,. \tag{1.59}$$

- Proof of Proposition 2.

Was used without shame derivation of Taylor expansions, which allows formal calculation, but assumes *a priori* approximations in "very regular" functional spaces. We deduce from (1.56) and (1.34)

$$(\varepsilon^*)_j^n = \psi(\rho_j^n) + \mathrm{O}(\Delta x)\,, \tag{1.60}$$

and we differentiate two times this relation with respect to the space (!):

$$\Big(\frac{\partial^2 \varepsilon^*}{\partial x^2}\Big)_j^n = \alpha\,\frac{\lambda^2}{2}\,\Big(\frac{\partial^2 \rho}{\partial x^2}\Big)_j^n + \mathrm{O}(\Delta x)\,. \tag{1.61}$$

We have also:

$$\frac{1}{2}\,(J_{j+1} - J_{j-1})^n \quad = \quad \Big(\frac{\partial J}{\partial x}\Big)_j^n\,\Delta x + \mathrm{O}(\Delta x^3) \tag{1.62}$$

$$\big(\varepsilon^*_{j+1} - 2\,\varepsilon^*_j + \varepsilon^*_{j-1}\big)^n \quad = \quad \Delta x^2\,\Big(\frac{\partial^2 \varepsilon^*}{\partial x^2}\Big)_j^n + \mathrm{O}(\Delta x^4)\,. \tag{1.63}$$

We deduce from the relation (1.53) and previous developments

$$\rho_j^n + \Delta t\,\Big(\frac{\partial \rho}{\partial t}\Big)_j^n + \mathrm{O}(\Delta t^2) = \rho_j^n - \Delta t\,\Big(\frac{\partial J}{\partial x}\Big)_j^n + \mathrm{O}(\Delta x^2)$$

which proves the relation (1.57). We do the same for the equation of the momentum (1.54):

$$J_j^n + \Delta t\,\Big(\frac{\partial J}{\partial t}\Big)_j^n + \mathrm{O}(\Delta t^2) = J_j^n + \frac{1}{2}\,\Big(\frac{\partial^2 J}{\partial x^2}\Big)_j^n\,\Delta x^2 - \frac{2\Delta x}{\lambda}\,\Big(\frac{\partial \varepsilon^*}{\partial x}\Big)_j^n + \mathrm{O}(\Delta x^3) = J_j^n - 2\,\Delta t\,\alpha\,\frac{\lambda^2}{2}\,\Big(\frac{\partial \rho}{\partial x}\Big)_j^n + \mathrm{O}(\Delta x^2)$$

which establishes (1.58) and the pressure law $p = \alpha\,\lambda^2\,\rho$ or (1.59). □

Proposition 3. Viscous fluid.

At second order, the density and the momentum are solutions of the system of diffusive acoustics

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = \mathrm{O}(\Delta x^2) \tag{1.64}$$

$$\frac{\partial J}{\partial t} + \frac{\partial p}{\partial x} - \lambda\,\Delta x\,(1-\alpha)\,\Big(\frac{1}{s} - \frac{1}{2}\Big)\,\frac{\partial^2 J}{\partial x^2} = \mathrm{O}(\Delta x^2) \tag{1.65}$$

with a pressure law still given by (1.59). We remark that the constraint $0 < s < 2$ implies that

$$\frac{1}{s} - \frac{1}{2} > 0\,. \tag{1.66}$$

- Proof of Proposition 3.

To establish (1.64), we share (1.53), pushing Taylor's formula one step further, that is to say at second order:

$$\rho + \Delta t\,\frac{\partial \rho}{\partial t} + \frac{\Delta t^2}{2}\,\frac{\partial^2 \rho}{\partial t^2} + \mathrm{O}(\Delta t^3) = \rho - \frac{\Delta x}{\lambda}\,\frac{\partial J}{\partial x} + \mathrm{O}(\Delta x^3) + \frac{\Delta x^2}{\lambda^2}\,\frac{\partial^2 \varepsilon^*}{\partial x^2} + \mathrm{O}(\Delta x^4)$$

and

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = -\frac{\Delta t}{2}\,\frac{\partial^2 \rho}{\partial t^2} + \frac{\Delta x^2}{\Delta t}\,\frac{\alpha}{2}\,\frac{\partial^2 \rho}{\partial x^2} + \mathrm{O}(\Delta x^2) = -\frac{\Delta t}{2}\,\Big(\frac{\partial^2 \rho}{\partial t^2} - \alpha\lambda^2\,\frac{\partial^2 \rho}{\partial x^2}\Big) + \mathrm{O}(\Delta x^2) = \mathrm{O}(\Delta x^2)$$

because the density ρ is the solution of the wave equation obtained by differentiating with respect to time equation (1.57), which is subtracted from the derivative with respect to the space of the equation (1.58).

For the momentum, we first develop the energy ε one step further. We leave (1.55), knowing that (1.56) expresses the energy ε in equilibrium at first order:

$$\varepsilon + \Delta t \frac{\partial \varepsilon}{\partial t} + \mathrm{O}(\Delta t^2) = \varepsilon^* + \frac{1}{2} \frac{\partial^2 \varepsilon^*}{\partial x^2} \Delta x^2 - \frac{\lambda}{2} \Delta x \frac{\partial J}{\partial x} + \mathrm{O}(\Delta x^3) = (1-s)\,\varepsilon + s\,\psi - \frac{\lambda}{2} \Delta x \frac{\partial J}{\partial x} + \mathrm{O}(\Delta x^2).$$

Then

$$s(\varepsilon - \psi) = -\Delta t \frac{\partial \psi}{\partial t} - \frac{\lambda}{2} \Delta x \frac{\partial J}{\partial x} + \mathrm{O}(\Delta x^2) = -\frac{\lambda \Delta x}{2} \Big(\alpha \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} \Big) + \mathrm{O}(\Delta x^2)$$

$$\varepsilon = \psi - \frac{\lambda \Delta x}{2s} \Big(\alpha \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} \Big) + \mathrm{O}(\Delta x^2). \tag{1.67}$$

We have now $\quad \varepsilon^* = (1-s)\,\varepsilon + s\,\psi \quad$ and we deduce

$$\varepsilon^* = \psi - \frac{1-s}{2s} \lambda \Delta x \Big(\alpha \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} \Big) + \mathrm{O}(\Delta x^2). \tag{1.68}$$

We finally develop both members of relation (1.54) by clarifying the terms of order two:

$$\begin{aligned} J + \Delta t \frac{\partial J}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 J}{\partial t^2} + \mathrm{O}(\Delta t^3) &= J + \frac{\Delta x^2}{2} \frac{\partial^2 J}{\partial x^2} + \mathrm{O}(\Delta x^4) - \frac{2\Delta x}{\lambda} \frac{\partial \varepsilon^*}{\partial x} + \mathrm{O}(\Delta x^3) \\ &= J + \frac{1}{2} \Delta x^2 \frac{\partial^2 J}{\partial x^2} - \Delta t \lambda^2 \alpha \frac{\partial \rho}{\partial x} + \frac{1-s}{s} \Delta x^2 \frac{\partial}{\partial x} \Big(\alpha \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} \Big) + \mathrm{O}(\Delta x^2). \end{aligned}$$

We deduce after division by Δt :

$$\begin{aligned} \frac{\partial J}{\partial t} + \alpha \lambda^2 \frac{\partial \rho}{\partial x} &= -\frac{\Delta t}{2} \frac{\partial^2 J}{\partial t^2} + \frac{\lambda \Delta x}{2} \frac{\partial^2 J}{\partial x^2} + \Big(\frac{1}{s} - 1 \Big) \lambda \Delta x \frac{\partial}{\partial x} \Big(\alpha \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} \Big) \\ &= -\frac{\Delta t}{2} \alpha \lambda^2 \frac{\partial^2 J}{\partial x^2} + \frac{\lambda \Delta x}{2} \frac{\partial^2 J}{\partial x^2} + \Big(\frac{1}{s} - 1 \Big) \lambda \Delta x (1-\alpha) \frac{\partial^2 J}{\partial x^2} + \mathrm{O}(\Delta x^3) \\ &= \lambda \Delta x (1-\alpha) \Big(\frac{1}{2} + \frac{1}{s} - 1 \Big) \frac{\partial^2 J}{\partial x^2} + \mathrm{O}(\Delta x^2) = \lambda \Delta x (1-\alpha) \Big(\frac{1}{s} - \frac{1}{2} \Big) \frac{\partial^2 J}{\partial x^2} + \mathrm{O}(\Delta x^2) \end{aligned}$$

and the relation (1.65) is established. □

1.4 ANNEX: SOME GAUSSIEN INTEGRALS

In the case of two-dimensional space, the continuous velocity distribution $f_0(v)$ at equilibrium is given by equation (1.3), that is to say

$$f_0(v) = \rho \frac{\beta}{2\pi} \exp\Big(-\frac{\beta}{2} |v-u|^2 \Big), \qquad v \in \mathbb{R}^2 \tag{1.69}$$

where $\beta > 0$ is homogeneous to the inverse square of a speed. We calculate in this Annex the values of several times m_{pq} of the form

$$m_{pq} = \int_{\mathbb{R}^2} v_1^p \, v_2^q \, f_0(v) \, \mathrm{d}v. \tag{1.70}$$

First calculate integrals to one dimension of space, knowing that

$$\int_{-\infty}^{\infty} \exp\Big(-\frac{\beta}{2}\theta^2\Big)\,\mathrm{d}\theta = \sqrt{\frac{2\pi}{\beta}}\,. \tag{1.71}$$

It was of course by antisymmetry

$$\int_{-\infty}^{\infty} \theta \exp\Big(-\frac{\beta}{2}\theta^2\Big)\,\mathrm{d}\theta = 0 \tag{1.72}$$

and we note that

$$\mathrm{d}\Big(\exp\Big(-\frac{\beta\theta^2}{2}\Big)\Big) = -\beta\theta \exp\Big(-\frac{\beta\theta^2}{2}\Big)\,\mathrm{d}\theta\,.$$

Then

$$\int_{-\infty}^{\infty} \theta^2 \exp\Big(-\frac{\beta\theta^2}{2}\Big)\,\mathrm{d}\theta = -\frac{1}{\beta}\int_{-\infty}^{\infty} \theta\,\mathrm{d}\Big(\exp\Big(-\frac{\beta\theta^2}{2}\Big)\Big) =$$

$$= -\frac{1}{\beta}\Big[\theta \exp\Big(-\frac{\beta\theta^2}{2}\Big)\Big]_{-\infty}^{\infty} + \frac{1}{\beta}\int_{-\infty}^{\infty} \mathrm{d}\theta \exp\Big(-\frac{\beta\theta^2}{2}\Big) = \frac{1}{\beta}\sqrt{\frac{2\pi}{\beta}}\,.$$

We deduce

$$\int_{-\infty}^{\infty} \theta^2 \exp\Big(-\frac{\beta\theta^2}{2}\Big)\,\mathrm{d}\theta = \frac{1}{\beta}\sqrt{\frac{2\pi}{\beta}}\,. \tag{1.73}$$

Always with the odd parity we have

$$\int_{-\infty}^{\infty} \theta^3 \exp\Big(-\frac{\beta\theta^2}{2}\Big)\,\mathrm{d}\theta = 0 \tag{1.74}$$

and

$$\int_{-\infty}^{\infty} \theta^4 \exp\Big(-\frac{\beta\theta^2}{2}\Big)\,\mathrm{d}\theta = -\frac{1}{\beta}\int_{-\infty}^{\infty} \theta^3\,\mathrm{d}\Big[\exp\Big(-\frac{\beta\theta^2}{2}\Big)\Big]$$

$$= -\frac{1}{\beta}\Big[\theta^3 \exp\Big(-\frac{\beta\theta^2}{2}\Big)\Big]_{-\infty}^{\infty} + \frac{3}{\beta}\int_{-\infty}^{\infty} \theta^2 \exp\Big(-\frac{\beta\theta^2}{2}\Big)\,\mathrm{d}\theta = 0 + \frac{3}{\beta}\,\frac{1}{\beta}\sqrt{\frac{2\pi}{\beta}}$$

$$\int_{-\infty}^{\infty} \theta^4 \exp\Big(-\frac{\beta\theta^2}{2}\Big)\,\mathrm{d}\theta = \frac{3}{\beta^2}\sqrt{\frac{2\pi}{\beta}}\,. \tag{1.75}$$

- At **two space dimensions**, the moment of zero order of $f_0(\bullet)$ is obtained without difficulty:

$$\int_{\mathbb{R}^2} f(v)\,\mathrm{d}v = \rho\,. \tag{1.76}$$

For the moment of order 1, m_{10} to fix ideas, we have:

$$m_{10} = \int_{\mathbb{R}^2} v_1\, f_0(v)\,\mathrm{d}v = \rho\,\frac{\beta}{2\pi}\Big(\int_{-\infty}^{\infty} (u_1+\theta) \exp\Big(-\frac{\beta\theta^2}{2}\Big)\,\mathrm{d}\theta\Big)\Big(\int_{-\infty}^{\infty} \exp\Big(-\frac{\beta}{2}\,|v_2-u_2|^2\Big)\,\mathrm{d}v\Big)$$

$$= \rho \, \frac{\beta}{2\pi} \Big(u_1 \sqrt{\frac{2\pi}{\beta}} + 0 \Big) \sqrt{\frac{2\pi}{\beta}} \; = \; \rho \, u_1$$

$$\int_{\mathbb{R}^2} v_j \, f_0(v) \, \mathrm{d}v = \rho \, u_j \,, \qquad 1 \leqslant j \leqslant 2 \,. \tag{1.77}$$

This is classic. For second order moments, we separe the case of m_{20} that of m_{11}. We have

$$m_{20} = \int_{\mathbb{R}^2} v_1^2 \, f_0(v) \, \mathrm{d}v = \frac{\rho\beta}{2\pi} \int_{-\infty}^{\infty} (u_1 + \theta)^2 \, e^{-\dfrac{\beta\theta^2}{2}} \, \mathrm{d}\theta \, \int_{-\infty}^{\infty} e^{-\dfrac{\beta |v_2 - u_2|^2}{2}} \, \mathrm{d}v_2$$

$$= \frac{\rho\beta}{2\pi} \Big(\int_{-\infty}^{\infty} \Big(u_1^2 + 2 u_1 \theta + \theta^2 \Big) \, e^{-\dfrac{\beta\theta^2}{2}} \, \mathrm{d}\theta \Big) \sqrt{\frac{2\pi}{\beta}} \; = \; \frac{\rho\beta}{2\pi} \Big(u_1^2 + \frac{1}{\beta} \Big) \, \frac{2\pi}{\beta} \; = \; \rho \, \Big(u_1^2 + \frac{1}{\beta} \Big) .$$

$$\int_{\mathbb{R}^2} v_j^2 \, f_0(v) \, \mathrm{d}v = \rho \, u_j^2 + \frac{\rho}{\beta} \, . \tag{1.78}$$

We have also

$$m_{11} = \int_{\mathbb{R}^2} v_1 \, v_2 \, f_0(v) \, \mathrm{d}v \; = \; \frac{\rho\beta}{2\pi} \Big(\int_{-\infty}^{\infty} (u_1 + \theta) \, e^{-\dfrac{\beta\theta^2}{2}} \, \mathrm{d}\theta \Big) \Big(\int_{-\infty}^{\infty} (u_2 + \theta) \, e^{-\dfrac{\beta\theta^2}{2}} \, \mathrm{d}\theta \Big)$$

$$= \frac{\rho\beta}{2\pi} \, (u_1 + 0) \sqrt{\frac{2\pi}{\beta}} \, (u_2 + 0) \sqrt{\frac{2\pi}{\beta}} \; = \; \rho \, u_1 \, u_2$$

$$\int_{\mathbb{R}^2} v_1 \, v_2 \, f_0(v) \, \mathrm{d}v = \rho \, u_1 \, u_2 \, . \tag{1.79}$$

The three-order moments are evaluated with the same approach:

$$m_{30} = \int_{\mathbb{R}^2} v_1^3 \, f_0(v) \, \mathrm{d}v = \frac{\rho\beta}{2\pi} \Big(\int_{-\infty}^{\infty} (u_1 + \theta)^3 \, e^{-\dfrac{\beta\theta^2}{2}} \, \mathrm{d}\theta \Big) \sqrt{\frac{2\pi}{\beta}}$$

$$= \frac{\rho\beta}{2\pi} \Big(\int_{-\infty}^{\infty} (u_1^3 + 3 \, u_1^2 \, \theta + 3 \, u_1 \, \theta^2 + \theta^3) \, e^{-\dfrac{\beta\theta^2}{2}} \, \mathrm{d}\theta \Big) \sqrt{\frac{2\pi}{\beta}} \; = \; \frac{\rho\beta}{2\pi} \Big(u_1^3 + 3 \, \frac{u_1}{\beta} \Big) \Big(\frac{2\pi}{\beta} \Big) = \rho \, u_1 \Big(u_1^2 + \frac{3}{\beta} \Big)$$

$$\int_{\mathbb{R}^2} v_j^3 \, f_0(v) \, \mathrm{d}v = \Big(\frac{3}{\beta} + u_j^2 \Big) \rho \, u_j \,, \qquad 1 \leqslant j \leqslant 2 \,. \tag{1.80}$$

For the discrete lattice Boltzmann schemes, we only keep the term the lowest order in u_j:

$$\int_{\mathbb{R}^2} v_j^3 \, f_0(v) \, \mathrm{d}v \simeq \frac{3}{\beta} \, \rho \, u_j \,, \qquad 1 \leqslant j \leqslant 2 \,. \tag{1.81}$$

On the other hand

$$m_{21} = \int_{\mathbb{R}^2} v_1^2 \, v_2 \, f_0(v) \, \mathrm{d}v \; = \; \rho \, \frac{\beta}{2\pi} \Big(\int_{-\infty}^{\infty} (u_1 + \theta)^2 \, e^{-\dfrac{\beta\theta^2}{2}} \, \mathrm{d}\theta \Big) \Big(\int_{-\infty}^{\infty} (u_2 + \theta) \, e^{-\dfrac{\beta\theta^2}{2}} \, \mathrm{d}\theta \Big) \; = \; \rho \, \Big(u_1^2 + \frac{1}{\beta} \Big) \, u_2$$

$$\int_{\mathbb{R}^2} v_1^2 \, v_2 \, f_0(v) \, \mathrm{d}v = \rho \Big(u_1^2 + \frac{1}{\beta} \Big) \, u_2 . \tag{1.82}$$

The D2Q9 model asked to evaluate the momentum associated to the square of the kinetic energy:

$$\int_{\mathbb{R}^2} \Big(\frac{1}{2}\,|v|^2\Big)^2 \, f_0(v)\,\mathrm{d}v = \frac{1}{4}\int_{\mathbb{R}^2} (v_1^2+v_2^2)^2\, f_0(v)\,\mathrm{d}v = \frac{1}{4}\int_{\mathbb{R}^2} (v_1^4+2\,v_1^2\,v_2^2+v_2^4)\, f_0(v)\,\mathrm{d}v$$

$$= \frac{1}{4}\,\frac{\rho\beta}{2\pi}\,\Big\{\Big(\int_{-\infty}^{\infty} (u_1^4+4\,u_1^3\,\theta+6\,u_1^2\,\theta^2+4\,u_1\,\theta^3+\theta^4)\, e^{-\dfrac{\beta\theta^2}{2}}\,\mathrm{d}\theta\Big)\times\sqrt{\frac{2\pi}{\beta}}$$

$$+2\Big(\int_{-\infty}^{\infty} (u_1^2+2\,u_1\,\theta+\theta^2)\, e^{-\dfrac{\beta\theta^2}{2}}\,\mathrm{d}\theta\Big)\Big(\int_{-\infty}^{\infty} (u_2^2+2\,u_2\,\theta+\theta^2)\, e^{-\dfrac{\beta\theta^2}{2}}\,\mathrm{d}\theta\Big)$$

$$+\sqrt{\frac{2\pi}{\beta}}\,\Big(\int_{-\infty}^{\infty} (u_2^4+4\,u_2^3\,\theta+6\,u_2^2\,\theta^2+4\,u_2\,\theta^3+\theta^4)\, e^{-\dfrac{\beta\theta^2}{2}}\,\mathrm{d}\theta\Big)\Big\}$$

$$= \frac{\rho}{4}\,\Big\{\Big(u_1^4+\frac{6}{\beta}\,u_1^2+\frac{3}{\beta^2}\Big)+2\Big(u_1^2+\frac{1}{\beta}\Big)\Big(u_2^2+\frac{1}{\beta}\Big)+\Big(u_2^4+\frac{6}{\beta}\,u_2^2+\frac{3}{\beta^2}\Big)\Big\} = \frac{\rho}{4}\,\Big(|u|^4+\frac{8}{\beta}\,|u|^2+\frac{8}{\beta^2}\Big)$$

and

$$\int_{\mathbb{R}^2} \Big(\frac{1}{2}\,|v|^2\Big)^2 \, f_0(v)\,\mathrm{d}v = \rho\,\Big(\frac{2}{\beta^2}+\frac{2}{\beta}\,|u|^2+\frac{1}{4}\,|u|^4\Big). \tag{1.83}$$

Referring to the relationship $\delta_4 = -18$ (equation (54b)) in Lallemand-Luo [95] page 6554 of volume 61, number 6 in *Physical Review E*, for the nine velocities two-dimensional model, everything happens as if

$$\int_{\mathbb{R}^2} \Big(\frac{1}{2}\,|v|^2\Big)^2 \, f_0(v)\,\mathrm{d}v \simeq \rho\,\Big(\frac{2}{\beta^2}+\frac{5}{4\,\beta}\,|u|^2\Big)\ ! \tag{1.84}$$

CHAPTER 2

SECOND ORDER ANALYSIS OF FLUID MODELS WITH LATTICE BOLTZMANN SCHEMES

We show [1] that when we formulate the lattice Boltzmann equation with a small time step Δt and an associated space scale Δx, a Taylor expansion joined with the so-called equivalent equation methodology leads to establish macroscopic fluid equations as a formal limit. We recover the Euler equations of gas dynamics at the first order and the compressible Navier-Stokes equations at the second order.

2.1 DISCRETE GEOMETRY

• We denote by d the dimension of space and by $\mathscr{L}$ a regular d-dimensional lattice. Such a lattice is composed by a set $\mathscr{L}^0$ of nodes or vertices and a set $\mathscr{L}^1$ of links or edges between two vertices. From a practical point of view, given a vertex x, there exists a set $V(x)$ of neighbouring nodes, including the node x itself. We consider here that the lattice $\mathscr{L}$ is parametrized by a space step $\Delta x > 0$. For the fundamental example called D2Q9 (see *e.g.* Qian, d'Humières and Lallemand [113]), the set $V(x)$ is given with the help of the family of vectors $(e_j)_{0 \leqslant j \leqslant J}$ defined by $J = 8$,

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

and the vicinity

$$V(x) = \{x + \Delta x\, e_j,\ 0 \leqslant j \leqslant J\}. \tag{2.1}$$

In the general case, we still suppose that the equation (2.1) holds but we do not make any precise definition concerning the integer J and the nondimensionalized vectors $(e_j)_{0 \leqslant j \leqslant J}$. Nevertheless if x is a node of the lattice ($x \in \mathscr{L}^0$), then $y^j = x + \Delta x\, e_j$ is an other node of the lattice, *i.e.* $y^j \in \mathscr{L}^0$.

2.2 LATTICE BOLTZMANN FRAMEWORK

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

$$\lambda = \frac{\Delta x}{\Delta t} \tag{2.2}$$

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

$$\Delta t\ v_j = \Delta x\, e_j\,, \quad 0 \leqslant j \leqslant J. \tag{2.3}$$

[1] in this contribution previously published in [43]

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

$$x \in \mathscr{L}^0 \implies x + \Delta t \; v_j \in \mathscr{L}^0 \,, \quad \forall j = 0, \dots J.$$

- According to D'Humières [80], the lattice Boltzmann scheme describes the dynamics of the density $f^j(x, t)$ of particles of velocity v_j at the node x and for the discrete time t. We introduce the $d+1$ scalar "conservative variables" $W(x, t)$ composed by the density ρ and the momentum q. Note that it is also possible to take into account the conservation of the total energy (see D'Humières's article for example). We have

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

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

and

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

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

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

in such a way that

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

- Following D'Humières [80], we introduce the "moment vector" m according to

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

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

$$m^0 \equiv \rho \,, \quad m^\alpha \equiv q^\alpha \,, \quad 1 \leqslant \alpha \leqslant d \,.$$

In other words, the matrix M satisfies

$$M_j^0 \equiv 1 \,, \quad M_j^\alpha \equiv v_j^\alpha \,, \quad 0 \leqslant j \leqslant J \,, \quad 1 \leqslant \alpha \leqslant d \,. \tag{2.10}$$

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

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

$$f^j = \sum_{k=0}^{J} (M^{-1})^j_k \, m^k , \quad 0 \leq j \leq J . \tag{2.11}$$

When f^j_{eq} is determined according to the relation (2.7), the associated equilibrium moments m^k_{eq} are given simply according to (2.9), *i.e.* in this case

$$m^k_{\rm eq} = \sum_{j=0}^{J} M^k_j \, f^j_{\rm eq} , \quad 0 \leq k \leq J . \tag{2.12}$$

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

$$m^i_{\rm eq} = m^i = W^i , \quad 0 \leq i \leq d . \tag{2.13}$$

2.3 COLLISION STEP

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

$$m^i_*(x,\,t) = m^i(x,\,t) , \quad 0 \leq i \leq d . \tag{2.14}$$

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

$$s_k = \frac{\Delta t}{\tau_k} , \quad d+1 \leq k \leq J .$$

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

$$m^k_*(x,\,t) = (1-s_k)\, m^k(x,\,t) + s_k \, m^k_{\rm eq} , \quad d+1 \leq k \leq J . \tag{2.15}$$

Proposition 1. Explicit Euler scheme.

The numerical scheme (2.15) is exactly the explicit Euler scheme relative to the continuous in time relaxation equation

$$\frac{\rm d}{{\rm d}t}\big(m^k - m^k_{\rm eq}\big) + \frac{1}{\tau_k}\big(m^k - m^k_{\rm eq}\big) = 0 , \quad d+1 \leq k \leq J . \tag{2.16}$$

Proof of Proposition 1.

Following *e.g.* Strang [127], we know that the explicit Euler scheme for the evolution (2.16) takes the form

$$\frac{1}{\Delta t}\Big[\big(m^k - m^k_{\rm eq}\big)(t+\Delta t) - \big(m^k - m^k_{\rm eq}\big)(t)\Big] + \frac{1}{\tau_k}\big(m^k - m^k_{\rm eq}\big)(t) = 0 . \tag{2.17}$$

We have by construction the relation (2.14), that is $m^i(t+\Delta t) = m^i(t)$ for $0 \leqslant i \leqslant d$ with these notations. Then $W(t+\Delta t) = W(t)$ and, due to the relation (2.7), $f^j_{\rm eq}(t+\Delta t) = f^j_{\rm eq}(t)$ after the collision step for all the components j of the particle distribution. Due to (2.12), we deduce that $m^k_{\rm eq}(t+\Delta t) = m^k_{\rm eq}(t)$ for all $k \leqslant J$. Thus the expression (2.17) takes the simpler form

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

which is exactly (2.15), except the change of notations: $m^k(t+\Delta t)$ is replaced by m^k_*. □

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

$$0 \leqslant \Delta t \leqslant 2\,\tau_k .$$

We will suppose in the following that

$$0 < s_k \leqslant 2, \quad d+1 \leqslant k \leqslant J.$$

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

- The particle distribution f^j_* after the collision step follows the relation (2.11). We have precisely after the collision step

$$f^j_* = \sum_{k=0}^{J} (M^{-1})^j_k \, m^k_*, \quad 0 \leqslant j \leqslant J. \tag{2.18}$$

2.4 ADVECTION STEP

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

$$f^j(x+v_j\,\Delta t,\, t+\Delta t) = f^j_*(x,\, t). \tag{2.19}$$

We re-write this relation in term of the "arrival" node $x+v_j\,\Delta t$. We set $\widetilde{x} = x+v_j\,\Delta t$, then we have $x = \widetilde{x} - v_j\,\Delta t$ and going back to the notation x, we write the relation (2.19) in the equivalent manner

$$f^j(x,\, t+\Delta t) = f^j_*(x - v_j\,\Delta t,\, t), \quad 0 \leqslant j \leqslant J, \quad x \in \mathscr{L}^0. \tag{2.20}$$

Proposition 2. Upwind scheme for the advection equation.

The scheme (2.20) for the advection step of the lattice Boltzmann method is nothing else that the explicit upwind scheme for the advection equation

$$\frac{\partial f^j}{\partial t} + v_j \bullet \nabla f^j = 0\,, \quad 0 \leqslant j \leqslant J\,,$$

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

$$\sigma_j \equiv \mid v_j \mid \frac{\Delta t}{\Delta x \mid e_j \mid}$$

equal, due to the definition (2.3), to unity: $\sigma_j = 1$.

Proof of Proposition 2.

When the Courant-Friedrichs-Lewy number σ_j is equal to unity, it is classical (see *e*.g. Strang [127]) that the upwind scheme is exact for the advection equation. □

2.5 EQUIVALENT EQUATION AT ZERO ORDER

• The lattice Boltzmann scheme is defined by the relations (2.4) to (2.9), (2.15) and (2.20). It is parametrized by the lattice step Δx, the matrix M linking the particle distribution f and the moment vector m, the choice of the conservative moments, the nonlinear equilibrium function $G(\bullet)$, the time step Δt and the ratios s_k between the time step and the collision time constants for nonequilibrium moments. In what follows, we fix the geometrical and topological structure of the lattice $\mathscr{L}$, we fix the matrix M and the equilibrium function $G(\bullet)$, we fix also the ratio λ defined in (2.2) and last but not least, we suppose that the parameters s_k for $k \geqslant d+1$ have a fixed value. Then the whole lattice Boltzmann scheme depends on the single parameter Δt.

• We explore now formally what are the partial differential equations associated with the Boltzmann numerical scheme, following the so-called "equivalent equation method" introduced and developed by Lerat-Peyret [100] and Warming-Hyett [133]. This approach is based on the assumption, that a sufficiently smooth function exists which satisfies the difference equation at the grid points. This assumption gives formal responses to put in evidence partial differential equations that minimimize the truncation errors of the numerical scheme. Nevertheless, we note here that this method of analysis fails to predict initial layers and boundary effects properly, as discussed by Griffiths and Sanz-Serna [72] or Chang [25]. The idea of the calculus is to suppose that all the data are sufficiently regular and to expand all the variables with the Taylor formula.

Proposition 3. Taylor expansion at zero order.

With the lattice Boltzmann defined previously, we have

$$f^j(x, t) = f^j_{eq}(x, t) + \mathrm{O}(\Delta t)\,, \quad 0 \leqslant j \leqslant J\,, \tag{2.21}$$

$$f^j_*(x, t) = f^j_{eq}(x, t) + \mathrm{O}(\Delta t)\,, \quad 0 \leqslant j \leqslant J\,, \tag{2.22}$$

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

Proof of Proposition 3.

The key point is to expand the relation (2.20) relative to the infinitesimal Δt. We have on one hand

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

and on the other hand

$$f_*^j(x - v_j\,\Delta t,\, t) \,=\, f_*^j(x,\, t) \,+\, \mathrm{O}(\Delta t)$$

Then $\quad m_*^k(x,\, t) \,=\, \sum_{j=0}^{J} M_j^k\, f_*^j(x,\, t) \;=\; m^k(x,\, t) + \mathrm{O}(\Delta t) \qquad$ and

$$m_*^k(x,\, t) \,-\, m^k(x,\, t) \,=\, \mathrm{O}(\Delta t)\,. \tag{2.23}$$

But, due to (2.15), we have

$$m_*^k(x,\, t) \,-\, m^k(x,\, t) \,=\, -s_k\big(m^k(x,\, t) - m_{\mathrm{e}q}^k(x,\, t)\big)\,. \tag{2.24}$$

From (2.23) and (2.24) we deduce, due to the fact that $s_k \neq 0$ when $k \geqslant d+1$:

$$m^k(x,\, t) \,=\, m_{\mathrm{e}q}^k(x,\, t) + \mathrm{O}(\Delta t)\,, \quad k \geqslant d+1\,. \tag{2.25}$$

We insert (2.25) into (2.23) and we deduce

$$m_*^k(x,\, t) \,=\, m_{\mathrm{e}q}^k(x,\, t) + \mathrm{O}(\Delta t)\,, \quad k \geqslant d+1\,. \tag{2.26}$$

Taking into account the relations (2.13) and (2.14) on one hand and (2.11) and (2.18) on the other hand, we deduce (2.21) and (2.22) from (2.25) and (2.26). □

2.6 TAYLOR EXPANSION AT FIRST ORDER

• We expand now the relation (2.20) one step further with respect to the time step Δt. We introduce the second order moment

$$F^{\alpha\,\beta} \equiv \sum_{j=0}^{J} v_j^\alpha\; v_j^\beta\; f_{\mathrm{e}q}^j\,, \quad 1 \leqslant \alpha,\, \beta \leqslant d\,. \tag{2.27}$$

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

Proposition 4. Euler equations of gas dynamics.

With the lattice Boltzmann scheme previously defined, we have the conservation of mass and momentum at the first order:

$$\partial_t \rho \,+\, \sum_{\beta=1}^{d} \partial_\beta\, q^\beta \;=\; \mathrm{O}(\Delta t) \tag{2.28}$$

$$\partial_t q^\alpha \,+\, \sum_{\beta=1}^{d} \partial_\beta\, F^{\alpha\,\beta} \;=\; \mathrm{O}(\Delta t)\,. \tag{2.29}$$

Proof of Proposition 4.

We expand both sides of relation (2.20) up to first order:

$f^j(x,\,t+\Delta t) = f^j(x,\,t) + \Delta t\,\partial_t f^j + \mathrm{O}(\Delta t^2)$

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

We take the moment of order k of this identity:

$$m^k(x,\,t) + \Delta t\,\partial_t m^k + \mathrm{O}(\Delta t^2) = = m_*^k(x,\,t) - \Delta t \sum_{j=0}^{J} M_j^k\, v_j^\beta\,\partial_\beta f_*^j + \mathrm{O}(\Delta t^2)$$

and we use the previous Taylor expansions (2.21) (2.22) at the order zero:

$$m^k(x,\,t) + \Delta t\,\partial_t m_{eq}^k = m_*^k(x,\,t) - \Delta t \sum_{j=0}^{J} M_j^k\, v_j^\beta\,\partial_\beta f_{eq}^j + \mathrm{O}(\Delta t^2)\,. \tag{2.30}$$

We take $k=0$ inside the relation (2.30). We get (2.28) since $m^0(x,\,t) \equiv m_*^0(x,\,t) \equiv \rho(x,\,t)$. Considering now the particular case $k=\alpha$ with $1 \leqslant \alpha \leqslant d$, we have also $m^\alpha(x,\,t) \equiv m_*^\alpha(x,\,t) \equiv q^\alpha(x,\,t)$ and the relation (2.29) is a direct consequence of the definition (2.27) and the property (2.10). □

Proposition 5. Technical lemma.

We introduce the "conservation defect" θ^k according to the relation

$$\theta^k(x,\,t) = \partial_t m_{eq}^k + \sum_{j=0}^{J} M_j^k\, v_j^\beta\,\partial_\beta f_{eq}^j \equiv \sum_{j=0}^{J} M_j^k\,(\partial_t f_{eq}^j + v_j^\beta\,\partial_\beta f_{eq}^j)\,. \tag{2.31}$$

Then we have the following properties:

$$m^k(x,\,t) = m_{eq}^k(x,\,t) - \frac{\Delta t}{s_k}\,\theta^k + \mathrm{O}(\Delta t^2)\,,\quad k \geqslant d+1\,, \tag{2.32}$$

$$m_*^k(x,\,t) = m_{eq}^k(x,\,t) - \Big(\frac{1}{s_k} - 1\Big)\,\Delta t\,\theta^k + \mathrm{O}(\Delta t^2)\,,\quad k \geqslant d+1\,, \tag{2.33}$$

$$\partial_\beta f_*^j = \partial_\beta f_{eq}^j - \Delta t \sum_{k=d+1}^{J} \Big(\frac{1}{s_k} - 1\Big)\,(M^{-1})_k^j\,\partial_\beta \theta^k + \mathrm{O}(\Delta t^2)\,. \tag{2.34}$$

Proof of Proposition 5.

We start from the relation (2.30) and we have observed at the previous proposition that

$$\theta^i = \mathrm{O}(\Delta t)\,,\quad 0 \leqslant i \leqslant d\,. \tag{2.35}$$

We remark also that from the relation (2.24), we have

$m^k(x,\,t) - m_{eq}^k(x,\,t) = \dfrac{1}{s_k}\big(m^k(x,\,t) - m_*^k(x,\,t)\big)\quad \text{if } k \geqslant d+1.$

Then the relation (2.32) is a direct consequence of (2.30) and the definition (2.31). In consequence, the relation (2.33) follows from (2.32) and (2.30). Due to (2.33), (2.35) and (2.18), we have

$$f_*^j(x,\,t) = f_{eq}^j(x,\,t) - \Delta t \sum_{k \geqslant d+1} \Big(\frac{1}{s_k} - 1\Big)\,(M^{-1})_k^j\,\theta^k + \mathrm{O}(\Delta t^2) \tag{2.36}$$

and the relation (2.34) follows from derivating (2.36) in the direction x_β. □

2.7 EQUIVALENT EQUATION AT SECOND ORDER

- We introduce the so-called "momentum-velocity tensor" $\Lambda_k^{\alpha\beta}$ according to

$$\Lambda_k^{\alpha\beta} \equiv \sum_{j=0}^{J} v_j^\alpha \, v_j^\beta \, (M^{-1})_k^j , \quad 1 \leqslant \alpha, \beta \leqslant d, \quad 0 \leqslant k \leqslant J. \tag{2.37}$$

We can now establish the major result of our contribution.

Proposition 6. Navier-Stokes equations of gas dynamics.

With the lattice Boltzmann method defined in previous sections and the conservation defect θ^k defined in 2.31), we have the following expansions up to second order accuracy:

$$\partial_t \rho + \sum_{\beta=1}^{d} \partial_\beta \, q^\beta = \mathrm{O}(\Delta t^2) \tag{2.38}$$

$$\partial_t q^\alpha + \sum_{\beta=1}^{d} \partial_\beta \Big(F^{\alpha\beta} - \Delta t \sum_{k \geqslant d+1} \Big(\frac{1}{s_k} - \frac{1}{2} \Big) \Lambda_k^{\alpha\beta} \, \theta^k \Big) = \mathrm{O}(\Delta t^2) . \tag{2.39}$$

- A consequence of relation (2.39) is the fact that a lattice Boltzmann scheme approximates at second order of accuracy a Navier-Stokes type equation with viscosities μ_k of the form

$$\mu_k = \Delta t \Big(\frac{1}{s_k} - \frac{1}{2} \Big) . \tag{2.40}$$

We refer for the details to D. D'Humières [80], Lallemand and Luo [95] or to the survey [42]. The relations (2.40) are known as the "Hénon's relations" [77]. We observe that in practice, the scalar μ_k is imposed by the physics and by the parameter Δt is constrained by the space discretization Δx and the relation (2.2). Then the parameter s_k must be chosen in order to satisfy the D'Humières relations (2.40).

Proof of Proposition 6.

We start again from the identity (2.20). We expand both terms up to second order accuracy:

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

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

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

$$\left\{ \begin{array}{l} m^i(x, t) + \Delta t \, \partial_t m^i + \frac{1}{2} \Delta t^2 \, \partial_{tt}^2 m^i + \mathrm{O}(\Delta t^3) = \\ m_*^i(x, t) - \Delta t \sum_{j=0}^{J} M_j^i \, v_j^\beta \, \partial_\beta f_*^j + \frac{1}{2} \Delta t^2 \sum_{j=0}^{J} M_j^i \, v_j^\beta \, v_j^\gamma \, \partial_{\beta\gamma}^2 f_*^j + \mathrm{O}(\Delta t^3) . \end{array} \right. \tag{2.41}$$

We use the microscopic conservation $m_*^i(x, t) \equiv m^i(x, t)$ in (2.41) and the previous Taylor expansion at order one, in particular the relation (2.34). We divide by Δt and we deduce:

$$\partial_t m^i + \frac{1}{2}\Delta t\, \partial^2_{tt} m^i = -\sum_{j=0}^{J} M^i_j\, v^\beta_j\, \partial_\beta f^j_{\text{eq}} + \Delta t \sum_{j=0}^{J} \sum_{k\geqslant d+1} M^i_j\, v^\beta_j \Big(\frac{1}{s_k} - 1\Big) (M^{-1})^j_k\, \partial_\beta \theta^k +$$

$$+ \frac{1}{2}\Delta t \sum_{j=0}^{J} M^i_j\, v^\beta_j\, v^\gamma_j\, \partial^2_{\beta\gamma} f^j_{\text{eq}} + \mathrm{O}(\Delta t^2)\,.$$

Then

$$\left\{ \begin{aligned} &\partial_t m^i + \sum_{\beta=1}^{d}\sum_{j=0}^{J} M^i_j\, v^\beta_j\, \partial_\beta f^j_{\text{eq}} = \Delta t \sum_{\beta=1}^{d}\sum_{j=0}^{J}\sum_{k\geqslant d+1} M^i_j\, v^\beta_j \Big(\frac{1}{s_k} - 1\Big)(M^{-1})^j_k\, \partial_\beta\theta^k + \\ &\qquad + \frac{\Delta t}{2}\Big(-\partial^2_{tt} m^i + \sum_{\beta=1}^{d}\sum_{j=0}^{J} M^i_j\, v^\beta_j\, v^\gamma_j\, \partial^2_{\beta\gamma} f^j_{\text{eq}} \Big) + \mathrm{O}(\Delta t^2)\,. \end{aligned} \right. \tag{2.42}$$

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

$$\partial^2_{tt} m^0 = \partial^2_{tt}\rho = -\sum_{\beta=1}^{d} \partial^2_{t\beta}\, q^\beta + \mathrm{O}(\Delta t) = -\sum_{\beta=1}^{d} \partial_\beta \partial_t\, q^\beta + \mathrm{O}(\Delta t) =$$

$$= \sum_{\beta=1}^{d}\sum_{\gamma=1}^{d} \partial^2_{\beta\gamma} F^{\beta\gamma} + \mathrm{O}(\Delta t) = \sum_{\beta=1}^{d}\sum_{\gamma=1}^{d}\sum_{j=0}^{J} v^\beta_j\, v^\gamma_j\, \partial^2_{\beta\gamma} f^j_{\text{eq}} + \mathrm{O}(\Delta t)$$

and the third line of (2.42) is null up to second order accuracy. Thus the conservation of mass (2.38) up to second order accuracy is established.

- We set $i = \alpha$ with $1 \leqslant \alpha \leqslant d$ and we look for the conservation of momentum. In this particular case, the relation (2.42) takes the form:

$$\left\{ \begin{aligned} &\partial_t q^\alpha + \sum_{\beta=1}^{d}\sum_{j=0}^{J} v^\alpha_j\, v^\beta_j\, \partial_\beta f^j_{\text{eq}} = \Delta t \sum_{k\geqslant d+1} \Big(\frac{1}{s_k} - 1\Big) \sum_{\beta=1}^{d} \Big[\sum_{j=0}^{J} v^\alpha_j\, v^\beta_j\, (M^{-1})^j_k \Big] \partial_\beta\theta^k + \\ &\qquad + \frac{\Delta t}{2}\Big(-\partial^2_{tt} q^\alpha + \sum_{\beta=1}^{d}\sum_{j=0}^{J} v^\alpha_j\, v^\beta_j\, v^\gamma_j\, \partial^2_{\beta\gamma} f^j_{\text{eq}} \Big) + \mathrm{O}(\Delta t^2)\,. \end{aligned} \right. \tag{2.43}$$

We have now to play with some algebra:

$$-\partial^2_{tt} q^\alpha + \sum_{\beta=1}^{d}\sum_{j=0}^{J} v^\alpha_j\, v^\beta_j\, v^\gamma_j\, \partial^2_{\beta\gamma} f^j_{\text{eq}} =$$

$$= \sum_{\beta=1}^{d} \Big(\partial_t \partial_\beta F^{\alpha\beta} + \sum_{j=0}^{J} v^\alpha_j\, v^\beta_j\, v^\gamma_j\, \partial^2_{\beta\gamma} f^j_{\text{eq}} \Big) + \mathrm{O}(\Delta t)$$

$$= \sum_{\beta=1}^{d} \partial_\beta \Big(\sum_{j=0}^{J} v^\alpha_j\, v^\beta_j \big(\partial_t f^j_{\text{eq}} + v^\gamma_j\, \partial_\gamma f^j_{\text{eq}} \big) \Big) + \mathrm{O}(\Delta t)$$

$$= \sum_{\beta=1}^{d} \partial_\beta \Big(\sum_{j=0}^{J} v^\alpha_j\, v^\beta_j \sum_{k=0}^{J} (M^{-1})^j_k\, \theta^k \Big) + \mathrm{O}(\Delta t)$$

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

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

due to the definition (2.37). We deduce from (2.27), (2.43) and the above calculus:

$$\partial_t q^\alpha + \sum_{\beta=1}^{d} \partial_\beta F^{\alpha\beta} = \Delta t \sum_{k \geqslant d+1} \Big(\frac{1}{s_k} - 1 \Big) \sum_{\beta=1}^{d} \Lambda_k^{\alpha\beta} \, \partial_\beta \theta^k + \frac{\Delta t}{2} \sum_{\beta=1}^{d} \partial_\beta \Big(\sum_{k \geqslant d+1} \Lambda_k^{\alpha\beta} \, \theta^k \Big) + \mathrm{O}(\Delta t^2)$$

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

and the relation (2.39) is established. □

CONCLUSION

- The previous propositions establish that the equivalent partial differential equations of a Boltzmann scheme are given up to second order accuracy by the same result as the formal Chapman-Enskog expansion. We find Euler type equation at the first order (Proposition 4) and Navier-Stokes type equation at the second order (Proposition 6). Note that with the above framework no *a priori* formal two-time multiple scaling is necessary to establish the Navier-Stokes equations from a lattice Boltzmann scheme, as done previously in the contribution of D'Humières. We remark also that a so-called diffusive scaling like $\frac{\Delta t}{\Delta x^2}$ = constant, instead of our condition (2.2) $\frac{\Delta t}{\Delta x}$ = constant, leads to the incompressible Navier-Stokes equations, as proposed by Junk, Klar and Luo [88]. In both cases, we have just to use the Taylor formula for a single infinitesimal parameter.

CHAPTER 3

A FUNDAMENTAL TWO-DIMENSIONAL FLUID LATTICE BOLTZMANN SCHEME

A lattice Boltzmann scheme contains many physical parameters to be set. Naturally, this requires a heavy investment. But this flexibility also allows the simulation of many physical phenomena, which makes the richness of the subject. We explore in this chapter the particular case of a conventional model for a Newtonian fluid. We detail the classical case of the nine velocities model on a bidimensional square lattice [1]. We first recall the basic features concerning the D2Q9 scheme. Then derive algebraic conditions to obtain the correct Euler equations of gas dynamics at first order of the Taylor expansion. We shortly recall a linearization methodology. Then consider the second order of the Taylor expansion octhe scheme and obtain conditions to enforce the approximation of the Navier Stokes equations of fluid dynamics in a baratropic approximation. We detail also the classical polynomial formulae to determine explicitly the particle distribution of the equilibrium state.

3.1 INTRODUCTION TO D2Q9

A lattice Boltzmann scheme contains many physical parameters to be set. Naturally, this requires a heavy investment. But this flexibility also allows the simulation of many physical phenomena, which makes the richness of the subject. We explore in this paragraph the particular case of a conventional model for a Newtonian fluid.

- Geometry.

The lattice is **two-dimensional** and associated to nine discrete velocities linking a given vertex to its **nine neighbours**. The notation "**D2Q9**", introduced by Qian in his thesis [112], gives a general and clear nomenclature. The lattice is cartesian and parameterized by a lenght Δx:

$$\mathcal{L} = (\Delta x\,\mathbb{Z}) \times (\Delta x\,\mathbb{Z})\,. \tag{3.1}$$

Nearby places of a given vertex $x \in \mathcal{L}$ are firstly x itself (with the number 0) and the other eight neighboring shown in Figure 3.1

$$y_j(x) = x + \Delta x\, e_j\,, \quad 0 \leqslant j \leqslant q-1 \equiv 8 \tag{3.2}$$

with

$$e_0 = \begin{pmatrix}0\\0\end{pmatrix},\ e_1 = \begin{pmatrix}1\\0\end{pmatrix},\ e_2 = \begin{pmatrix}0\\1\end{pmatrix},\ e_3 = \begin{pmatrix}-1\\0\end{pmatrix},\ e_4 = \begin{pmatrix}0\\-1\end{pmatrix},\ e_5 = \begin{pmatrix}1\\1\end{pmatrix},\ e_6 = \begin{pmatrix}-1\\1\end{pmatrix},\ e_7 = \begin{pmatrix}-1\\-1\end{pmatrix},\ e_8 = \begin{pmatrix}1\\-1\end{pmatrix}. \tag{3.3}$$

[1] A part of this chapter is the english translation of a part of the reference [42].

A numerical scale velocity is defined from the datum of a time step Δt:

$$\lambda = \frac{\Delta x}{\Delta t}. \tag{3.4}$$

In the following, we suppose that this parameter is fixed.

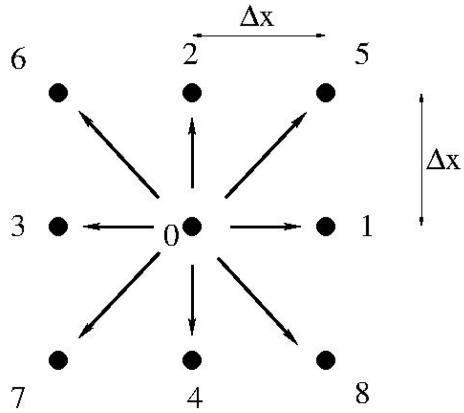

Figure 3.1 – *Discrete velocity vectors $(e_j)_{0\leqslant j\leqslant J}$ for the D2Q9 lattice.*

- Moments at equilibrium

For a classical fluid problem, the moments at equilibrium are the density ρ and the two components of the momentum J. We have $W \equiv (\rho\,, J_x\,, J_x) \equiv (\rho\,, J_1\,, J_2) \equiv (m_0, m_1, m_2)$:

$$\rho \;=\; m_0 \equiv \sum_{j=0}^{8} f_j \tag{3.5}$$

$$J_\alpha \;=\; m_\alpha \equiv \sum_{j=0}^{8} e_j^\alpha\,\lambda\, f_j\,, \quad 1 \leqslant \alpha \leqslant 2 \tag{3.6}$$

where e_j^α are the cartesian components of the vectors e_j introduced in (3.3). We will also denote the discrete velocity $\lambda\, e_j$ with the notation v_j:

$$v_j = \lambda\, e_j\,.$$

We have

$$J_x = J_1 \;=\; \lambda\,(f_1 - f_3 + f_5 - f_6 - f_7 + f_8) \tag{3.7}$$

$$J_y = J_2 \;=\; \lambda\,(f_2 - f_4 + f_5 + f_6 - f_7 - f_8)\,. \tag{3.8}$$

- Nonconserved moments

We basically follow the work of Lallemand and Luo [95], although our ratings may be different. We construct an other representation of the particle distribution f with so-called moments m through a fixed invertible matrix M. We have

$$m_k = \sum_{j=0}^{8} M_{kj}\, f_j\,. \tag{3.9}$$

The first lines of the matrix M are associated to the conserved moments $\rho,\ J_x$ and J_y. From (3.5), (3.7) and (3.8) we have

$$M_{0j} = 1\,, \quad M_{1j} = v_j^1\,, \quad M_{2j} = v_j^2\,.$$

The nonconserved moments are numbered 3 to 8 and have to be constructed. The philosophy is to consider moments of the discrete particle distribution $\big(f_j\big)_{0\leqslant j\leqslant 8}$ of higher and higher degree that respect invariance properties. Non strictly correct algebraic formulas are given according to

$$\left\{\begin{array}{l} \varepsilon = m_3 \simeq \sum\limits_{j=0}^{8} \dfrac{1}{2}\,|v_j|^2 f_j\,, \quad XX = m_4 \simeq \sum\limits_{j=0}^{8} \Big[\big(v_j^1\big)^2 - \big(v_j^2\big)^2\Big] f_j\,, \quad XY = m_5 \simeq \sum\limits_{j=0}^{8} v_j^1\, v_j^2\, f_j\,, \\ q_x = m_6 \simeq \sum\limits_{j=0}^{8} \dfrac{1}{2}\,|v_j|^2\, v_j^1 f_j\,, \quad q_y = m_7 \simeq \sum\limits_{j=0}^{8} \dfrac{1}{2}\,|v_j|^2\, v_j^2 f_j\,, \quad \varepsilon_2 = m_8 \simeq \sum\limits_{j=0}^{8} \dfrac{1}{2}\Big(\dfrac{1}{2}\,|v_j|^2\Big)^2 f_j \end{array}\right. \tag{3.10}$$

and we have the usual nomenclature

$$m = \big(\rho, J_x, J_y, \varepsilon, XX, XY, q_x, q_y, \varepsilon_2\big)^{\rm t}\,.$$

We observe that ε is the total energy and $q_x\,,\, q_y$ the two components of the heat flux. Following the usual framework developped by Lallemand and Luo [95], we impose for the matrix M to have orthogonal rows:

$$\sum_j M_{kj}\, M_{pj} = 0\,, \qquad 0 \leqslant k \neq p \leqslant 8\,. \tag{3.11}$$

We implement a Gram-Schmidt algorithm in order to satisfy the condition (3.11) with an initial family given by (3.5), (3.7), (3.8) and (3.10). The calculus is elementary, presented in a very close form in [42]. We have:

Proposition 1. Orthogonal matrix for the D2Q9 scheme.

After Gram-Schmidt orthogonalisation, the family (3.10) can be written as

$$\left\{\begin{array}{l} \varepsilon = m_3 = 3 \sum\limits_{j=0}^{8} |v_j|^2 f_j - 4\,\lambda^2 \sum\limits_{j=0}^{8} f_j \\ XX = m_4 = \sum\limits_{j=0}^{8} \Big[\big(v_j^1\big)^2 - \big(v_j^2\big)^2\Big] f_j \\ XY = m_5 = \sum\limits_{j=0}^{8} v_j^1\, v_j^2\, f_j \\ q_x = m_6 = 3 \sum\limits_{j=0}^{8} |v_j|^2\, v_j^1 f_j - 5\lambda^2 \sum\limits_{j=0}^{8} v_j^1 f_j \\ q_y = m_7 = 3 \sum\limits_{j=0}^{8} |v_j|^2\, v_j^2 f_j - 5\lambda^2 \sum\limits_{j=0}^{8} v_j^2 f_j \\ \varepsilon_2 = m_8 = \dfrac{9}{2} \sum\limits_{j=0}^{8} |v_j|^4 f_j - \dfrac{21}{2}\,\lambda^2 \sum\limits_{j=0}^{8} |v_j|^2 f_j + 4\,\lambda^4 \sum\limits_{j=0}^{8} f_j \end{array}\right. \tag{3.12}$$

and the matrix M is finally given by:

$$M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 \\ 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \\ 0 & -2\lambda^3 & 0 & 2\lambda^3 & 0 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 \\ 0 & 0 & -2\lambda^3 & 0 & 2\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 4\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \end{pmatrix}. \tag{3.13}$$

The inverse M^-1 of the matrix (3.13) is given by

$$M^{-1} = \begin{pmatrix} \frac{1}{9} & 0 & 0 & -\frac{1}{9\lambda^2} & 0 & 0 & 0 & 0 & \frac{1}{9\lambda^4} \\ \frac{1}{9} & \frac{1}{6\lambda} & 0 & -\frac{1}{36\lambda^2} & \frac{1}{4\lambda^2} & 0 & -\frac{1}{6\lambda^3} & 0 & -\frac{1}{18\lambda^4} \\ \frac{1}{9} & 0 & \frac{1}{6\lambda} & -\frac{1}{36\lambda^2} & -\frac{1}{4\lambda^2} & 0 & 0 & -\frac{1}{6\lambda^3} & -\frac{1}{18\lambda^4} \\ \frac{1}{9} & -\frac{1}{6\lambda} & 0 & -\frac{1}{36\lambda^2} & \frac{1}{4\lambda^2} & 0 & \frac{1}{6\lambda^3} & 0 & -\frac{1}{18\lambda^4} \\ \frac{1}{9} & 0 & -\frac{1}{6\lambda} & -\frac{1}{36\lambda^2} & -\frac{1}{4\lambda^2} & 0 & 0 & \frac{1}{6\lambda^3} & -\frac{1}{18\lambda^4} \\ \frac{1}{9} & \frac{1}{6\lambda} & \frac{1}{6\lambda} & \frac{1}{18\lambda^2} & 0 & \frac{1}{4\lambda^2} & \frac{1}{12\lambda^3} & \frac{1}{12\lambda^3} & \frac{1}{36\lambda^4} \\ \frac{1}{9} & -\frac{1}{6\lambda} & \frac{1}{6\lambda} & \frac{1}{18\lambda^2} & 0 & -\frac{1}{4\lambda^2} & -\frac{1}{12\lambda^3} & \frac{1}{12\lambda^3} & \frac{1}{36\lambda^4} \\ \frac{1}{9} & -\frac{1}{6\lambda} & -\frac{1}{6\lambda} & \frac{1}{18\lambda^2} & 0 & \frac{1}{4\lambda^2} & -\frac{1}{12\lambda^3} & -\frac{1}{12\lambda^3} & \frac{1}{36\lambda^4} \\ \frac{1}{9} & \frac{1}{6\lambda} & -\frac{1}{6\lambda} & \frac{1}{18\lambda^2} & 0 & -\frac{1}{4\lambda^2} & \frac{1}{12\lambda^3} & -\frac{1}{12\lambda^3} & \frac{1}{36\lambda^4} \end{pmatrix}. \tag{3.14}$$

- Equilibrium and relaxation of the nonconserved moments.

During the relaxation step, the conserved variables $W \equiv (\rho, J_x, J_y)$ are not modified; the nonconserved moments m_3 to m_8 relax towards an equilibrium value m_k^{eq}. This equilibrium value is a function of the conserved variables:

$$m_k^{\text{eq}} = \psi_k(W), \qquad k \geqslant 3. \tag{3.15}$$

These functions $\psi_k(\bullet)$ are precised in the following of this chapter. In first approaches, we can suppose if necessary that the functions $\psi_k(\bullet)$ are linear functions of the conserved moments:

$$\psi_k(W) = C_{k0}\,\rho + C_{k1}\,J_1 + C_{k2}\,J_2, \qquad k \geqslant 3. \tag{3.16}$$

Moreover, the relaxation step $m \longrightarrow m^*$ needs also parameters s_k for $k \geqslant 3$ such that

$$m_k^* = m_k + s_k\big(m_k^{\text{eq}} - m_k\big). \tag{3.17}$$

The parameters σ_k introduced by Hénon [77] in the context of cellular automata are defined according to

$$\sigma_k = \frac{1}{s_k} - \frac{1}{2}. \tag{3.18}$$

We will denote also with a specialized nomenclature

$$\begin{cases} \varepsilon^{\mathrm{eq}} \equiv m_3^{\mathrm{eq}}, & XX^{\mathrm{eq}} \equiv m_4^{\mathrm{eq}}, & YY^{\mathrm{eq}} \equiv m_5^{\mathrm{eq}}, & q_x^{\mathrm{eq}} \equiv m_6^{\mathrm{eq}}, & q_y^{\mathrm{eq}} \equiv m_7^{\mathrm{eq}}, & \varepsilon_2^{\mathrm{eq}} \equiv m_8^{\mathrm{eq}} \\ \varepsilon^* \equiv m_3^*, & XX^* \equiv m_4^*, & YY^* \equiv m_5^*, & q_x^* \equiv m_6^*, & q_y^* \equiv m_7^*, & \varepsilon_2^* \equiv m_8^* \\ s_\varepsilon \equiv s_3, & s_{xx} \equiv s_4, & s_{xy} \equiv s_5, & s_{qx} \equiv s_6, & s_{qy} \equiv s_7, & s_{\varepsilon 2} \equiv s_8 \\ \sigma_\varepsilon \equiv \sigma_3, & \sigma_{xx} \equiv \sigma_4, & \sigma_{xy} \equiv \sigma_5, & \sigma_{qx} \equiv \sigma_6, & \sigma_{qy} \equiv \sigma_7, & \sigma_{\varepsilon 2} \equiv \sigma_8. \end{cases}$$

3.2 FIRST ORDER PARTIAL DIFFERENTIAL EQUATIONS

When using a lattice Boltzmann scheme, a grail is to have a precise approximation of the Navier-Stokes equations:

$$\partial_t \rho + \partial_x J_x + \partial_y J_y = 0 \tag{3.19}$$

$$\partial_t J_x + \partial_x\Big(\frac{J_x^2}{\rho} + p\Big) + \partial_x\Big(\frac{J_x J_y}{\rho}\Big) - \partial_x\big(\mu \partial_x u_x\big) - \partial_y\big(\mu \partial_y u_x\big) - \partial_x\big(\zeta\, \mathrm{div} u\big) = 0 \tag{3.20}$$

$$\partial_t J_y + \partial_x\Big(\frac{J_x J_y}{\rho}\Big) + \partial_y\Big(\frac{J_y^2}{\rho} + p\Big) - \partial_x\big(\mu \partial_x u_y\big) - \partial_y\big(\mu \partial_y u_y\big) - \partial_y\big(\zeta\, \mathrm{div} u\big) = 0 \tag{3.21}$$

with p the pressure field, $u \equiv \dfrac{J}{\rho} = (u_x\,,\, u_y)$ the velocity and $\mathrm{div} u \equiv \partial_x u_x + \partial_y u_y$.

- We want now to know if it is possible to fit some equilibrium functions ψ_k of the D2Q9 scheme in order to approximate the nonlinear first order Euler equations. We introduce the tensor Λ_{kp}^l of momentum-velocity (see also (2.37):

$$\Lambda_{kp}^l \equiv \sum_{j=0}^{q-1} M_{kj}\, M_{pj}\, (M^{-1})_{jl}\,, \quad 0 \leqslant k\,,\, p\,,\, l \leqslant 8\,. \tag{3.22}$$

Then the equivalent equations at first order of the lattice Boltzmann scheme can be written, with an implicit summation on (1, 2) for the repeted greek indices and from 0 to 8 for the latin indices, as

$$\partial_t \rho + \partial_\alpha J_\alpha = \mathrm{O}(\Delta t) \tag{3.23}$$

$$\partial_t J_\alpha + \Lambda_{\alpha\beta}^l\, \partial_\beta m_l^{\mathrm{eq}} = \mathrm{O}(\Delta t)\,, \qquad 1 \leqslant \alpha \leqslant 2\,. \tag{3.24}$$

- We introduce "reduced" two by two matrices Λ^l according to

$$\Lambda^l \equiv \Big(\Lambda_{\alpha\beta}^l\Big)_{1 \leqslant \alpha,\, \beta \leqslant 2} \tag{3.25}$$

Then from (3.13) and (3.22) we obtain without difficulty:

$$\begin{cases} \Lambda^\rho \equiv \Lambda^0 = \dfrac{2}{3}\lambda^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \Lambda^1 = \Lambda^2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \Lambda^\varepsilon \equiv \Lambda^3 = \dfrac{1}{6}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ \Lambda^{xx} \equiv \Lambda^4 = \dfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \Lambda^{xy} \equiv \Lambda^5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \Lambda^6 = \Lambda^7 = \Lambda^8 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}. \end{cases} \tag{3.26}$$

In the sum on the left hand side of (3.24), only the indexes $l = 0,\ 3,\ 4$ and 5 are active *id est* are associated to a nontrivial expansion. The equations (3.24) can in consequence be written as

$$\left\{ \begin{array}{l} \partial_t J_x + \partial_x \Big(\dfrac{2}{3} \lambda^2 \rho + \dfrac{1}{6} \varepsilon^{\rm eq} + \dfrac{1}{2} XX^{\rm eq} \Big) + \partial_y XY^{\rm eq} = {\rm O}(\Delta t) \\ \partial_t J_y + \partial_x XY^{\rm eq} + \partial_y \Big(\dfrac{2}{3} \lambda^2 \rho + \dfrac{1}{6} \varepsilon^{\rm eq} - \dfrac{1}{2} XX^{\rm eq} \Big) = {\rm O}(\Delta t) \,. \end{array} \right. \tag{3.27}$$

We identify the equations (3.27) and the first order terms of the Navier-Stokes equations (3.20) and (3.21). We obtain the conditions

$$\left\{ \begin{array}{rcl} \dfrac{2}{3} \lambda^2 \rho + \dfrac{1}{6} \varepsilon^{\rm eq} + \dfrac{1}{2} XX^{\rm eq} &=& \rho \, u_x^2 + p \\ XY^{\rm eq} &=& \rho \, u_x \, u_y \\ \dfrac{2}{3} \lambda^2 \rho + \dfrac{1}{6} \varepsilon^{\rm eq} - \dfrac{1}{2} XX^{\rm eq} &=& \rho \, u_y^2 + p \,. \end{array} \right. \tag{3.28}$$

By solving the linear system (3.28), we have proved the following

Proposition 2. Equilibrium function of second order moments

The Euler equations of gas dynamics are recovered by the D2Q9 fluid lattice Bolzmann scheme at first order if and only if the second order moments ε, XX and XY have equilibrium values that satisfy

$$\left\{ \begin{array}{rcl} \varepsilon^{\rm eq} &=& 6 \, p - 4 \lambda^2 \rho + 3 \rho \, (u_x^2 + u_y^2) \\ XX^{\rm eq} &=& \rho \, (u_x^2 - u_y^2) \\ XY^{\rm eq} &=& \rho \, u_x \, u_y \,. \end{array} \right. \tag{3.29}$$

3.3 ADVECTIVE DISSIPATIVE LINEAR ACOUSTICS

- We will eventually consider an acoustic approximation, by linearization of the Navier-Stokes equations (3.19), (3.20) and (3.21) around a constant state $W_0 \equiv (\rho_0 \,, \rho_0 \, u_0 \,, \rho_0 \, v_0)$:

$$\rho = \rho_0 + \widetilde{\rho} \,, \quad J_x = \rho_0 \, u_0 + \widetilde{J}_x \,, \quad J_y = \rho_0 \, v_0 + \widetilde{J}_y \,.$$

The variation of pressure is a linear function of the variation of density and the related coefficient is exactly the square of the sound velocity:

$$\widetilde{p} = c_0^2 \, \widetilde{\rho} \tag{3.30}$$

and we have also the following elementary calculus, with the notation $\overrightarrow{u_0} = (u_0 \,, v_0)$:

$$\left\{ \begin{array}{rcl} \widetilde{u_x} &=& \widetilde{\dfrac{J_x}{\rho}} \;=\; -\dfrac{u_0}{\rho_0} \widetilde{\rho} + \dfrac{1}{\rho_0} \widetilde{J}_x \\ \widetilde{\dfrac{J_x^2}{\rho}} &=& -\dfrac{J_{x0}^2}{\rho_0^2} \widetilde{\rho} + 2 \dfrac{J_{x0}}{\rho_0} \widetilde{J}_x \;=\; -u_0^2 \, \widetilde{\rho} + 2 \, u_0 \, \widetilde{J}_x \\ \widetilde{\dfrac{J_x J_y}{\rho}} &=& -u_0 \, v_0 \, \widetilde{\rho} + v_0 \, \widetilde{J}_x + u_0 \, \widetilde{J}_y \\ \widetilde{\partial_x u_x} &=& \partial_x \Big(-\dfrac{u_0}{\rho_0} \widetilde{\rho} + \dfrac{1}{\rho_0} \widetilde{J}_x \Big) \;=\; -\dfrac{u_0}{\rho_0} \partial_x \widetilde{\rho} + \dfrac{1}{\rho_0} \partial_x \widetilde{J}_x \\ \partial_x \widetilde{(\mu \, \partial_x u_x)} &=& -\partial_x \left(\dfrac{\mu_0 \, u_0}{\rho_0} \, \partial_x \widetilde{\rho} \right) + \partial_x \left(\dfrac{\mu_0}{\rho_0} \, \partial_x \widetilde{J}_x \right) \\ \widetilde{{\rm div} u} &=& -\dfrac{1}{\rho_0} \, \overrightarrow{u_0} \bullet \nabla \widetilde{\rho} + \dfrac{1}{\rho_0} \, {\rm div} \widetilde{J} \end{array} \right.$$

and associated relations by changing the numbering of the coordinate. Dropping away the “tilda” notation, we can now write the linear equations of advective acoustics for the conservation of momentum:

$$\left\{ \begin{array}{l} \partial_t J_x + (c_0^2 - u_0^2)\,\partial_x \rho + 2\,u_0\,\partial_x J_x - u_0\,v_0\,\partial_y \rho + v_0\,\partial_y J_x + u_0\,\partial_y J_y \\ \qquad - \partial_x\Big(\dfrac{\mu_0}{\rho_0}\,\partial_x J_x\Big) - \partial_y\Big(\dfrac{\mu_0}{\rho_0}\,\partial_y J_x\Big) + \partial_x\Big(\dfrac{\mu_0\,u_0}{\rho_0}\,\partial_y \rho\Big) + \partial_y\Big(\dfrac{\mu_0\,u_0}{\rho_0}\,\partial_y \rho\Big) \\ \qquad - \partial_x\Big(\dfrac{\zeta_0}{\rho_0}\,\mathrm{div} J\Big) - \partial_x\Big(\dfrac{\zeta_0}{\rho_0}\,\overrightarrow{u_0}\bullet\nabla\rho\Big) = 0 \end{array} \right. \tag{3.31}$$

$$\left\{ \begin{array}{l} \partial_t J_y - u_0\,v_0\,\partial_x \rho + v_0\,\partial_x J_x + u_0\,\partial_x J_y + (c_0^2 - u_0^2)\,\partial_y \rho + 2\,u_0\,\partial_y J_y \\ \qquad - \partial_x\Big(\dfrac{\mu_0}{\rho_0}\,\partial_x J_y\Big) - \partial_y\Big(\dfrac{\mu_0}{\rho_0}\,\partial_y J_y\Big) + \partial_x\Big(\dfrac{\mu_0\,v_0}{\rho_0}\,\partial_x \rho\Big) + \partial_y\Big(\dfrac{\mu_0\,v_0}{\rho_0}\,\partial_y \rho\Big) \\ \qquad - \partial_y\Big(\dfrac{\zeta_0}{\rho_0}\,\mathrm{div} J\Big) - \partial_y\Big(\dfrac{\zeta_0}{\rho_0}\,\overrightarrow{u_0}\bullet\nabla\rho\Big) = 0 \end{array} \right. \tag{3.32}$$

A natural question is to know if it is possible to fit the various parameters C_{ki} of (3.16) and σ_k of (3.17) of the D2Q9 scheme in order to approximate the second order linearized advective acoustics composed by the equations (3.19), (3.31) and (3.32). Yhis approach is very usefull for an implementation with formal calculus.

3.4 SECOND ORDER PARTIAL DIFFERENTIAL EQUATIONS

In this section, we do our best to recover the Navier Stokes equations of gas dynamics in a barotropic regime. Mass and momentum are conserved. We do not consider the conservation of energy and thermodynamics is reduced to a simple relation between pressure and density. The method is to apply the Taylor expansion method developed in the chapter 2.

We introduce the so-called “conservation defect” θ_k (see also (2.31)) according to:

$$\theta_k \equiv \partial_t m_k^{\mathrm{eq}} + \Lambda_{k\beta}^l\,\partial_\beta m_l^{\mathrm{eq}}, \qquad k \geqslant 3. \tag{3.33}$$

The second order equivalent partial differential equations take the form (see (2.39)):

$$\partial_t \rho + \partial_\alpha J_\alpha = \mathrm{O}(\Delta t^2) \tag{3.34}$$

$$\partial_t J_\alpha + \Lambda_{\alpha\beta}^l\,\partial_\beta m_l^{\mathrm{eq}} - \Delta t \sum_{l\geqslant 3} \sigma_l\,\Lambda_{\alpha\beta}^l\,\partial_\beta \theta_l = \mathrm{O}(\Delta t^2)\,. \tag{3.35}$$

In order to explicit the left hand side of the equations (3.35), we first observe that the matrices Λ^l are all reduced to zero, except for $l = 3, 4$ and 5 as observed in (3.26). We must in consequence explicit the conservation defects $\theta_\varepsilon \equiv \theta_3$, $\theta_{xx} \equiv \theta_4$ and $\theta_{xy} \equiv \theta_5$. For doing this, we have to consider the coefficients $\Lambda_{k\beta}^l$ for all the values $0 \leqslant k \leqslant 8$ and $1 \leqslant \beta \leqslant 2$. We introduce new reduced matrices Λ_k (with an index at a lower position), that are matrices with 2 lines and 9 columns:

$$\Lambda_k \equiv \Big(\Lambda_{k\beta}^l\Big)_{1\leqslant\beta\leqslant 2,\,0\leqslant l\leqslant 8} \tag{3.36}$$

and after some lignes of elementary algebra, we have

$$\left\{\begin{array}{l} \Lambda_\varepsilon \equiv \Lambda_3 = \begin{pmatrix} 0 & \lambda^2 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \lambda^2 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \\ \Lambda_{xx} \equiv \Lambda_4 = \begin{pmatrix} 0 & \frac{\lambda^2}{3} & 0 & 0 & 0 & 0 & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & -\frac{\lambda^2}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 \end{pmatrix}, \\ \Lambda_{xy} \equiv \Lambda_5 = \begin{pmatrix} 0 & 0 & \frac{2\lambda^2}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 \\ 0 & \frac{2\lambda^2}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 \end{pmatrix}. \end{array}\right. \tag{3.37}$$

We deduce from the expression (3.33) of the conservation defects and from the previous expressions (3.37) of the reduced momentum-velocity tensors the following

Proposition 3. First expression of the conservation defect for the second order moments

We have, with $q \equiv (q_x\,,\, q_y)$,

$$\left\{\begin{array}{rcl} \theta_\varepsilon &=& \partial_t \varepsilon^{\rm eq} + \lambda^2\, {\rm div} J + {\rm div} q \\ \theta_{xx} &=& \partial_t XX^{\rm eq} + \dfrac{\lambda^2}{3}\big(\partial_x J_x - \partial_y J_y\big) + \dfrac{1}{3}\big(-\partial_x q_x^{\rm eq} + \partial_y q_y^{\rm eq}\big) \\ \theta_{xy} &=& \partial_t XY^{\rm eq} + \dfrac{2\lambda^2}{3}\big(\partial_y J_x + \partial_x J_y\big) + \dfrac{1}{3}\big(\partial_y q_x^{\rm eq} + \partial_x q_y^{\rm eq}\big). \end{array}\right. \tag{3.38}$$

Proposition 4. Second expression of the conservation defect for the second order moments

Taking into account on one hand the expression (3.29) of the equilibrium momenta $\varepsilon^{\rm eq}$, $XX^{\rm eq}$ and $XY^{\rm eq}$, and on the other hand the D2Q9 first order equivalent equations (3.23) (3.24) and the Euler equations issued from (3.19), (3.20) and (3.21), with $\mu = \zeta = 0$, we have the following expressions for the three useful defects of conservation θ_ε, θ_{xx} and θ_{xy}, with $c^2 \equiv {\rm d}p/{\rm d}\rho$ the square of the sound velocity:

$$\theta_\varepsilon = \left\{\begin{array}{l} -6\,c^2\big(u_x\,\partial_x\rho + u_y\,\partial_y\rho\big) + (5\,\lambda^2 - 6\,c^2)\,{\rm div}J \\ \qquad + \partial_x\big(q_x^{\rm eq} - 3|u|^2 J_x\big) + \partial_y\big(q_y^{\rm eq} - 3|u|^2 J_y\big) + {\rm O}(\Delta t) \end{array}\right. \tag{3.39}$$

$$\theta_{xx} = \left\{\begin{array}{l} -2\,c^2\big(u_x\,\partial_x\rho - u_y\,\partial_y\rho\big) + \partial_x\Big[\Big(\dfrac{\lambda^2}{3} + u_y^2 - u_x^2\Big)J_x - \dfrac{1}{3}\,q_x^{\rm eq}\Big] \\ \qquad - \partial_y\Big[\Big(\dfrac{\lambda^2}{3} + u_y^2 - u_x^2\Big)J_y - \dfrac{1}{3}\,q_y^{\rm eq}\Big] + {\rm O}(\Delta t) \end{array}\right. \tag{3.40}$$

$$\theta_{xy} = \left\{\begin{array}{l} -c^2\big(u_y\,\partial_x\rho + u_x\,\partial_y\rho\big) + \partial_x\Big(-u_x\,u_y\,J_x + \dfrac{2\,\lambda^2}{3}\,J_y + \dfrac{1}{3}\,q_y^{\rm eq}\Big) \\ \qquad + \partial_y\Big(-u_x\,u_y\,J_y + \dfrac{2\,\lambda^2}{3}\,J_x + \dfrac{1}{3}\,q_x^{\rm eq}\Big) + {\rm O}(\Delta t) \end{array}\right. \tag{3.41}$$

Proof of Proposition 4.

We have

$$\begin{aligned} \partial_t\varepsilon^{\rm eq} &= \partial_t\Big(6\,p - 4\,\lambda^2\,\rho + 3\,\frac{j_x^2 + J_y^2}{\rho}\Big) \\ &= \big(6\,c^2 - 4\,\lambda^2\big)\,\partial_t\rho - 3\,\big(u_x^2 + u_y^2\big)\,\partial_t\rho + 6\,(u_x\,\partial_t J_x + u_y\,\partial_t J_y) \end{aligned}$$

$$= \big(4\,\lambda^2-6\,c^2+3\,|u|^2\big)\,(\partial_x J_x+\partial_y J_x) - 6u_x\left[\partial_x\Big(\frac{J_x^2}{\rho}+p\Big)+\partial_y\Big(\frac{J_x J_y}{\rho}\Big)\right] - 6u_y\left[\partial_x\Big(\frac{J_x J_y}{\rho}\Big)+\partial_y\Big(\frac{J_y^2}{\rho}+p\Big)\right]$$

$$= \big(4\,\lambda^2-6\,c^2+3\,|u|^2\big)\,(\partial_x J_x+\partial_y J_x) - 6u_x\left[(c^2-u_x^2)\,\partial_x\rho+2\,u_x\,\partial_x J_x - u_x\,u_y\,\partial_y\rho + u_y\,\partial_y J_x + u_x\,\partial_y J_x\right]$$
$$- 6u_y\left[-u_x\,u_y\,\partial_x\rho + u_y\,\partial_x J_x + u_x\,\partial_x J_y + (c^2-u_y^2)\,\partial_y\rho + 2\,u_y\,\partial_y J_y\right] + \mathrm{O}(\Delta t)$$

$$= 6\big(u_x^3+u_x\,u_y^2-u_x\,c^2\big)\,\partial_x\rho + 6\big(u_x^2\,u_y+u_y^3-u_y\,c^2\big)\,\partial_y\rho + \big(4\,\lambda^2-6\,c^2-9\,u_x^2-3\,u_y^2\big)\,\partial_x J_x$$
$$- 6\,u_x\,u_y\,\partial_y J_x - 6\,u_x\,u_y\,\partial_x J_y + \big(4\,\lambda^2-6\,c^2-3\,u_x^2-9\,u_y^2\big)\,\partial_y J_y + \mathrm{O}(\Delta t)$$

$$= -6\,c^2\,(u_x\,\partial_x\rho+u_y\,\partial_y\rho) + \big(4\,\lambda^2-6\,c^2\big)\,\mathrm{div}J - 3\,\partial_x\big(|u|^2\,J_x\big) - 3\,\partial_y\big(|u|^2\,J_y\big) + \mathrm{O}(\Delta t)$$

and the expression (3.39) is a direct consequence of the previous expresion $\partial_t\varepsilon^{\mathrm{eq}}$ and the first relation of (3.38). For the second moment of second order, we have

$$\partial_t XX^{\mathrm{eq}} = \partial_t\left(\frac{J_x^2-J_y^2}{\rho}\right) = -\big(u_x^2-u_y^2\big)\,\partial_t\rho + 2\,u_x\,\partial_t J_x + 2\,u_y\,\partial_t J_y$$

$$= -\big(u_x^2-u_y^2\big)\,\mathrm{div}J - 2\,u_x\left[(c^2-u_x^2)\,\partial_x\rho + 2\,u_x\,\partial_x J_x - u_x\,u_y\,\partial_y\rho + u_y\,\partial_y J_x + u_x\,\partial_y J_x\right]$$
$$+ 2\,u_y\left[-u_x\,u_y\,\partial_x\rho + u_y\,\partial_x J_x + u_x\,\partial_x J_y + (c^2-u_y^2)\,\partial_y\rho + 2\,u_y\,\partial_y J_y\right] + \mathrm{O}(\Delta t)$$

$$= 2\big(u_x^3-u_x\,u_y^2-u_x\,c^2\big)\,\partial_x\rho + 2\big(u_x^2\,u_y-u_y^3+u_y\,c^2\big)\,\partial_y\rho + \big(u_y^2-3\,u_x^2\big)\,\partial_x J_x + 2\,u_x\,u_y\,\partial_x J_y$$
$$- 2\,u_x\,u_y\,\partial_y J_x + \big(3\,u_y^2-u_x^2\big)\,\partial_x J_x + \mathrm{O}(\Delta t)$$

$$= -2\,c^2\,(u_y\,\partial_x\rho+u_x\,\partial_y\rho) + \partial_x\Big[\big(u_y^2-u_x^2\big)\,J_x\Big] + \partial_y\Big[\big(u_x^2-u_y^2\big)\,J_y\Big] + \mathrm{O}(\Delta t)$$

and the expression (3.40) is a direct consequence of the previous expresion of $\partial_t XX^{\mathrm{eq}}$ and the second relation of (3.38). For the third moment of second order, we have

$$\partial_t XY^{\mathrm{eq}} = \partial_t\left(\frac{J_x J_y}{\rho}\right) = -u_x\,u_y\,\partial_t\rho + u_y\,\partial_t J_x + u_x\,\partial_t J_y$$

$$= u_x\,u_y\,(\partial_x J_x+\partial_y J_x) - u_y\left[\partial_x\Big(\frac{J_x^2}{\rho}+p\Big)+\partial_y\Big(\frac{J_x J_y}{\rho}\Big)\right] - u_x\left[\partial_x\Big(\frac{J_x J_y}{\rho}\Big)+\partial_y\Big(\frac{J_y^2}{\rho}+p\Big)\right] + \mathrm{O}(\Delta t)$$

$$= u_x\,u_y\,\mathrm{div}J - u_y\left[(c^2-u_x^2)\,\partial_x\rho + 2\,u_x\,\partial_x J_x - u_x\,u_y\,\partial_y\rho + u_y\,\partial_y J_x + u_x\,\partial_y J_x\right]$$
$$- u_x\left[-u_x\,u_y\,\partial_x\rho + u_y\,\partial_x J_x + u_x\,\partial_x J_y + (c^2-u_y^2)\,\partial_y\rho + 2\,u_y\,\partial_y J_y\right] + \mathrm{O}(\Delta t)$$

$$= -c^2\,(u_y\,\partial_x\rho+u_x\,\partial_y\rho) - 2\,u_x\,u_y\,\partial_x J_x - u_x^2\,\partial_x J_y + 2\,u_x^2\,u_y\,\partial_x\rho + 2\,u_x\,u_y^2\,\partial_y\rho - 2\,u_x\,u_y\,\partial_y J_y + \mathrm{O}(\Delta t)$$

$$= -c^2\,(u_y\,\partial_x\rho+u_x\,\partial_y\rho) - \partial_x\big(u_x\,u_y\,J_x\big) - \partial_y\big(u_x\,u_y\,J_y\big) + \mathrm{O}(\Delta t)$$

and the expression (3.41) is a direct consequence of the previous expresion $\partial_t XY^{\mathrm{eq}}$ and the third relation of (3.38). The proof is completed. □

Proposition 5. Second order terms for the D2Q9 scheme

The second order terms $D_\alpha \equiv \Delta t\,\sum_{l\geqslant 3}\sigma_l\,\Lambda^l_{\alpha\beta}\,\partial_\beta\theta_l$ of the equivalent partial differential equations

(3.35) of the D2Q9 fluid scheme admit the following expressions:

$$
D_x = \left\{ \begin{array}{l}
\Delta t \Big\{ \sigma_\varepsilon \, \partial_x \Big[\Big(\frac{5\lambda^2}{6} - c^2 \Big) \big(\partial_x J_x + \partial_y J_y \big) + \frac{1}{6} \big(\partial_x q_x^{\rm eq} + \partial_y q_y^{\rm eq} \big) \Big] \\
\qquad + \sigma_{xx} \, \partial_x \Big[\partial_x \Big(\frac{\lambda^2}{6} J_x - \frac{1}{6} q_x^{\rm eq} \Big) - \partial_y \Big(\frac{\lambda^2}{6} J_y - \frac{1}{6} q_y^{\rm eq} \Big) \Big] \\
\qquad + \sigma_{xy} \, \partial_y \Big[\partial_x \Big(\frac{2\lambda^2}{3} J_y + \frac{1}{3} q_y^{\rm eq} \Big) + \partial_y \Big(\frac{2\lambda^2}{3} J_x + \frac{1}{3} q_x^{\rm eq} \Big) \Big] \\
\qquad + \sigma_\varepsilon \, \partial_x \big[- c^2 \big(u_x \partial_x \rho + u_y \partial_y \rho \big) \big] \\
\qquad + \sigma_{xx} \, \partial_x \big[- c^2 \big(u_x \partial_x \rho - u_y \partial_y \rho \big) \big] \; + \; \sigma_{xy} \, \partial_y \big[- c^2 \big(u_y \partial_x \rho + u_x \partial_y \rho \big) \big] \\
\qquad + \sigma_\varepsilon \; \Big[\partial_x^2 \big(- \frac{1}{2} |u|^2 J_x \big) \; + \; \partial_x \partial_y \big(- \frac{1}{2} |u|^2 J_y \big) \Big] \\
\qquad + \sigma_{xx} \Big[\partial_x^2 \big(\frac{u_y^2 - u_x^2}{2} J_x \big) - \partial_x \partial_y \big(\frac{u_y^2 - u_x^2}{2} J_y \big) \Big] + \sigma_{xy} \; \big[- \partial_x \partial_y \big(u_x u_y J_x \big) - \partial_y^2 \big(u_x u_y J_y \big) \big] \Big\}
\end{array} \right. \tag{3.42}
$$

$$
D_y = \left\{ \begin{array}{l}
\Delta t \Big\{ \sigma_\varepsilon \, \partial_y \Big[\Big(\frac{5\lambda^2}{6} - c^2 \Big) \big(\partial_x J_x + \partial_y J_y \big) + \frac{1}{6} \big(\partial_x q_x^{\rm eq} + \partial_y q_y^{\rm eq} \big) \Big] \\
\qquad + \sigma_{xx} \, \partial_y \Big[\partial_x \Big(- \frac{\lambda^2}{6} J_x + \frac{1}{6} q_x^{\rm eq} \Big) - \partial_y \Big(- \frac{\lambda^2}{6} J_y + \frac{1}{6} q_y^{\rm eq} \Big) \Big] \\
\qquad + \sigma_{xy} \, \partial_x \Big[\partial_x \Big(\frac{2\lambda^2}{3} J_y + \frac{1}{3} q_y^{\rm eq} \Big) + \partial_y \Big(\frac{2\lambda^2}{3} J_x + \frac{1}{3} q_x^{\rm eq} \Big) \Big] \\
\qquad + \sigma_\varepsilon \, \partial_y \big[- c^2 \big(u_x \partial_x \rho + u_y \partial_y \rho \big) \big] \\
\qquad + \sigma_{xx} \, \partial_y \big[c^2 \big(u_x \partial_x \rho - u_y \partial_y \rho \big) \big] \; + \; \sigma_{xy} \, \partial_x \big[- c^2 \big(u_y \partial_x \rho + u_x \partial_y \rho \big) \big] \\
\qquad + \sigma_\varepsilon \; \Big[\partial_x \partial_y \big(- \frac{1}{2} |u|^2 J_x \big) \; + \; \partial_y^2 \big(- \frac{1}{2} |u|^2 J_y \big) \Big] \\
\qquad + \sigma_{xx} \Big[- \partial_x \partial_y \big(\frac{u_y^2 - u_x^2}{2} J_x \big) + \partial_y^2 \big(\frac{u_y^2 - u_x^2}{2} J_y \big) \Big] + \sigma_{xy} \; \big[- \partial_x^2 \big(u_x u_y J_x \big) - \partial_x \partial_y \big(u_x u_y J_y \big) \big] \Big\} .
\end{array} \right. \tag{3.43}
$$

Proof of Proposition 5.

We have, taking into account the relations (3.39), (3.40) and (3.41),

$$
\begin{array}{l}
\dfrac{D_x}{\Delta t} = \displaystyle\sum_{l \geqslant 3} \sigma_l \, \Lambda_{1\beta}^l \, \partial_\beta \theta_l \; = \; \frac{\sigma_\varepsilon}{6} \partial_x \theta_\varepsilon + \frac{\sigma_{xx}}{2} \partial_x \theta_{xx} + \sigma_{xy} \partial_y \theta_{xy} \\
\quad = \sigma_\varepsilon \partial_x \Big[- c^2 \big(u_x \partial_x \rho + u_y \partial_y \rho \big) + \Big(\dfrac{5\lambda^2}{6} \; - \; c^2 \Big) {\rm div} J + \partial_x \Big(\dfrac{1}{6} q_x^{\rm eq} - \dfrac{1}{2} |u|^2 J_x \Big) + \partial_y \Big(\dfrac{1}{6} q_y^{\rm eq} - \dfrac{1}{2} |u|^2 J_y \Big) \Big] \\
\qquad + \sigma_{xx} \partial_x \Big[- c^2 \big(u_x \partial_x \rho - u_y \partial_y \rho \big) + \partial_x \Big[\Big(\dfrac{\lambda^2}{6} + \dfrac{1}{2} \big(u_y^2 - u_x^2 \big) \Big) J_x - \dfrac{1}{6} q_x^{\rm eq} \Big] \\
\qquad\qquad - \partial_y \Big[\Big(\dfrac{\lambda^2}{6} + \dfrac{1}{2} \big(u_y^2 - u_x^2 \big) \Big) J_y - \dfrac{\lambda^2}{3} q_y^{\rm eq} \Big] \Big] \\
\qquad + \sigma_{xy} \partial_y \Big[- c^2 \big(u_y \partial_x \rho + u_x \partial_y \rho \big) + \partial_x \Big(\dfrac{2\lambda^2}{3} J_y + \dfrac{1}{3} q_y^{\rm eq} \Big) + \partial_y \Big(\dfrac{2\lambda^2}{3} J_x + \dfrac{1}{3} q_x^{\rm eq} \Big) \\
\qquad\qquad - \partial_x \big(u_x u_y J_x \big) - \partial_y \big(u_x u_y J_y \big) \Big]
\end{array}
$$

and the relation (3.42) is just a re-ordering of the previous expression following the increasing powers of the velocity. In a similar way,

$$
\begin{array}{l}
\dfrac{D_y}{\Delta t} = \displaystyle\sum_{l \geqslant 3} \sigma_l \, \Lambda_{2\beta}^l \, \partial_\beta \theta_l \; = \; \frac{\sigma_\varepsilon}{6} \partial_y \theta_\varepsilon - \frac{\sigma_{xx}}{2} \partial_y \theta_{xx} + \sigma_{xy} \partial_x \theta_{xy} \\
\quad = \sigma_\varepsilon \partial_y \Big[- c^2 \big(u_x \partial_x \rho + u_y \partial_y \rho \big) + (\dfrac{5\lambda^2}{6} \; - \; c^2) \, {\rm div} J + \partial_x \Big(\dfrac{1}{6} q_x^{\rm eq} - \dfrac{1}{2} |u|^2 J_x \Big) + \partial_y \Big(\dfrac{1}{6} q_y^{\rm eq} - \dfrac{1}{2} |u|^2 J_y \Big) \Big] \\
\qquad - \sigma_{xx} \partial_y \Big[- c^2 \big(u_x \partial_x \rho - u_y \partial_y \rho \big) + \partial_x \Big[\Big(\dfrac{\lambda^2}{6} + \dfrac{1}{2} \big(u_y^2 - u_x^2 \big) \Big) J_x - \dfrac{1}{6} q_x^{\rm eq} \Big]
\end{array}
$$

$$
\begin{aligned}
&\qquad - \partial_y \Big[\Big(\frac{\lambda^2}{6} + \frac{1}{2} \big(u_y^2 - u_x^2\big) \Big) J_y - \frac{\lambda^2}{3}\, q_y^{\rm eq} \Big] \Big] \\
&+ \sigma_{xy}\, \partial_x \Big[- c^2 \big(u_y\, \partial_x \rho + u_x\, \partial_y \rho \big) + \partial_x \Big(\frac{2\,\lambda^2}{3}\, J_y + \frac{1}{3}\, q_y^{\rm eq} \Big) + \partial_y \Big(\frac{2\,\lambda^2}{3}\, J_x + \frac{1}{3}\, q_x^{\rm eq} \Big) \\
&\qquad - \partial_x \big(u_x\, u_y\, J_x \big) - \partial_y \big(u_x\, u_y\, J_y \big) \Big]
\end{aligned}
$$

and the relation (3.43) follow without difficulty. The proof of Proposition 5 is completed. □

- We have now to compare the expressions (3.42) (3.43) and the second order dissipation terms proposed by the Navier-Stokes equations in (3.20) and (3.21):

$$
D_x^{\rm NS} = \left\{ \begin{array}{l} \partial_x \Big(\frac{\mu}{\rho}\, \partial_x J_x \Big) + \partial_y \Big(\frac{\mu}{\rho}\, \partial_y J_x \Big) + \partial_x \Big(\frac{\zeta}{\rho} \big(\partial_x J_x + \partial_y J_y \big) \Big) \\ \quad - \partial_x \Big(\frac{\mu}{\rho}\, u_x\, \partial_x \rho \Big) - \partial_y \Big(\frac{\mu}{\rho}\, u_x\, \partial_y \rho \Big) - \partial_x \Big(\frac{\zeta}{\rho} \big(u_x\, \partial_x \rho + u_y\, \partial_y \rho \big) \Big) \end{array} \right. \tag{3.44}
$$

$$
D_y^{\rm NS} = \left\{ \begin{array}{l} \partial_x \Big(\frac{\mu}{\rho}\, \partial_x J_y \Big) + \partial_y \Big(\frac{\mu}{\rho}\, \partial_y J_y \Big) + \partial_y \Big(\frac{\zeta}{\rho} \big(\partial_x J_x + \partial_y J_y \big) \Big) \\ \quad - \partial_x \Big(\frac{\mu}{\rho}\, u_y\, \partial_x \rho \Big) - \partial_y \Big(\frac{\mu}{\rho}\, u_y\, \partial_y \rho \Big) - \partial_y \Big(\frac{\zeta}{\rho} \big(u_x\, \partial_x \rho + u_y\, \partial_y \rho \big) \Big) . \end{array} \right. \tag{3.45}
$$

Proposition 6. Identification of the second order terms at order zero in velocity

When we identify the second order dissipations given by the expressions (3.42) and (3.44) on one hand, (3.43) and (3.45) on the other hand, we obtain a necessary value for the shear viscosity

$$
\frac{\mu}{\rho} = \lambda^2\, \Delta t\, \frac{\sigma_{xx}\, \sigma_{xy}}{\sigma_{xx} + 2\, \sigma_{xy}} \tag{3.46}
$$

and for the bulk viscosity:

$$
\frac{\zeta}{\rho} = \lambda^2\, \Delta t\, \sigma_\varepsilon \left(\frac{\sigma_{xx}\, \sigma_{xy}}{\sigma_{xx} + 2\, \sigma_{xy}} - \frac{c^2}{\lambda^2} \right). \tag{3.47}
$$

Moreover, we have

$$
\frac{\partial q_x^{\rm eq}}{\partial J_x} = \frac{\partial q_y^{\rm eq}}{\partial J_y} = \frac{\sigma_{xx} - 4\, \sigma_{xy}}{\sigma_{xx} + 2\, \sigma_{xy}}\, \lambda^2 . \tag{3.48}
$$

Proof of Proposition 6.

At the ordre zero in velocity, the relation (3.44) shows that the coefficient $\frac{\mu+\zeta}{\rho}$ of $\partial_x^2 J_x$ is equal to the coefficient $\frac{\mu}{\rho}$ of $\partial_y^2 J_x$ plus the coefficient $\frac{\zeta}{\rho}$ of $\partial_x \partial_y J_y$. We have also an analogous relation in the equation (3.45) : the coefficient $\frac{\mu+\zeta}{\rho}$ of $\partial_y^2 J_y$ is equal to the coefficient $\frac{\mu}{\rho}$ of $\partial_x^2 J_y$ plus the coefficient $\frac{\zeta}{\rho}$ of $\partial_x \partial_y J_x$. We write this isotropy property for the relations (3.42) and (3.43), with the notation

$$
P \equiv \frac{\partial q_x^{\rm eq}}{\partial J_x} , \quad Q \equiv \frac{\partial q_y^{\rm eq}}{\partial J_y} .
$$

We have

$$\begin{aligned}
\mathrm{coeff}\Big(\partial_x^2 J_x\Big) &= \Big[\Big(\frac{5}{6}\,\lambda^2 - c^2\Big) + \frac{P}{6}\Big]\,\sigma_\varepsilon + \Big(\frac{\lambda^2}{6} - \frac{P}{6}\Big)\,\sigma_{xx} = \frac{\mu+\zeta}{\rho\,\Delta t} \\
\mathrm{coeff}\Big(\partial_y^2 J_x\Big) &= \Big(\frac{2}{3}\,\lambda^2 + \frac{P}{3}\Big)\,\sigma_{xy} = \frac{\mu}{\rho\,\Delta t} \\
\mathrm{coeff}\Big(\partial_x\partial_y J_y\Big) &= \Big[\Big(\frac{5}{6}\,\lambda^2 - c^2\Big) + \frac{Q}{6}\Big]\,\sigma_\varepsilon - \Big(\frac{\lambda^2}{6} - \frac{Q}{6}\Big)\,\sigma_{xx} + \Big(\frac{2}{3}\,\lambda^2 + \frac{Q}{3}\Big)\,\sigma_{xy} = \frac{\zeta}{\rho\,\Delta t}\,.
\end{aligned}$$

Then we have from the previous isotropy property:

$$\frac{\sigma_\varepsilon}{6}\,P + \frac{\lambda^2\,\sigma_{xx}}{6} - \frac{\sigma_{xx}}{6}\,P = \frac{2}{3}\,\lambda^2\,\sigma_{xy} + \frac{\sigma_{xy}}{3}\,P + \frac{1}{6}\big(\sigma_\varepsilon + \sigma_{xx} + 2\,\sigma_{xy}\big)\,Q - \frac{\lambda^2}{6}\,\sigma_{xx} + \frac{2}{3}\,\lambda^2\,\sigma_{xy}$$

and this relation can be written as

$$\frac{1}{6}\big(-\sigma_\varepsilon + \sigma_{xx} + 2\,\sigma_{xy}\big)\,P + \frac{1}{6}\big(\sigma_\varepsilon + \sigma_{xx} + 2\,\sigma_{xy}\big)\,Q = \frac{\lambda^2}{3}\,\big(\sigma_{xx} - 4\,\sigma_{xy}\big)\,. \tag{3.49}$$

We focus now on the equation (3.45):

$$\begin{aligned}
\mathrm{coeff}\Big(\partial_y^2 J_y\Big) &= \Big[\Big(\frac{5}{6}\,\lambda^2 - c^2\Big) + \frac{Q}{6}\Big]\,\sigma_\varepsilon + \Big(\frac{\lambda^2}{6} - \frac{Q}{6}\Big)\,\sigma_{xx} = \frac{\mu+\zeta}{\rho\,\Delta t} \\
\mathrm{coeff}\Big(\partial_x^2 J_y\Big) &= \Big(\frac{2}{3}\,\lambda^2 + \frac{Q}{3}\Big)\,\sigma_{xy} = \frac{\mu}{\rho\,\Delta t} \\
\mathrm{coeff}\Big(\partial_x\partial_y J_x\Big) &= \Big[\Big(\frac{5}{6}\,\lambda^2 - c^2\Big) + \frac{P}{6}\Big]\,\sigma_\varepsilon + \Big(-\frac{\lambda^2}{6} + \frac{P}{6}\Big)\,\sigma_{xx} + \Big(\frac{2}{3}\,\lambda^2 + \frac{P}{3}\Big)\,\sigma_{xy} = \frac{\zeta}{\rho\,\Delta t}\,.
\end{aligned}$$

and the second isotropy property takes the form

$$\frac{\sigma_\varepsilon}{6}\,Q + \frac{\lambda^2\,\sigma_{xx}}{6} - \frac{\sigma_{xx}}{6}\,Q = \frac{2}{3}\,\lambda^2\,\sigma_{xy} + \frac{\sigma_{xy}}{3}\,Q + \frac{1}{6}\big(\sigma_\varepsilon + \sigma_{xx} + 2\,\sigma_{xy}\big)\,P - \frac{\lambda^2}{6}\,\sigma_{xx} + \frac{2}{3}\,\lambda^2\,\sigma_{xy}$$

and we have a second relation

$$\frac{1}{6}\big(\sigma_\varepsilon + \sigma_{xx} + 2\,\sigma_{xy}\big)\,P + \frac{1}{6}\big(-\sigma_\varepsilon + \sigma_{xx} + 2\,\sigma_{xy}\big)\,Q = \frac{\lambda^2}{3}\,\big(\sigma_{xx} - 4\,\sigma_{xy}\big)\,. \tag{3.50}$$

We solve the linear system without difficulty:

$$P \equiv \frac{\partial q_x^{\mathrm{eq}}}{\partial J_x} = Q \equiv \frac{\partial q_y^{\mathrm{eq}}}{\partial J_y} = \frac{\sigma_{xx} - 4\,\sigma_{xy}}{\sigma_{xx} + 2\,\sigma_{xy}}\,\lambda^2\,. \tag{3.51}$$

and the relation (3.48) is established. Then we have

$$\frac{\mu}{\rho\,\Delta t} = \Big(\frac{2}{3}\,\lambda^2 + \frac{P}{3}\Big)\,\sigma_{xy} = \lambda^2\,\frac{\sigma_{xx}\,\sigma_{xy}}{\sigma_{xx} + 2\,\sigma_{xy}}$$

and the relation (3.46) is proven. On the other hand,

$$
\begin{aligned}
\frac{\zeta}{\rho\,\Delta t} &= \Big[\Big(\frac{5}{6}\lambda^2 - c^2\Big) + \frac{P}{6}\Big]\,\sigma_\varepsilon - \Big(-\frac{\lambda^2}{6} + \frac{P}{6}\Big)\,\sigma_{xx} + \Big(\frac{2}{3}\lambda^2 + \frac{P}{3}\Big)\,\sigma_{xy} \\
&= \Big(\frac{5}{6}\lambda^2 - c^2\Big)\sigma_\varepsilon - \frac{\lambda^2}{6}\,\sigma_{xx} + \frac{2}{3}\lambda^2\sigma_{xy} + \frac{1}{6}\big(\sigma_\varepsilon + \sigma_{xx} + 2\sigma_{xy}\big)\,P \\
&= \Big(\frac{5}{6}\lambda^2 - c^2\Big)\sigma_\varepsilon - \frac{\lambda^2}{6}\,\sigma_{xx} + \frac{2}{3}\lambda^2\sigma_{xy} + \frac{1}{6}\big(\sigma_\varepsilon + \sigma_{xx} + 2\sigma_{xy}\big)\,\frac{\sigma_{xx} - 4\sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}\,\lambda^2 \\
&= \sigma_\varepsilon\,\Big(\frac{5}{6}\lambda^2 - c^2 + \frac{1}{6}\,\frac{\sigma_{xx} - 4\sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}\,\lambda^2\Big) \;=\; \lambda^2\sigma_\varepsilon\,\Big(\frac{\sigma_{xx} + \sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}} - \frac{c^2}{\lambda^2}\Big)
\end{aligned}
$$

that establishes the relation (3.47) and the proposition is established. □

Proposition 7. Identification of the second order terms at order one in velocity

When we identify the second order dissipations given by the expressions (3.42) and (3.44) on one hand, (3.43) and (3.45) on one hand at order 1 relative to the velocity in a linearized approach, we obtain the following expressions for the sound velocity

$$c^2 = \frac{\lambda^2}{3}\,, \tag{3.52}$$

for the bulk viscosity:

$$\frac{\zeta}{\rho} = \lambda^2\,\Delta t\,\frac{\sigma_\varepsilon}{3}\,\frac{2\sigma_{xx} + \sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}\,. \tag{3.53}$$

and for the heat flux:

$$q_x^{\rm eq} = C_1\,J_x + \xi\,u\,\rho\,, \qquad q_y^{\rm eq} = C_1\,J_y + \xi\,v\,\rho\,, \tag{3.54}$$

with the coefficients C_1 and ξ determined according to

$$C_1 = \frac{\sigma_{xx} - 4\sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}\,\lambda^2\,, \qquad \xi = 6\,\frac{\sigma_{xy} - \sigma_{xx}}{\sigma_{xx} + 2\sigma_{xy}}\;c^2\,. \tag{3.55}$$

Proof of Proposition 7.

If we consider a linearized approach around a given state $W_0 = (\rho_0\,, \rho_0\,u_0\,\rho_0\,v_0)$, we have from the relation (3.48) of the previous proposition the developments

$$
\left\{
\begin{aligned}
q_x^{\rm eq} &= C_1\,J_x + u_0\,\xi_x + v_0\,\eta_x \\
q_y^{\rm eq} &= C_1\,J_y + u_0\,\xi_y + v_0\,\eta_y
\end{aligned}
\right. \tag{3.56}
$$

with C_1 proposed at the relation (3.55). We introduce this representation inside the expression (3.42). The term of order one relative to the advective velocity takes the form

$$D_x^1 = \left\{ \begin{array}{l} \Delta t \left\{ \dfrac{\sigma_\varepsilon}{6} \Big[u_0 \big(\partial_x^2 \xi_x + \partial_x \partial_y \xi_y \big) + v_0 \big(\partial_x^2 \eta_x + \partial_x \partial_y \eta_y \big) \Big] \right. \\ \qquad + \dfrac{\sigma_{xx}}{6} \Big[u_0 \big(- \partial_x^2 \xi_x + \partial_x \partial_y \xi_y \big) + v_0 \big(- \partial_x^2 \eta_x + \partial_x \partial_y \eta_y \big) \Big] \\ \qquad + \dfrac{\sigma_{xy}}{3} \Big[u_0 \big(\partial_x \partial_y \xi_y + \partial_y^2 \xi_x \big) + v_0 \big(\partial_x \partial_y \eta_y + \partial_y^2 \eta_x \big) \Big] \\ \qquad + c^2 \sigma_\varepsilon \Big(- u_0 \partial_x^2 \rho - v_0 \partial_x \partial_y \rho \Big) + c^2 \sigma_{xx} \Big(- u_0 \partial_x^2 \rho + v_0 \partial_x \partial_y \rho \Big) \\ \qquad \left. + c^2 \sigma_{xy} \Big(- u_0 \partial_y^2 \rho - v_0 \partial_x \partial_y \rho \Big) \right\} . \end{array} \right. \tag{3.57}$$

We identify the terms relative to u and v in (3.44) and (3.57). We obtain:

$$\left\{ \begin{array}{l} \dfrac{\sigma_\varepsilon}{6} \big(\partial_x^2 \xi_x + \partial_x \partial_y \xi_y \big) + \dfrac{\sigma_{xx}}{6} \big(- \partial_x^2 \xi_x + \partial_x \partial_y \xi_y \big) + \dfrac{\sigma_{xy}}{3} \big(\partial_x \partial_y \xi_y + \partial_y^2 \xi_x \big) \\ - c^2 \sigma_\varepsilon \partial_x^2 \rho - c^2 \sigma_{xx} \partial_x^2 \rho - c^2 \sigma_{xy} \partial_y^2 \rho = \dfrac{1}{\Delta t} \Big(- \dfrac{\mu_0}{\rho_0} \Delta \rho - \dfrac{\zeta_0}{\rho_0} \partial_x^2 \rho \Big) \end{array} \right. \tag{3.58}$$

$$\left\{ \begin{array}{l} \dfrac{\sigma_\varepsilon}{6} \big(\partial_x^2 \eta_x + \partial_x \partial_y \eta_y \big) + \dfrac{\sigma_{xx}}{6} \big(- \partial_x^2 \eta_x + \partial_x \partial_y \eta_y \big) + \dfrac{\sigma_{xy}}{3} \big(\partial_x \partial_y \eta_y + \partial_y^2 \eta_x \big) \\ - c^2 \sigma_\varepsilon \partial_x \partial_y \rho + c^2 \sigma_{xx} \partial_x \partial_y \rho - c^2 \sigma_{xy} \partial_x \partial_y \rho = \dfrac{1}{\Delta t} \Big(- \dfrac{\zeta_0}{\rho_0} \partial_x \partial_y \rho \Big) . \end{array} \right. \tag{3.59}$$

The relations (3.58) and (3.59) are identities between functions. The right hand side of (3.58) does not contain cross derivatives. So we deduce

$$\Big(\frac{\sigma_\varepsilon}{6} + \frac{\sigma_{xx}}{6} + \frac{\sigma_{xy}}{3} \Big) \partial_x \partial_y \xi_y \equiv 0 . \tag{3.60}$$

All the σ's coefficients are strictly positive. The relation (3.60) is an identity between functions and it implies that $\xi_y \equiv 0$. In an analogous way, the right hand side of (3.59) contains only cross derivatives. We identify the ∂_y^2 terms of the left hand side:

$$\frac{\sigma_{xy}}{3} \partial_y^2 \eta_x \equiv 0 \tag{3.61}$$

and $\eta_x \equiv 0$.

- In an analogous way, the function ξ_x *a priori* depends on ρ, J_x and J_y. But only the variable ρ is present in the right hand side of (3.58). Then the functional ξ_x is only a function of the variable ρ that we can *a priori* suppose linear taking into account our actual linear framework. Similarly, the functional η_y can not depend on the variables J_x and J_y that are absent at the right hand side of (3.59). It is only a function of the variable ρ. We have finally

$$\xi_x \equiv \xi \rho , \qquad \eta_y \equiv \eta \rho , \qquad \xi_y \equiv 0 , \qquad \eta_x \equiv 0 . \tag{3.62}$$

With the framework (3.62), we write again the relations (3.58) and (3.59). We get

$$\sigma_\varepsilon \Big(\frac{\xi}{6} - c^2 \Big) \partial_x^2 \rho + \sigma_{xx} \Big(- \frac{\xi}{6} - c^2 \Big) \partial_x^2 \rho + \sigma_{xy} \Big(\frac{\xi}{3} - c^2 \Big) \partial_y^2 \rho = \frac{1}{\Delta t} \Big(- \frac{\mu_0}{\rho_0} \Delta \rho - \frac{\zeta_0}{\rho_0} \partial_x^2 \rho \Big) \tag{3.63}$$

$$\sigma_\varepsilon\Big(\frac{\eta}{6}-c^2\Big)+\sigma_{xx}\Big(\frac{\eta}{6}+c^2\Big)+\sigma_{xy}\Big(\frac{\eta}{3}-c^2\Big)=-\frac{1}{\Delta t}\,\frac{\zeta_0}{\rho_0}\,. \tag{3.64}$$

The relation (3.63) generates two distinct relations because $\partial_x^2\rho$ and $\partial_y^2\rho$ are two independent variables:

$$\sigma_\varepsilon\Big(\frac{\xi}{6}-c^2\Big)+\sigma_{xx}\Big(-\frac{\xi}{6}-c^2\Big) = \frac{1}{\Delta t}\Big(-\frac{\mu_0}{\rho_0}-\frac{\zeta_0}{\rho_0}\Big) \tag{3.65}$$

$$\sigma_{xy}\Big(\frac{\xi}{3}-c^2\Big) = -\frac{1}{\Delta t}\,\frac{\mu_0}{\rho_0}\,. \tag{3.66}$$

• When we do the same treatment for the other equation of momentum conservation along the y direction, we obtain relations that are analogous to (3.64), (3.65) and (3.66), except that the parameters ξ and η are exchanged:

$$\sigma_\varepsilon\Big(\frac{\xi}{6}-c^2\Big)+\sigma_{xx}\Big(\frac{\xi}{6}+c^2\Big)+\sigma_{xy}\Big(\frac{\xi}{3}-c^2\Big) = -\frac{1}{\Delta t}\,\frac{\zeta_0}{\rho_0} \tag{3.67}$$

$$\sigma_\varepsilon\Big(\frac{\eta}{6}-c^2\Big)+\sigma_{xx}\Big(-\frac{\eta}{6}-c^2\Big) = \frac{1}{\Delta t}\Big(-\frac{\mu_0}{\rho_0}-\frac{\zeta_0}{\rho_0}\Big) \tag{3.68}$$

$$\sigma_{xy}\Big(\frac{\eta}{3}-c^2\Big) = -\frac{1}{\Delta t}\,\frac{\mu_0}{\rho_0}\,. \tag{3.69}$$

We deduce immediately

$$\eta\equiv\xi\,. \tag{3.70}$$

We use the relations (3.65), (3.66) and (3.67) for writing that $\mu_0+\zeta_0=\mu_0+\zeta_0$. It comes

$$-\sigma_{xx}\Big(\frac{\xi}{3}+2\,c^2\Big)-2\,\sigma_{xy}\Big(\frac{\xi}{3}-c^2\Big)=0$$

and finally

$$\xi = 6\,\frac{-\sigma_{xx}+\sigma_{xy}}{\sigma_{xx}+2\sigma_{xy}}\,c^2\,.$$

The relation (3.55) is established. We inject the expression (3.55) inside (3.66). We have

$$\sigma_{xy}\Big(c^2-\frac{\xi}{3}\Big)=\sigma_{xy}\,c^2\Big(1+2\,\frac{\sigma_{xx}-\sigma_{xy}}{\sigma_{xx}+2\sigma_{xy}}\Big)=3\,c^2\,\frac{\sigma_{xx}\,\sigma_{xy}}{\sigma_{xx}+2\sigma_{xy}}=\frac{1}{\Delta t}\,\frac{\mu_0}{\rho_0}\equiv\lambda^2\,\frac{\sigma_{xx}\,\sigma_{xy}}{\sigma_{xx}+2\sigma_{xy}}$$

due to the relation (3.46). We deduce from the previous line the necessary expression (3.52) of the sound velocity: $c^2=\lambda^2/3$.

• We focus now on a part of the left hand side of the relation (3.67):

$$\sigma_{xx}\Big(\frac{\xi}{6}+c^2\Big)+\sigma_{xy}\Big(\frac{\xi}{3}-c^2\Big)=\Big[\sigma_{xx}\Big(\frac{\sigma_{xy}-\sigma_{xx}}{\sigma_{xx}+2\sigma_{xy}}+1\Big)+\sigma_{xy}\Big(2\,\frac{\sigma_{xy}-\sigma_{xx}}{\sigma_{xx}+2\sigma_{xy}}-1\Big)\Big]\,c^2$$

$$=\Big(\frac{3\sigma_{xx}\,\sigma_{xy}}{\sigma_{xx}+2\sigma_{xy}}-\frac{3\sigma_{xy}\,\sigma_{xx}}{\sigma_{xx}+2\sigma_{xy}}\Big)\,c^2=0$$

and the relation (3.67) is reduced to

$$\sigma_\varepsilon \Big(\frac{\xi}{6} - c^2\Big) = -\frac{1}{\Delta t}\,\frac{\zeta_0}{\rho_0}\,.$$

We have now

$$\frac{1}{\Delta t}\,\frac{\zeta_0}{\rho_0} = \sigma_\varepsilon \Big(c^2 - \frac{\xi}{6}\Big) = \sigma_\varepsilon\, c^2 \Big(1 + \frac{\sigma_{xx} - \sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}\Big) = \sigma_\varepsilon\, c^2\, \frac{2\sigma_{xx} + \sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}} = \sigma_\varepsilon\, \frac{\lambda^2}{3}\, \frac{2\sigma_{xx} + \sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}$$

and the relation (3.53) is established. Observe also that if we inject the expression (3.52) of the sound velocity inside the relation (3.47), we have

$$\frac{1}{\Delta t}\,\frac{\zeta_0}{\rho_0} = \sigma_\varepsilon\, \lambda^2 \Big(\frac{\sigma_{xx} + \sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}} - \frac{1}{3}\Big) = \sigma_\varepsilon\, \frac{\lambda^2}{3}\, \frac{2\sigma_{xx} + \sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}$$

in coherence with the previous expression. The proposition 7 is established. □

Proposition 8. Towards nonlinearity

If we want to generalize the previous framework for nonlinear fluid mechanics, we must have

$$\sigma_{xx} = \sigma_{xy} \tag{3.71}$$

$$\frac{\mu}{\rho} = \frac{\mu_0}{\rho_0} = \frac{\lambda^2\,\Delta t}{3}\,\sigma_{xx} \tag{3.72}$$

$$\frac{\zeta}{\rho} = \frac{\zeta_0}{\rho_0} = \frac{\lambda^2\,\Delta t}{3}\,\sigma_\varepsilon \tag{3.73}$$

and the heat flux has the expression

$$q = -\lambda^2\, J. \tag{3.74}$$

Proof of Proposition 8.

The expression (3.54) of the heat flux is now nonlinear and has to be considered as a differential:

$$\mathrm{d}q_x^{\mathrm{eq}} = C_1\, \mathrm{d}J_x + \xi\, \frac{J_x}{\rho}\, \mathrm{d}\rho\,, \qquad \mathrm{d}q_y^{\mathrm{eq}} = C_1\, \mathrm{d}J_y + \xi\, \frac{J_y}{\rho}\, \mathrm{d}\rho\,,$$

with $C_1 = \frac{\sigma_{xx} - 4\sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}\, \lambda^2$ a true constant and $\xi = 6\, \frac{\sigma_{xx} - \sigma_{xy}}{\sigma_{xx} + 2\sigma_{xy}}\, c^2$ (*c.f.* (3.55) only function only of the density. We enforce the Schwarz relations in the previous expressions:

$$\frac{\partial C_1}{\partial \rho} = \frac{\partial}{\partial J_x}\Big(\xi\, \frac{J_x}{\rho}\Big) \tag{3.75}$$

Because $\frac{\partial C_1}{\partial \rho} = 0$ and $\frac{\partial \xi}{\partial J_x} = 0$ as observed previously, the relation (3.75) implies $\frac{\xi}{\rho} = 0$ and the relation (3.71) is established. Joined with the expressions (3.46) and (3.53), the constraint (3.71) immediatly establishes (3.72) and (3.73). In consequence of (3.71), we have also $C_1 = -\lambda^2$. Moreover, the condition $\xi = 0$ shows that $\mathrm{d}q_x^{\mathrm{eq}} = -\lambda^2\, \mathrm{d}J_x$ and the first component of (3.74) is clear. The proof is identical for the second component and the proposition is established. □

3.5 EQUILIBRIUM STATE

In the previous section, we have proved that the satisfaction of Navier Stokes equations at second order equivalent equations of the D2Q9 scheme with conservation of the moments ρ, J_x and J_y implies the knowledge of the following equilibria for the moments numbered from 4 to 7:

$$\left\{ \begin{array}{l} \varepsilon^{\mathrm{eq}} = -2\lambda^2 \rho + 3\,\dfrac{J_x^2 + J_y^2}{\rho}, \quad XX^{\mathrm{eq}} = \dfrac{J_x^2 - J_y^2}{\rho}, \quad YY^{\mathrm{eq}} = \dfrac{J_x J_y}{\rho}, \\ q_x^{\mathrm{eq}} = -\lambda^2 J_x, \quad q_y^{\mathrm{eq}} = -\lambda^2 J_y. \end{array} \right. \tag{3.76}$$

The equilibrium value of the last momentum ε_2 defined in (3.12) has no direct influence on the equivalent equations. In the following, we show that the most reasonable value is the following one:

$$\varepsilon_2^{\mathrm{eq}} = \lambda^4 \rho - 3\lambda^2 \,\frac{J_x^2 + J_y^2}{\rho}. \tag{3.77}$$

If this relation is satisfied, the family f_j^{eq} of particle distribution at equilibrium is given by the following proposition.

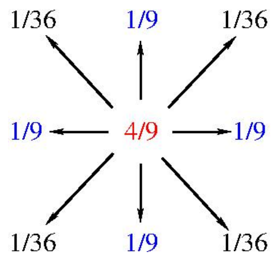

Figure 3.2 – *Ponderations ω_j (c.f. (3.79)) for the particle distribution of the D2Q9 lattice Boltzmann scheme.*

Proposition 9. Equilibrium particle distribution for the D2Q9 lattice Boltzmann scheme.

If the momenta m are defined with the relation $m \equiv M f$ and the matrix M explicited in (3.14), the equilibrium values (3.76) and (3.77) induces the following Qian's equilibrium [112, 113] for the particle distribution:

$$f_j^{\mathrm{eq}} = \rho\, \omega_j\, \psi_j(\rho, u), \qquad 0 \leqslant j \leqslant 8, \tag{3.78}$$

where the coefficients ω_j are illustrated on Figure 3.2

$$\omega_j = \left\{ \begin{array}{ll} \dfrac{4}{9}, & j = 0 \\ \dfrac{1}{9}, & 1 \leqslant j \leqslant 4 \\ \dfrac{1}{36}, & 5 \leqslant j \leqslant 8 \end{array} \right. \tag{3.79}$$

and the functions $\psi_j(\rho, u)$ defined from the elementary vectors introduced in (3.3):

$$\psi_j(\rho, u) = 1 + 3\,\frac{u \bullet e_j}{\lambda} + \frac{9}{2}\Big(\frac{u \bullet e_j}{\lambda}\Big)^2 - \frac{3}{2}\,\frac{|u|^2}{\lambda^2}. \tag{3.80}$$

Proof of Proposition 9.

The tedious by elementary product of the matrix M of (3.14) by the vector f^{eq} whose components are explicited in (3.78) is equal to the vector

$$m^{\mathrm{eq}} = \left\{ \begin{array}{c} \Big(\rho\,,\, \rho\, u_x\,,\, \rho\, u_y\,,\, -2\,\rho\,\lambda^2 + 3\rho\,(u_x^2 - 3 + u_y^2)\,,\, \rho\,(u_x^2 - u_y^2)\,,\, \rho\, u_x\, u_y\,, \\ -\lambda^2\,\rho\, u_x\,,\, -\lambda^2\,\rho\, u_y\,,\, \rho\,\lambda^4 - 3\,\rho\,\lambda^2\left(u_x^2 + u_y^2\right)\Big)^{\mathrm{t}} \end{array} \right. \tag{3.81}$$

and the proposition 9 is proved. □

The explicitation of all components of the vector f^{eq} is useful for the treatment of boundary conditions:

$$f^{\mathrm{eq}} = \left\{ \begin{array}{lcl} f_0^{\mathrm{eq}} & = & \dfrac{2\,\rho}{9}\,\left[2 - \dfrac{3}{\lambda^2}\left(u_x^2 + u_y^2\right)\right] \\ f_1^{\mathrm{eq}} & = & \dfrac{\rho}{18}\,\left[2 + \dfrac{3}{\lambda^2}\left(2\,u_x\,\lambda + 2\,u_x^2 - u_y^2\right)\right] \\ f_2^{\mathrm{eq}} & = & \dfrac{\rho}{18}\,\left[2 + \dfrac{3}{\lambda^2}\left(2\,u_y\,\lambda + 2\,u_y^2 - u_x^2\right)\right] \\ f_3^{\mathrm{eq}} & = & \dfrac{\rho}{18}\,\left[2 + \dfrac{3}{\lambda^2}\left(-2\,u_x\,\lambda + 2\,u_x^2 - u_y^2\right)\right] \\ f_4^{\mathrm{eq}} & = & \dfrac{\rho}{18}\,\left[2 + \dfrac{3}{\lambda^2}\left(-2\,u_y\,\lambda + 2\,u_y^2 - u_x^2\right)\right] \\ f_5^{\mathrm{eq}} & = & \dfrac{\rho}{36}\,\left[1 + \dfrac{3}{\lambda^2}\left(u_x\,\lambda + u_y\,\lambda + u_x^2 + 3\,u_x\,u_y + u_y^2\right)\right] \\ f_6^{\mathrm{eq}} & = & \dfrac{\rho}{36}\,\left[1 + \dfrac{3}{\lambda^2}\left(-\,u_x\,\lambda + u_y\,\lambda + u_x^2 - 3\,u_x\,u_y + u_y^2\right)\right] \\ f_7^{\mathrm{eq}} & = & \dfrac{\rho}{36}\,\left[1 + \dfrac{3}{\lambda^2}\left(-\,u_x\,\lambda - u_y\,\lambda + u_x^2 + 3\,u_x\,u_y + u_y^2\right)\right] \\ f_8^{\mathrm{eq}} & = & \dfrac{\rho}{36}\,\left[1 + \dfrac{3}{\lambda^2}\left(u_x\,\lambda - u_y\,\lambda + u_x^2 - 3\,u_x\,u_y + u_y^2\right)\right]. \end{array} \right. \tag{3.82}$$

CHAPTER 4

THIRD ORDER EQUIVALENT EQUATION OF LATTICE BOLTZMANN SCHEMES

We recall in this contribution [1] the origin of lattice Boltzmann scheme and detail the version due to D'Humières [80]. 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.

4.1 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 [131] and Ulam [130]. Nevertheless, this idea became very popular with the so-called "Conway's game of life" described by Gardner [60]. 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

$$\frac{\partial f}{\partial t} + v \bullet \nabla_x f = Q(f). \tag{4.1}$$

The left hand side of equation (4.1) 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 [26]) that the so-called equilibrium distribution f^{eq} that is defined by $Q(f^{eq}) = 0$ is a Maxwellian distribution.

Due to the difficulties to handle equation (4.1), two important ideas for simplifying the dynamics have been proposed. The first one with Bhatnagar, Gross and Krook [9], consists in a linearization around the equilibrium distribution f^{eq} and in replacing the collision operator by a linear development around f^{eq}:

$$Q^{BGK}(f) = S \bullet (f - f^{eq}), \tag{4.2}$$

[1] initially published in [45]

where S is the linearized collision operator at the equilibrium:

$$S = \mathrm{d}Q(f^{\mathrm{eq}})\,. \tag{4.3}$$

On the other hand with Carleman [24] and Broadwell [18], one reduces the space of velocities $\mathbb{R}^3$ into a discrete set $\mathcal{V}$. Following this approach, the Boltzmann equation (4.1) is replaced by a system of partial differential equations. This methodology of studying Boltzmann equation with discrete velocities has been developed by Cabannes [22] and Gatignol [62].

In their pioneering work, Hardy, Pomeau and De Pazzis [73] 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,

$$x \in \mathcal{L}^0 \quad \text{and} \quad v \in \mathcal{V} \qquad \Longrightarrow \qquad x + \Delta t\, v \in \mathcal{L}^0\,. \tag{4.4}$$

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, Hardy *e*t al [73] 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:

$$\left\{ \begin{array}{rcl} \dfrac{\partial \rho}{\partial t} + \mathrm{div} q & = & 0 \\ \dfrac{\partial q}{\partial t} + \mathrm{div}\big(P(\rho,\, q)\big) & = & 0 \end{array} \right. \tag{4.5}$$

With the next generation of cellular automata proposed by Frisch, Hasslacher and Pomeau [59] a two-dimensional triangular lattice (D2Q6) was introduced and pressure tensor $P(\bullet,\bullet)$ of relation (4.5) 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 [84]. 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 [101] , 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

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

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 (4.1). Then Higuera, Succi and Benzi

[79] proposed to use a BGK approximation of the type (4.2) for the collision operator and Qian, D’Humières and Lallemand [113] introduced a polynomial equilibrium distribution f^{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 (4.1)), based on method of characteristic as an **e**xact time integration operator (due to (4.4)). Then the scheme can finally be written as:

$$f_j(x,\, t+\Delta t) = f_j^*(x - v_j\, \Delta t,\, t)\,, \qquad v_j \in \mathcal{V}\,, \quad x \in \mathcal{L}^0\,. \tag{4.6}$$

We refer to Lallemand and Luo [95] or to our lecture notes [42] 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 [80]) instead of the expression “multiple relaxation times” often used as in D’Humières *a*t al [83]. 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 [80] and to the new point of view proposed by Junk and Rheinländer [89]. We prefer to use the method of equivalent partial differential equation proposed by Lerat and Peyret [100] and Warming and Hyett [133] 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 [42] and after the second ICMMES conference [43]. We propose to apply previous ideas to advective thermics in section 5 and diffusive acoustics in section 6.

4.2 LATTICE BOLTZMANN “MRT” 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 (4.4) 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 (4.6) couples linearly a vertex x with its neighbors $x + v_j\, \Delta t$ for $0 \leqslant j \leqslant J$. 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

$$\rho(x,\, t) \equiv \sum_{j=0}^{J} f_j(x,\, t) \equiv m_0(x,\, t) \tag{4.7}$$

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

$$q_\alpha(x,\,t) \equiv \sum_{j=0}^{J} v_j^\alpha\, f_j(x,\,t) \equiv m_\alpha(x,\,t). \tag{4.8}$$

We set $M_{0j} \equiv 1$ and $M_{\alpha j} \equiv v_j^\alpha$ for $1 \leqslant \alpha \leqslant d$. We suppose that we have completed the matrix M into $(M_{kj})_{0\leqslant j,k\leqslant J}$ in such a way that M is **i**nvertible. From particle distribution $f \in \mathbb{R}^q$ at vertex x and time t, D'Humières [80] introduces the vector of momenta $m \in \mathbb{R}^q$ defined by

$$m_k = \sum_{j=0}^{J} M_{kj}\, f_j\,, \qquad 0 \leqslant k \leqslant J. \tag{4.9}$$

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 $0 \leqslant i \leqslant N-1$, we have conservation of momentum number i during the relaxation process. The i^{o} momentum after relaxation, denoted by m_i^* is equal to m_i and by definition coincides with the equilibrium value m_i^{eq} also denoted by W_i:

$$m_i^* = m_i \equiv m_i^{\text{e}q} \equiv W_i\,, \qquad 0 \leqslant i \leqslant N-1\,. \tag{4.10}$$

We construct with the above hypothesis a **c**onserved vector $W \in \mathbb{R}^N$. For $k \geqslant N$, the momentum m_k is **n**ot at thermodynamical equilibrium. It relaxes towards an equilibrium value m_k^{eq} which is a **g**iven nonlinear function ψ_k of vector W of conserved variables:

$$m_k^{\text{e}q} \equiv \psi_k(W)\,, \qquad k \geqslant N. \tag{4.11}$$

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 (4.2) and (4.3). 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

$$m_k^* = (1-s_k)\, m_k + s_k\, m_k^{\text{e}q}\,, \qquad k \geqslant N\,, \qquad s_k > 0. \tag{4.12}$$

Remark that $s_k < 0$ is excluded because it corresponds to a repulsion by $m_k^{\text{e}q}$ and $s_k = 0$ refers to equilibrium, considered by convention for the other indices. It is classical (see *e*.g. Lallemand and Luo, [95]) that $s_k \leqslant 2$ for stability of forward Euler scheme (4.12). After relaxation, distribution f^* is re-constructed thanks to elementary linear algebra:

$$f_j^* = \sum_{\ell=0}^{J} M_{j\ell}^{-1}\, m_\ell^*\,, \qquad 0 \leqslant j \leqslant J. \tag{4.13}$$

4.3 TENSOR OF MOMENTUM-VELOCITY

Following our previous contributions [42] [43], we introduce the so-called "tensor of momentum-velocity" Λ_{kp}^ℓ according to

$$\Lambda_{kp}^\ell \equiv \sum_{j=0}^{J} M_{kj}\, M_{pj}\, (M^{-1})_{j\ell}\,, \qquad 0 \leqslant k,\, p,\, \ell \leqslant J. \tag{4.14}$$

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

$$Z^{\ell}_{kpq} \equiv \sum_{j=0}^{J} M_{kj}\, M_{pj}\, M_{qj}\, (M^{-1})_{j\ell}\,, \qquad 0 \leqslant k,\, p,\, q,\, \ell \leqslant J\,, \tag{4.15}$$

$$\Xi^{\ell}_{kpqr} \equiv \sum_{j=0}^{J} M_{kj}\, M_{pj}\, M_{qj}\, M_{rj}\, (M^{-1})_{j\ell}\,, \qquad 0 \leqslant k,\, p,\, q,\, r,\, \ell \leqslant J\,. \tag{4.16}$$

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

$$\left\{ \begin{array}{rclccccc} \Lambda^{\ell}_{0p} & = & \delta^{\ell}_{p}\,, & 0 & \leqslant & p,\, \ell & \leqslant & J \\ Z^{\ell}_{0pq} & = & \Lambda^{\ell}_{pq}\,, & 0 & \leqslant & p,\, q,\, \ell & \leqslant & J \\ \Xi^{\ell}_{0pqr} & = & Z^{\ell}_{pqr}\,, & 0 & \leqslant & p,\, q,\, r,\, \ell & \leqslant & J\,. \end{array} \right. \tag{4.17}$$

We have also the not so intuitive following property.

Proposition 4.3.1. Algebraic property. *The tensors* Λ, Z *and* Ξ *satisfy the two following relations:*

$$\sum_{r} \Lambda^{r}_{kp}\, \Lambda^{\ell}_{rq} \;=\; Z^{\ell}_{kpq}\,, \quad 0 \leqslant k,\, p,\, q,\, \ell \leqslant J\,, \tag{4.18}$$

$$\sum_{s,t} \Lambda^{s}_{kp}\, \Lambda^{t}_{sq}\, \Lambda^{\ell}_{tr} \;=\; \Xi^{\ell}_{kpqr}\,, \quad 0 \leqslant k,\, p,\, q,\, r,\, \ell \leqslant J\,. \tag{4.19}$$

Proof. We replace the tensor Λ in left hand side of relation (4.18) by its definition (4.14):

$$\begin{aligned} \sum_{r} \Lambda^{r}_{kp}\, \Lambda^{\ell}_{rq} &= \sum_{r,j,\nu} M_{kj}\, M_{pj}\, M^{-1}_{jr}\, M_{r\nu}\, M_{q\nu}\, M^{-1}_{\nu\ell} \\ &= \sum_{j,\nu} M_{kj}\, M_{pj}\, \delta_{j\nu}\, M_{q\nu}\, M^{-1}_{\nu\ell} \\ &= \sum_{j} M_{kj}\, M_{pj}\, M_{qj}\, M^{-1}_{j\ell} \\ &= Z^{\ell}_{kpq} \quad \text{due to definition (4.15).} \end{aligned}$$

We use a similar methodology for left hand side of (4.19):

$$\begin{aligned} \sum_{s,t} \Lambda^{s}_{kp}\, \Lambda^{t}_{sq}\, \Lambda^{\ell}_{tr} &= \sum_{s,t,j,\nu,\mu} M_{kj}\, M_{pj}\, M^{-1}_{js}\, M_{s\nu}\, M_{q\nu}\, M^{-1}_{\nu t}\, M_{t\mu}\, M_{r\mu}\, M^{-1}_{\mu\ell} \\ &= \sum_{j,\nu\mu} M_{kj}\, M_{pj}\, \delta_{j\nu}\, M_{q\nu}\, \delta_{\nu\mu}\, M_{r\mu}\, M^{-1}_{\mu\ell} \\ &= \sum_{j} M_{kj}\, M_{pj}\, M_{qj}\, M_{rj}\, M^{-1}_{j\ell} \\ &= \Xi^{\ell}_{kpqr} \end{aligned}$$

using simply definition (4.16). □

4.4 EQUIVALENT EQUATIONS OF LATTICE BOLTZMANN MRT 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 (4.9) between particle distribution f and momenta m, equilibrium functions

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

that define the equilibrium momenta m_k^{eq} according to (4.11), the discrete relaxation step (4.10)-(4.12) and the final advective step (4.6). In what follows, we fix the geometrical and topological structure of lattice $\mathscr{L}$, we fix the matrix M and the equilibrium function $\psi_k(\bullet)$, and last but not least, we suppose that parameters s_k for $k \geqslant N$ 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 [100] and Warming and Hyett [133]. 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 4.4.1. General development at third order of accuracy. *With the lattice Boltzmann precised previously, we have the following formal development:*

$$\left\{ \begin{array}{l} m^k + \Delta t\, \partial_t m^k + \dfrac{1}{2} \Delta t^2\, \partial_t^2 m^k + \dfrac{1}{6} \Delta t^3\, \partial_t^3 m^k + O(\Delta t^4) \;=\; m_k^* \\ -\Delta t\, \Lambda_{k\alpha}^{\ell}\, \partial_\alpha m_\ell^* + \dfrac{\Delta t^2}{2}\, Z_{k\alpha\beta}^{\ell}\, \partial_\alpha \partial_\beta m_\ell^* - \dfrac{\Delta t^3}{6}\, \Xi_{k\alpha\beta\gamma}^{\ell}\, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^* + O(\Delta t^4), \qquad 0 \leqslant k \leqslant J. \end{array} \right. \tag{4.20}$$

Proof. We apply matrix M (relation (4.9)) to the scheme (4.6) and obtain in this way:

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

and the result comes from a classical Taylor expansion of left hand side of relation (4.6). □

Proposition 4.4.2. Equilibrium at order zero. *With the lattice Boltzmann defined previously, we have*

$$f_j(x,\, t) = f_j^{eq}(x,\, t) + O(\Delta t) = f_j^*(x,\, t) + O(\Delta t), \qquad 0 \leqslant j \leqslant J, \tag{4.21}$$

$$m_k(x,\, t) = m_k^{eq}(x,\, t) + O(\Delta t) = m_k^*(x,\, t) + O(\Delta t), \qquad 0 \leqslant j \leqslant J. \tag{4.22}$$

Proof. The relation (4.22) is clear for $k < N$ due to (4.10). If $k \geqslant N$, we apply the relation (4.20) by restricting ourselves to order zero and we get:

$$m_k = m_k^* + \mathrm{O}(\Delta t), \quad k \geqslant N. \tag{4.23}$$

The relation (4.23) joined with (4.12) clearly implies (4.22). Then (4.21) is a consequence of (4.22) by applying the fixed matrix M^{-1}. □

Proposition 4.4.3. First order expansion of mass conservation law. *With the lattice Boltzmann scheme previously defined, we have the conservation of mass at first order:*

$$\partial_t \rho + \partial_\alpha q_\alpha^{eq} = O(\Delta t). \tag{4.24}$$

When $N = d+1$, $q_\alpha^{eq} = q_\alpha$ *in relation (4.24).*

Proof. We have from the relation (4.20) 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 (4.17) and (4.22),

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

The relation (4.24) is established. □

Proposition 4.4.4. Nonequilibrium momenta at first order. *For* $k \geqslant N$, *we introduce the so-called "defect of conservation" according to*

$$\theta_k \equiv \partial_t m_k^{eq} + \Lambda_{k\alpha}^{\ell}\, \partial_\alpha m_\ell^{eq}, \qquad k \geqslant N \tag{4.25}$$

and the viscosity coefficient

$$\sigma_k \equiv \frac{1}{s_k} - \frac{1}{2}, \qquad k \geqslant N \tag{4.26}$$

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

$$m_k = m_k^{eq} - \Delta t\Big(\frac{1}{2} + \sigma_k\Big)\theta_k + O(\Delta t^2), \qquad k \geqslant N \tag{4.27}$$

$$m_k^* = m_k^{eq} + \Delta t\Big(\frac{1}{2} - \sigma_k\Big)\theta_k + O(\Delta t^2), \qquad k \geqslant N. \tag{4.28}$$

Proof. We consider relation (4.20) up to first order accuracy with the hypothesis that $k \geqslant N$ i.e. $m_k \neq m_k^*$:

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

Then we use definition (4.12) of momentum m_k^* after relaxation:

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

and obtain the intermediate relation (see also [42])

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

Then relation (4.27) is an elementary consequence of (4.26). After relaxation we use again relation (4.12) and obtain

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

Thus relation (4.28) is a direct consequence of previous relation and (4.26). □

The viscosity coefficient $\sigma_k \equiv \frac{1}{s_k} - \frac{1}{2}$ has been introduced by Hénon [77] in the context of cellular automata. It has been re-discovered and explicited for lattice Boltzmann scheme by D'Humières [80].

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 [80] and introduce the associated Chapman-Enskog expansion for the discrete particle distribution f_j :

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

In terms of moments m_k, we have after the linear mapping (4.9):

$$m_k = m_k^{eq} + \Delta t\; m_k^1 + \mathrm{O}(\Delta t^2)\,. \tag{4.29}$$

If the moment of label k is at equilibrium ($k < N$), we have from relation (4.10) $m_k \equiv m_k^{eq}$ and in consequence

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

If moment m_k is not at thermodynamical equilibrium, expansions (4.27) and (4.29) are necessarily identical and it comes taking into account (4.26)

$$m_k^1 = -\frac{1}{s_k}\,\theta_k\,, \qquad k \geqslant N\,.$$

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

Proposition 4.4.5. Second order expansion of mass conservation law. *With the lattice Boltzmann scheme previously defined, we have the conservation of mass at second order:*

$$\partial_t \rho + \partial_\alpha q_\alpha^{eq} - \Delta t\, \sigma_\alpha\, \partial_\alpha \theta_\alpha = O(\Delta t^2)\,. \tag{4.30}$$

When $N = d+1$, *relation (4.30) is equivalent to*

$$\partial_t \rho + \partial_\alpha q_\alpha = O(\Delta t^2)\,. \tag{4.31}$$

Proof. We first evaluate second order time derivative of density as a function of space derivatives. We differentiate relation (4.24) relatively to time and relation (4.25) with $k = \alpha$ relatively to space. We obtain

$$\mathrm{O}(\Delta t) = \partial_t^2 \rho + \partial_\alpha \partial_t q_\alpha^{\mathrm{e}q} = \partial_t^2 \rho + \partial_\alpha \big(\theta_\alpha - \Lambda_{\alpha\beta}^{\ell} \partial_\beta m_\ell^{\mathrm{e}q}\big)$$

and we deduce the intermediate lemma:

$$\partial_t^2 \rho + \partial_\alpha \theta_\alpha - \Lambda_{\alpha\beta}^{\ell} \partial_\alpha \partial_\beta m_\ell^{\mathrm{e}q} = \mathrm{O}(\Delta t)\,. \tag{4.32}$$

We now apply relation (4.20) up to second order accuracy with $i = 0$:

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

We have according to (4.28) with $k = \alpha$:

$$q_\alpha^* = q_\alpha^{\mathrm{e}q} + \Delta t \Big(\frac{1}{2} - \sigma_\alpha\Big) \theta_\alpha + \mathrm{O}(\Delta t^2)$$

and we use relation (4.17) to simplify the expression of $Z_{0\alpha\beta}^{\ell}$. It comes

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

We inject also relation (4.32) for second time derivative of density up to first order. We deduce:

$$\begin{aligned} &\partial_t \rho + \frac{\Delta t}{2} \big(\Lambda_{\alpha\beta}^{\ell} \partial_\alpha \partial_\beta m_\ell^{\mathrm{e}q} - \partial_\alpha \theta_\alpha\big) + \mathrm{O}(\Delta t^2) \\ &= -\partial_\alpha \Big[q_\alpha^{\mathrm{e}q} + \Delta t \Big(\frac{1}{2} - \sigma_\alpha\Big) \theta_\alpha \Big] + \frac{\Delta t}{2} \Lambda_{\alpha\beta}^{\ell} \partial_\alpha \partial_\beta m_\ell^{\mathrm{e}q} + \mathrm{O}(\Delta t^2) \end{aligned}$$

and relation (4.30) is a simple consequence of the previous equation and relation (4.18). When momenta q_α are at equilibrium ($N = d + 1$), the "defect of conservation" θ_α is of order $\mathrm{O}(\Delta t)$ and the term $\Delta t\, \sigma_\alpha\, \partial_\alpha \theta_\alpha$ inside equation (4.30) is of order $\mathrm{O}(\Delta t^2)$. Thus relation (4.31) is proven and the proposition is established. □

Proposition 4.4.6. Nonequilibrium momenta at second order. *We can be more specific about relations (4.27) and (4.28) up to second order accuracy for non-conserved momenta, i.e. $k \geqslant N$:*

$$m_k = m_k^{eq} - \Delta t \big(\frac{1}{2} + \sigma_k\big) \big[\theta_k - \Delta t \big(\sigma_k \partial_t \theta_k + \sigma_\ell \Lambda_{k\alpha}^{\ell} \partial_\alpha \theta_\ell\big)\big] + O(\Delta t^3) \tag{4.33}$$

$$m_k^* = m_k^{eq} + \Delta t \big(\frac{1}{2} - \sigma_k\big) \big[\theta_k - \Delta t \big(\sigma_k \partial_t \theta_k + \sigma_\ell \Lambda_{k\alpha}^{\ell} \partial_\alpha \theta_\ell\big)\big] + O(\Delta t^3)\,. \tag{4.34}$$

Proof. We consider relation (4.20) up to second order accuracy:

$$\begin{aligned} &m_k + \Delta t\, \partial_t m_k + \tfrac{\Delta t^2}{2} \partial_t^2 m_k + \mathrm{O}(\Delta t^3) \\ &= m_k^* - \Delta t\, \Lambda_{k\alpha}^{\ell} \partial_\alpha m_\ell^* + \tfrac{\Delta t^2}{2} Z_{k\alpha\beta}^{\ell} \partial_\alpha \partial_\beta m_\ell^* + \mathrm{O}(\Delta t^3)\,. \end{aligned}$$

We transform the expression $\partial_t^2 m_k$ by deriving in time the expression (4.25). It comes

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

with implicit summation over repeted indices. Then from relaxation definition (4.12), we obtain

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

by taking into account relations (4.25) and (4.18). Then relation (4.33) is a direct consequence of above expression and of first order development (4.27). The expresion (4.34) of momentum of order k after relaxation step follows from analogous considerations. □

Proposition 4.4.7. Third order mass conservation for thermal problem. *When only one conservation is present ($N = 1$), conservation of mass (4.30) admits the following expression up to third order accuracy:*

$$\partial_t \rho + \partial_\alpha q_\alpha^{eq} - \Delta t \, \sigma_\alpha \, \partial_\alpha \theta_\alpha + \Delta t^2 \Big[\Big(\sigma_\alpha^2 - \frac{1}{6} \Big) \partial_\alpha \partial_t \theta_\alpha + \Big(\sigma_\alpha \, \sigma_\ell - \frac{1}{12} \Big) \Lambda_{\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta \theta_\ell \Big] = O(\Delta t^3) \, . \quad (4.35)$$

Proof. 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 (4.30) relatively to time:

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

Then by inserting inside the previous expression derivation towards space of relation (4.25):

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

we obtain

$$\partial_t^2 \rho + \partial_\alpha \theta_\alpha - \Lambda_{\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta m_\ell^{\mathrm{eq}} - \Delta t \, \sigma_\alpha \, \partial_\alpha \partial_t \theta_\alpha = \mathrm{O}(\Delta t^2) \, . \quad (4.36)$$

We now derive relatively to time relation (4.36) and neglect the last term:

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

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

$$\partial_t^3 \rho + \partial_\alpha \partial_t \theta_\alpha - \Lambda_{\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta \theta_\ell + \Lambda_{\alpha\beta}^{p} \, \Lambda_{p\gamma}^{\ell} \, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^{\mathrm{eq}} = \mathrm{O}(\Delta t) \, . \quad (4.37)$$

We consider now the expression (4.20) up to third order in the particular case $i = 0$:

$$\begin{aligned}
&\rho + \Delta t \, \partial_t \rho + \frac{\Delta t^2}{2} \, \partial_t^2 \rho + \frac{\Delta t^3}{6} \, \partial_t^3 \rho + \mathrm{O}(\Delta t^4) \\
&= \rho - \Delta t \, \partial_\alpha q_\alpha^* + \frac{\Delta t^2}{2} \, Z_{0\alpha\beta}^{\ell} \, \partial_\alpha \partial_\beta m_\ell^* - \frac{\Delta t^3}{6} \, \Xi_{0\alpha\beta\gamma}^{\ell} \, \partial_\alpha \partial_\beta \partial_\gamma m_\ell^* + \mathrm{O}(\Delta t^4) \, .
\end{aligned}$$

We insert in left hand side the previous expressions (4.36) and (4.37) for high order time derivatives and in right hand side the momentum q^*_α with the help of (4.28). We take also into account remarks (4.17). We obtain:

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

We simplify the above expression by taking into account relation (4.19). We obtain:

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

and the relation (4.35) 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 4.4.2 is still valid and we have equilibrium at order zero (relations (4.21) and (4.22)).

Proposition 4.4.8. 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*

$$\partial_t q_\alpha + \Lambda^\ell_{\alpha\beta}\partial_\beta m^{eq}_\ell = O(\Delta t) \qquad 1 \leqslant \alpha \leqslant d\,. \tag{4.38}$$

Proof. We detail relation (4.20) at order one for $k = \alpha$. It comes

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

and conclusion (4.38) comes directly from (4.22). □

We recall that, according to Proposition 6, conservation of mass can be written as (4.31) at second order of accuracy. Moreover, expression of nonequilibrium momenta at first order are still given according to relations (4.27) and (4.28). We can precise now the conservation of momentum up to second order.

Proposition 4.4.9. 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*

$$\partial_t q_\alpha + \Lambda^\ell_{\alpha\beta}\partial_\beta m^{eq}_\ell - \sigma_\ell\,\Delta t\,\Lambda^\ell_{\alpha\beta}\partial_\beta\theta_\ell = O(\Delta t^2)\,, \qquad 1 \leqslant \alpha \leqslant d\,. \tag{4.39}$$

Proof. We first precise second order time derivative of conserved variables. We have by derivation of (4.31) relatively to time and of (4.38) relatively to space:

$$\partial_t^2 \rho = \Lambda_{\alpha\beta}^{\ell} \partial_\alpha \partial_\beta \rho + \mathrm{O}(\Delta t) .$$

In an analogous way, we differentiate (4.38) relatively to time and replace $\partial_t m_\ell^{eq}$ by expression obtained from definition (4.25):

$$\partial_t^2 q_\alpha + \Lambda_{\alpha\beta}^{\ell} \partial_\beta \big(\theta_\ell - \Lambda_{\ell\gamma}^{p} \partial_\gamma m_p^{\mathrm{eq}}\big) = \mathrm{O}(\Delta t) .$$

Then

$$\partial_t^2 q_\alpha = -\Lambda_{\alpha\beta}^{\ell} \partial_\beta \theta_\ell + \Lambda_{\alpha\beta}^{p} \Lambda_{p\gamma}^{\ell} \partial_\beta \partial_\gamma m_\ell^{\mathrm{eq}} + \mathrm{O}(\Delta t) .$$

We consider now relation (4.20) with $k = \alpha$ up to second order accuracy:

$$\begin{aligned} q_\alpha + \Delta t\, \partial_t q_\alpha + \frac{\Delta t^2}{2} \partial_t^2 q_\alpha + \mathrm{O}(\Delta t^3) = \\ q_\alpha - \Delta t\, \Lambda_{\alpha\beta}^{\ell} \partial_\beta m_\ell^* + \frac{\Delta t^2}{2} Z_{\alpha\beta\gamma}^{\ell} \partial_\beta \partial_\gamma m_\ell^* + \mathrm{O}(\Delta t^3) . \end{aligned}$$

We substitute in the right hand side the expression (4.28) of momenta after relaxation:

$$\begin{aligned} \partial_t q_\alpha + \frac{\Delta t}{2} \Big(-\Lambda_{\alpha\beta}^{\ell} \partial_\beta \theta_\ell + \Lambda_{\alpha\beta}^{p} \Lambda_{p\gamma}^{p} \partial_\beta \partial_\gamma m_\ell^{\mathrm{eq}} \Big) \\ + \Lambda_{\alpha\beta}^{\ell} \partial_\beta \Big[m_\ell^{\mathrm{eq}} + \Delta t \Big(\frac{1}{2} - \sigma_\ell \Big) \theta_\ell \Big] - \frac{\Delta t}{2} Z_{\alpha\beta\gamma}^{\ell} \partial_\beta \partial_\gamma m_\ell^{\mathrm{eq}} = \mathrm{O}(\Delta t^2) \end{aligned}$$

and relation (4.39) is a direct consequence of identity (4.18). □

Proposition 4.4.10. Third order equivalent equations for fluid model. *When $N = d+1$ conservation laws are present, second order conservation of mass (4.31) and momentum (4.39) admit the following expressions up to third order accuracy:*

$$\partial_t \rho + \sum_\alpha \partial_\alpha q_\alpha - \frac{\Delta t^2}{12} \sum_{\alpha\beta\ell} \Lambda_{\alpha\beta}^{\ell} \partial_\alpha \partial_\beta \theta_\ell = O(\Delta t^3) \tag{4.40}$$

$$\begin{aligned} \partial_t q_\alpha + \sum_{\beta\ell} \Lambda_{\alpha\beta}^{\ell} \partial_\beta m_\ell^{eq} - \sum_{\beta\ell} \sigma_\ell \Delta t\, \Lambda_{\alpha\beta}^{\ell} \partial_\beta \theta_\ell + \Delta t^2 \Big[\sum_{\beta\ell} \Big(\sigma_\ell^2 - \frac{1}{6} \Big) \Lambda_{\alpha\beta}^{\ell} \partial_t \partial_\beta \theta_\ell \\ + \sum_{\beta\gamma p\ell} \Big(\sigma_\ell \sigma_p - \frac{1}{12} \Big) \Lambda_{\alpha\beta}^{p} \Lambda_{p\gamma}^{\ell} \partial_\beta \partial_\gamma \theta_\ell \Big] = O(\Delta t^3) , \qquad 1 \leqslant \alpha \leqslant d . \end{aligned} \tag{4.41}$$

Proof. First, the nonconserved momenta still admit the developments (4.33) and (4.34) as previously. Second, we precise second order and third order time derivative of conserved variables. >From (4.31) and (4.39), we have

$$\partial_t^2 \rho = \Lambda_{\alpha\beta}^{\ell} \partial_\alpha \partial_\beta m_\ell^{\mathrm{eq}} - \sigma_\ell \Delta t\, \Lambda_{\alpha\beta}^{\ell} \partial_\alpha \partial_\beta \theta_\ell + \mathrm{O}(\Delta t^2) \tag{4.42}$$

$$\partial_t^3 \rho = \Lambda_{\alpha\beta}^{\ell} \partial_\alpha \partial_\beta \theta_\ell - \Lambda_{\alpha\beta}^{p} \Lambda_{p\gamma}^{\ell} \partial_\alpha \partial_\beta \partial_\gamma m_\ell^{\mathrm{eq}} + \mathrm{O}(\Delta t) \tag{4.43}$$

$$\partial_t^2 q_\alpha = -\Lambda^\ell_{\alpha\beta}\partial_\beta\theta_\ell + \Lambda^p_{\alpha\beta}\Lambda^\ell_{p\gamma}\partial_\beta\partial_\gamma m^{\rm eq}_\ell + \sigma_\ell\,\Delta t\,\Lambda^\ell_{\alpha\beta}\partial_t\partial_\beta\theta_\ell + {\rm O}(\Delta t^2) \tag{4.44}$$

$$\partial_t^3 q_\alpha = -\Lambda^\ell_{\alpha\beta}\partial_t\partial_\beta\theta_\ell + \Lambda^p_{\alpha\beta}\Lambda^\ell_{p\gamma}\partial_\beta\partial_\gamma\theta_\ell - \Lambda^p_{\alpha\beta}\Lambda^q_{p\gamma}\Lambda^\ell_{q\zeta}\partial_\beta\partial_\gamma\partial_\zeta m^{\rm eq}_\ell + {\rm O}(\Delta t)\,. \tag{4.45}$$

We look for development (4.20) when $i = 0$:

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

We replace $\partial_t^2\rho$ and $\partial_t^3\rho$ by their values (4.42) and (4.43) obtained from previous Taylor expansions, we use relations (4.17) and introduce development (4.34) for nonconserved momenta. We get

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

First order terms vanish and we have a simplification due to (4.18). Coefficient of $\Lambda^\ell_{\alpha\beta}\partial_\alpha\partial_\beta\theta_\ell\,\Delta t^2$ is equal to $-\frac{\sigma_\ell}{2} + \frac{1}{6} + \frac{1}{2}(\sigma_\ell - \frac{1}{2}) = -\frac{1}{12}$ and relation (4.40) is established.
We explicit relation (4.20) 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 (4.44), (4.45) and (4.34) 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

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

We replace $Z^\ell_{\alpha\beta\gamma}$ and $\Xi^\ell_{\alpha\beta\gamma\zeta}$ by their values obtained from relations (4.18) and (4.19) 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 $\frac{\sigma_\ell}{2} - \frac{1}{6} + \sigma_\ell\,(\sigma_\ell - \frac{1}{2}) = \sigma_\ell^2 - \frac{1}{6}$ and the coefficient of $\Lambda^p_{\alpha\beta}\Lambda^\ell_{p\gamma}\partial_\beta\partial_\gamma\theta_\ell\,\Delta t^2$ is simply: $\frac{1}{6} + \sigma_\ell\,(\sigma_p - \frac{1}{2}) + \frac{1}{2}\,(\sigma_\ell - \frac{1}{2}) = \sigma_\ell\,\sigma_p - \frac{1}{12}$. Then relation (4.41) is proven. □

If we compare third order mass conservation (4.35) for a single conservation law and third order momentum conservation (4.41) 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 (4.41) contains one more factor of the type "Λ" than relation (4.35). Nevertheless, a structure is clearly appearing!

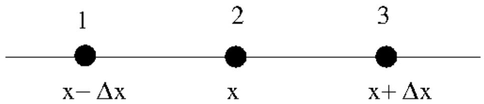

Figure 4.1 – *Neighboring nodes for D1Q3 lattice Boltzmann scheme*

4.5 APPLICATION TO ADVECTIVE THERMICS

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

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

$$\lambda \equiv \frac{\Delta x}{\Delta t}.$$

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 (4.7). There is only one component of momentum:

$$q \equiv -\lambda f_- + \lambda f_+ . \tag{4.46}$$

We choose internal energy according to

$$\epsilon \equiv \frac{\lambda^2}{2}\left(f_- + f_+\right) \tag{4.47}$$

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

$$M = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \frac{\lambda^2}{2} & 0 & \frac{\lambda^2}{2} \end{pmatrix}. \tag{4.48}$$

It is therefore easy to explicit the tensor of mementum-velocity Λ defined at relation (4.14). We have for D1Q3 model

$$\Lambda^0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Lambda^1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & \frac{\lambda^2}{2} \\ 0 & \frac{\lambda^2}{2} & 0 \end{pmatrix}, \quad \Lambda^2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & \frac{\lambda^2}{2} \end{pmatrix} \tag{4.49}$$

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 [30], Shan [121], Chen-Doolen [28] and Ginzburg [64]. 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):

$$q^{eq} = v\lambda\rho, \qquad \epsilon^{eq} = \zeta\frac{\lambda^2}{2}\rho. \tag{4.50}$$

Due to equilibrium values (4.50), defects of conservation θ introduced in (4.25) take the simple algebraic form

$$\theta_1 \equiv v\,\lambda\,\frac{\partial\rho}{\partial t} + \zeta\,\lambda^2\,\frac{\partial\rho}{\partial x}\,, \qquad \theta_2 \equiv \frac{\lambda^2}{2}\Big(\zeta\,\frac{\partial\rho}{\partial t} + v\,\lambda\,\frac{\partial\rho}{\partial x}\Big). \tag{4.51}$$

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 (4.26). Then relations (4.10) and (4.12) can be summarized in a single matricial relation. The momenta after relaxation satisfy

$$m^* = J_0 \bullet m\,, \tag{4.52}$$

with

$$J_0 = \begin{pmatrix} 1 & 0 & 0 \\ s_1\,v\,\lambda & 1-s_1 & 0 \\ \zeta\,s_2\,\frac{\lambda^2}{2} & 0 & 1-s_2 \end{pmatrix}. \tag{4.53}$$

Proposition 4.5.1. Third order equivalent equation for advective thermal D1Q3 lattice Boltzmann scheme. *With notations explicited previously, the D1Q3 scheme defined by (4.6), (4.9), (4.52) and (4.53) satisfy the following partial equivalent equation*

$$\begin{aligned} &\frac{\partial\rho}{\partial t} + v\,\lambda\,\frac{\partial\rho}{\partial x} - \sigma_1\,\Delta t\,\lambda^2\,(\zeta - v^2)\,\frac{\partial^2\rho}{\partial x^2} \\ &-\Delta t^2\,v\,\lambda^3\Big[2\Big(\sigma_1^2 - \frac{1}{12}\Big)(\zeta - v^2) + \Big(\frac{1}{12} - \sigma_1\,\sigma_2\Big)(1-\zeta)\Big]\frac{\partial^3\rho}{\partial x^3} = O(\Delta t^3)\,. \end{aligned} \tag{4.54}$$

Proof. Due to (4.50) and (4.24), we write the equivalent equation at order one:

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

and we report this expression to precise defects of equilibrium:

$$\theta_1 = (\zeta - v^2)\,\lambda^2\,\frac{\partial\rho}{\partial x} + \mathrm{O}(\Delta t)\,, \qquad \theta_2 = \frac{\lambda^3}{2}\,v\,(1-\zeta)\,\frac{\partial\rho}{\partial x} + \mathrm{O}(\Delta t)\,. \tag{4.55}$$

We replace expression (4.55) of θ_1 inside relation (4.30) and obtain mass conservation at second order:

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

This expression for $\frac{\partial\rho}{\partial t}$ allows us to precise θ_1 defined in (4.51):

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

We use relation (4.55) for complementary third order terms of relation (4.35). Then conservation law at third order takes the form:

$$\begin{aligned} &\frac{\partial\rho}{\partial t} + v\,\lambda\,\frac{\partial\rho}{\partial x} - \sigma_1\,\Delta t\,\frac{\partial}{\partial x}\Big[(\zeta - v^2)\,\lambda^2\,\frac{\partial\rho}{\partial x} + \sigma_1\,\Delta t\,\lambda^2\,(\zeta - v^2)\,\frac{\partial^2\rho}{\partial x^2}\Big] \\ &\quad + \Delta t^2\Big[\Big(\sigma_1^2 - \frac{1}{6}\Big)(-v\,\lambda)\,\lambda^2\,(\zeta - v^2)\,\frac{\partial^3\rho}{\partial x^3} + \Big(\sigma_1\,\sigma_2 - \frac{1}{12}\Big)\,v\,\lambda^3\,(1-\zeta)\,\frac{\partial^2}{\partial x^2}\Big(\frac{\partial\rho}{\partial x}\Big)\Big] = \mathrm{O}(\Delta t^3) \end{aligned}$$

and relation (4.54) is a consequence of factorization of $\Delta t^2\,v\,\lambda^3$ in the previous expression. □

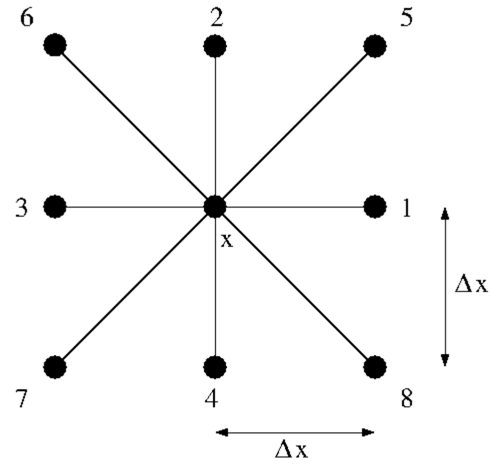

Figure 4.2 – *Neighboring nodes for the D2Q9 lattice Boltzmann scheme*

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.

The moments m satisfy relation (4.9) with a 9×9 matrix M classically (see Lallemand and Luo [95]) given by the relation

$$M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & +1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}. \tag{4.56}$$

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 (4.35), (4.40) and (4.41):

$$\begin{aligned} &\Lambda^0_{\alpha\beta} = \frac{2}{3}\lambda^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \Lambda^1_{\alpha\beta} = \Lambda^2_{\alpha\beta} = 0, \ \Lambda^3_{\alpha\beta} = \frac{1}{6}\lambda^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ &\Lambda^4_{\alpha\beta} = \Lambda^5_{\alpha\beta} = \Lambda^6_{\alpha\beta} = 0, \ \Lambda^7_{\alpha\beta} = \frac{1}{2}\lambda^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ \Lambda^8_{\alpha\beta} = \lambda^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad 1 \leq \alpha, \beta \leq 2. \end{aligned} \tag{4.57}$$

The equilibrium momenta are linear functions of the only conserved variable ρ. It is classical (see Lallemand and Luo [95]) 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 $\sum_j |v_j|^2 \, v_j \, f_j$, *i*d 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

$$q_x^{eq} = u\,\lambda\,\rho\,, \quad q_y^{eq} = v\,\lambda\,\rho\,. \tag{4.58}$$

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

$$m_5^{eq} = a_5\,u\,\rho\,, \quad m_6^{eq} = a_6\,v\,\rho\,. \tag{4.59}$$

We complete this equilibrium distribution in a very simple manner:

$$m_3^{eq} = a_3\,\rho\,, \quad m_4^{eq} = a_4\,\rho\,, \quad m_7^{eq} = a_7\,\rho\,, \qquad m_8^{eq} = a_8\,\rho\,. \tag{4.60}$$

The momenta m^* after equilibrium satisfy the relation (4.52) 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:

$$J_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ u\,\lambda\,s_1 & 1{-}s_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v\,\lambda\,s_1 & 0 & 1{-}s_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_3\,s_3 & 0 & 0 & 1{-}s_3 & 0 & 0 & 0 & 0 & 0 \\ a_4\,s_4 & 0 & 0 & 0 & 1{-}s_4 & 0 & 0 & 0 & 0 \\ a_5\,u\,s_5 & 0 & 0 & 0 & 0 & 1{-}s_5 & 0 & 0 & 0 \\ a_6\,v\,s_5 & 0 & 0 & 0 & 0 & 0 & 1{-}s_5 & 0 & 0 \\ a_7\,s_7 & 0 & 0 & 0 & 0 & 0 & 0 & 1{-}s_7 & 0 \\ a_8\,s_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1{-}s_8 \end{pmatrix}. \tag{4.61}$$

We have the first following property:

Proposition 4.5.2. Second order scheme for D2Q9 advective thermal lattice Boltzmann scheme. *With notations explicited previously, the D2Q9 scheme defined by (4.6), (4.9), (4.52) and (4.61) is equivalent to the following advective thermal model*

$$\frac{\partial \rho}{\partial t} + \lambda\Big(u\,\frac{\partial \rho}{\partial x} + v\,\frac{\partial \rho}{\partial y}\Big) - \lambda^2\,\xi\,\sigma_1\,\Delta t\Big(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2}\Big) = O(\Delta t)^2 \tag{4.62}$$

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

$$a_3 = 3\,(u^2 + v^2) - 4 + 6\,\xi\,, \quad a_7 = u^2 - v^2\,, \quad a_8 = u\,v\,. \tag{4.63}$$

Proof. From Proposition 4, the relation (4.62) is true at order one, due to the particular choice of conservated momenta (4.58), (4.59) and (4.60). We apply now Proposition 6 (relation (4.30)). We just have to evaluate the defects of conservation θ_1 and θ_2. Due to the relations (4.25) and (4.57), 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 (4.62) at order one:

$$\theta_1 = \Big(\frac{2}{3} + \frac{a_3}{6} + \frac{a_7}{2} - u^2\Big)\,\lambda^2\,\frac{\partial \rho}{\partial x} + \Big(a_8 - u\,v\Big)\,\lambda^2\,\frac{\partial \rho}{\partial y} + \mathrm{O}(\Delta t)^2\,. \tag{4.64}$$

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

$$\theta_2 = \Big(a_8 - u\,v\Big)\,\lambda^2\,\frac{\partial\rho}{\partial x} + \Big(\frac{a_3}{6} - \frac{a_7}{2} + \frac{2}{3} - v^2\Big)\,\lambda^2\,\frac{\partial\rho}{\partial y} + \mathrm{O}(\Delta t)^2 . \tag{4.65}$$

Then due to relation (4.30),

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

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 (4.63) is clear and the proposition is established. □

The expression (4.61) 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 (4.61). For development of the algebraic consequences of representations of lattice symmetry group for the conception of lattice Boltzmann scheme, we refer to Lallemnd-Luo [96] and Rubinstein [117]. We precise now the equivalent equation of the Boltzmann scheme at order three.

Proposition 4.5.3. Third order scheme for D2Q9 advective thermal lattice Boltzmann scheme. *With previous notations and hypotheses, the D2Q9 Boltzmann scheme defined by (4.6), (4.9), (4.52) and (4.61) is equivalent at third order to the following partial differential equation*

$$\begin{aligned}
&\frac{\partial\rho}{\partial t} + \lambda\Big(u\,\frac{\partial\rho}{\partial x} + v\,\frac{\partial\rho}{\partial y}\Big) - \lambda^2\,\xi\,\sigma_1\,\Delta t\Big(\frac{\partial^2\rho}{\partial x^2} + \frac{\partial^2\rho}{\partial y^2}\Big) - \lambda^3\,\Delta t^2\,\Big\{\,\frac{1}{6}\Big(2\,\sigma_1^2 - \frac{1}{6}\Big)\,\xi\,\Big(u\,\frac{\partial}{\partial x} + v\,\frac{\partial}{\partial y}\Big)\big(\Delta\rho\big)\\
&+ \frac{1}{6}\Big(\sigma_1\,\sigma_3 - \frac{1}{12}\Big)\Big[\Big(3\,(u^2+v^2) + (6\,\xi - 5) - a_5\Big)\,u\,\frac{\partial}{\partial x} + \Big(3\,(u^2+v^2) + (6\,\xi - 5) - a_6\Big)\,v\,\frac{\partial}{\partial y}\Big]\big(\Delta\rho\big)\\
&+ \frac{1}{6}\Big(\sigma_1\,\sigma_7 - \frac{1}{12}\Big)\Big[\Big(3\,(u^2 - v^2) - 1 + a_5\Big)\,u\,\frac{\partial}{\partial x} + \Big(3\,(u^2 - v^2) + 1 - a_6\Big)\,v\,\frac{\partial}{\partial y}\Big]\Big(\frac{\partial^2\rho}{\partial x^2} - \frac{\partial^2\rho}{\partial y^2}\Big)\\
&+ \frac{2}{3}\Big(\sigma_1\,\sigma_8 - \frac{1}{12}\Big)\Big[\big(3\,u^2 - 2 - a_6\big)\,v\,\frac{\partial}{\partial x} + \big(3\,v^2 - 2 - a_5\big)\,u\,\frac{\partial}{\partial y}\Big]\,\frac{\partial^2\rho}{\partial x\partial y}\Big\} \;=\; O(\Delta t)^3 .
\end{aligned} \tag{4.66}$$

Proof. We complete the relation (4.62) by the two extra terms present in relation (4.35) and we take into account an expansion of defect of conservation θ_1 and θ_2 at order 2. On one side, from (4.36), (4.64) and (4.65), taking into account the equation (4.62), we have easily

$$\sigma_1\,\Delta t\,\frac{\partial\theta_1}{\partial x} + \sigma_2\,\Delta t\,\frac{\partial\theta_2}{\partial y} = \lambda^2\,\xi\,\sigma_1\,\Delta t\Big(\frac{\partial^2\rho}{\partial x^2} + \frac{\partial^2\rho}{\partial y^2}\Big) + \sigma_1^2\,\Delta t^2\,\lambda^3\,\xi\,\Big(u\,\frac{\partial}{\partial x} + v\,\frac{\partial}{\partial y}\Big)\big(\Delta\rho\big) + \mathrm{O}(\Delta t)^3 . \tag{4.67}$$

On the other side,

$$\begin{aligned}\Delta t^2 \Big(\sigma_\alpha^2 - \frac{1}{6}\Big) \partial_\alpha \partial_t \theta_\alpha &= \Delta t^2 \Big(\sigma_1^2 - \frac{1}{6}\Big) \Big[\frac{\partial^2 \theta_1}{\partial x \partial t} + \frac{\partial^2 \theta_2}{\partial y \partial t} \Big] \\ &= \Delta t^2 \Big(\sigma_1^2 - \frac{1}{6}\Big) \xi \lambda^2 \Delta\Big(\frac{\partial \rho}{\partial t}\Big) + \mathrm{O}(\Delta t)^3 \\ &= -\Delta t^2 \Big(\sigma_1^2 - \frac{1}{6}\Big) \xi \lambda^3 \Big(u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y}\Big) (\Delta \rho) + \mathrm{O}(\Delta t)^3\end{aligned}$$

and due to (4.67), the first four terms in (4.35) expand as the first two lines of (4.66) 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 (4.35). We remark that due to (4.57) 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 (4.25) and (4.56):

$$\begin{aligned}\theta_3 &= -\lambda \Big[\big(3(u^2+v^2) + (6\xi - 5) - a_5\big) u \frac{\partial \rho}{\partial x} + \big(3(u^2+v^2) + (6\xi - 5) - a_6\big) v \frac{\partial \rho}{\partial y} \Big] + \mathrm{O}(\Delta t) \\ \theta_7 &= -\frac{\lambda}{3} \Big[\big(3(u^2 - v^2) - 1 + a_5\big) u \frac{\partial \rho}{\partial x} + \big(3(u^2 - v^2) + 1 - a_6\big) v \frac{\partial \rho}{\partial y} \Big] + \mathrm{O}(\Delta t) \\ \theta_8 &= -\frac{\lambda}{3} \Big[\big(3u^2 - 2 - a_6\big) v \frac{\partial \rho}{\partial x} + \big(3v^2 - 2 - a_5\big) u \frac{\partial \rho}{\partial y} \Big] + \mathrm{O}(\Delta t).\end{aligned}$$

The proposition is established. □

4.6 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 (4.7)), momentum (see (4.46)) and kinetic energy (*c.f.* (4.47)). Then matrix M proposed at relation (4.48) remains valid for this new physical model and in consequence the tensor of momentum-velocity Λ is still given according to the relation (4.49). For acoustics, density (4.7) and momentum (4.46) are in equilibrium. Kinetic energy ϵ admits an equilibrium value ϵ^{eq} given as in (4.50) in order to respect Galilean invariance. We suppose

$$\epsilon^{eq} = \zeta \frac{\lambda^2}{2} \rho.$$

The present model is linear and relation (4.52) is still valid but matrix J_0 is no longer given by relation (4.53) and we suppose now

$$J_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \zeta s \lambda^2/2 & 0 & 1-s \end{pmatrix}. \tag{4.68}$$

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

$$\theta \equiv \zeta \frac{\lambda^2}{2} \frac{\partial \rho}{\partial t} + \frac{\lambda^2}{2} \frac{\partial q}{\partial x}.$$

Proposition 4.6.1. Third order scheme for D1Q3 diffusive acoustics lattice Boltzmann scheme. *With previous notations, the D1Q3 Boltzmann scheme defined by (4.6), (4.9), (4.52) and (4.68) admits the following partial differential equations for conservation of mass and conservation of momentum at third order of accuracy:*

$$\frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} - \frac{1}{12}(1-\zeta)\,\lambda^2\,\Delta t^2\,\frac{\partial^3 q}{\partial x^3} = O(\Delta t^3) \tag{4.69}$$

$$\begin{aligned}\frac{\partial q}{\partial t} + \zeta\,\lambda^2\,\frac{\partial \rho}{\partial x} - \sigma\,\lambda^2\,\Delta t\,(1-\zeta)\,\frac{\partial^2 q}{\partial x^2}& \\ - \frac{\lambda^4\,\Delta t^2}{6}\,\zeta\,(1-\zeta)\,(6\sigma^2-1)\,\frac{\partial^3 \rho}{\partial x^3} &= O(\Delta t^3)\,.\end{aligned} \tag{4.70}$$

Proof. We have the relation (4.69) at first order of accuracy, due to Proposition 4 (relation (4.24)). Conservation of momentum at first order is a consequence of Proposition 9 (relation (4.38)) and of the expression (4.49) 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

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

and the relation (4.69) is true at first order.

Conservation of mass (4.40) implies that no first order term in Δt is present. We deduce an expansion of the defect of conservation θ at second order :

$$\theta = (1-\zeta)\,\frac{\lambda^2}{2}\,\frac{\partial q}{\partial x} + \mathrm{O}(\Delta t^2)\,. \tag{4.71}$$

Conservation of momentum (4.39) 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 (4.24). In consequence, relations (4.69) and (4.70) 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 (4.40) and (4.41). 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

$$\begin{aligned}\Big(\sigma_\ell^2 - \frac{1}{6}\Big)\,\Lambda^\ell_{\alpha\beta}\,\partial_t\partial_\beta\theta_\ell &= \Big(\sigma^2 - \frac{1}{6}\Big)\,\Lambda^2_{11}\,\frac{\partial^2\theta}{\partial x\,\partial t} \\ &= \Big(\sigma^2 - \frac{1}{6}\Big)\,(1-\zeta)\,\lambda^2\,\frac{\partial^2}{\partial x^2}\Big(\frac{\partial q}{\partial x}\Big) + \mathrm{O}(\Delta t^2) \quad \text{due to (4.71)} \\ &= -\Big(\sigma^2 - \frac{1}{6}\Big)\,(1-\zeta)\,\lambda^4\,\frac{\partial^3 q}{\partial x^3} + \mathrm{O}(\Delta t^2)\,,\end{aligned}$$

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 (4.70) is completely established and the proposition is proved. □

We adapt now the D2Q9 Boltzmann scheme presented at second sub-section 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 (4.56). In consequence, the momentum-velocity tensor Λ is still obtained according to relations (4.57). This model conserves mass and the two components of momentum. Then following Lallemand and Luo [95], relations (4.58) to (4.60) have to be replaced by

$$m_3^{\mathrm{e}q} = -2\rho\,,\quad m_4^{\mathrm{e}q} = \rho\,,\quad m_5^{\mathrm{e}q} = -\frac{q_x}{\lambda}\,,\quad m_6^{\mathrm{e}q} = -\frac{q_6}{\lambda}\,,\quad m_7^{\mathrm{e}q} = m_8^{\mathrm{e}q} = 0$$

and in consequence the matrix J_0 takes the form

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

Due to relation (4.57), only three defects of conservation play an active role for determining the equivalent equations. We have now (see details *e*.g. [42])

$$\theta_3 \equiv -2\,\frac{\partial\rho}{\partial t}\,,\quad \theta_7 \equiv \frac{2}{3}\Big(\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y}\Big),\quad \theta_8 \equiv \frac{1}{3}\Big(\frac{\partial q_y}{\partial x} + \frac{\partial q_x}{\partial y}\Big). \tag{4.72}$$

Proposition 4.6.2. Third order scheme for D2Q9 diffusive acoustics lattice Boltzmann scheme. *With previous notations, the D2Q9 Boltzmann scheme defined by (4.6), (4.9), (4.52) and (4.71) admits the following partial differential equations for conservation of mass and momentum at third order of accuracy:*

$$\frac{\partial\rho}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} - \frac{1}{18}\,\lambda^2\,\Delta t^2\,\Delta\big(di\,v q\big) \;=\; O(\Delta t^3)\,, \tag{4.73}$$

$$\frac{\partial q_x}{\partial t} + \frac{\lambda^2}{3}\,\frac{\partial\rho}{\partial x} - \frac{\lambda^2}{3}\,\Delta t\Big[\sigma_3\,\frac{\partial}{\partial x}di\,v q + \sigma_8\,\Delta q_x\Big] - \frac{\lambda^4\,\Delta t^2}{9}\Big(\sigma_3^2 + \sigma_8^2 - \frac{1}{3}\Big)\frac{\partial}{\partial x}\Delta\rho \;=\; O(\Delta t^3)\,, \tag{4.74}$$

$$\frac{\partial q_x}{\partial t} + \frac{\lambda^2}{3}\,\frac{\partial\rho}{\partial x} - \frac{\lambda^2}{3}\,\Delta t\Big[\sigma_3\,\frac{\partial}{\partial x}di\,v q + \sigma_8\,\Delta q_x\Big] - \frac{\lambda^4\,\Delta t^2}{9}\Big(\sigma_3^2 + \sigma_8^2 - \frac{1}{3}\Big)\frac{\partial}{\partial y}\Delta\rho \;=\; O(\Delta t^3)\,. \tag{4.75}$$

Proof. We have to go step by step as in the other examples. Equation of mass (4.73) is valid at first order. Second, due to (4.39) and (4.57),

$$\begin{aligned}\Lambda^{\ell}_{\alpha\beta}\partial_\beta m^{eq}_{\ell} &= \Lambda^{0}_{\alpha\beta}\partial_\beta m^{eq}_{0} + \Lambda^{3}_{\alpha\beta}\partial_\beta m^{eq}_{3} + \Lambda^{7}_{\alpha\beta}\partial_\beta m^{eq}_{7} + \Lambda^{8}_{\alpha\beta}\partial_\beta m^{eq}_{8} \\ &= \frac{2}{3}\lambda^2\partial_\alpha\rho + \frac{1}{6}\lambda^2\partial_\alpha\big(m^{eq}_3\big) = \frac{2}{3}\lambda^2\partial_\alpha\rho + \frac{1}{6}\lambda^2(-2)\partial_\alpha\rho \;=\; \frac{1}{3}\lambda^2\partial_\alpha\rho\end{aligned}$$

and relations (4.74) and (4.75) 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 (4.72) and (4.73) at second order:

$$\theta_3 = 2\,\mathrm{d}iv\,q + \mathrm{O}(\Delta t^2)\,.$$

For momentum transfer, we have from (4.39)

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

In particular for $\alpha = 1$ we have

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

and for $\alpha = 2$

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

These expressions prove that momentum conservation (4.74) and (4.75) is established at order two.

The extension to third order of accuracy follow (4.40) and (4.41). Due to relation (4.40),

$$\begin{aligned}\frac{\Delta t^2}{12}\,\Lambda^{\ell}_{\alpha\beta}\partial_\alpha\partial_\beta\theta_\ell &= \frac{\Delta t^2}{12}\,\Big(\Lambda^{3}_{\alpha\beta}\partial_\alpha\partial_\beta\theta_3 + \Lambda^{7}_{\alpha\beta}\partial_\alpha\partial_\beta\theta_7 + \Lambda^{8}_{\alpha\beta}\partial_\alpha\partial_\beta\theta_8\Big) \\ &= \frac{\lambda^2\,\Delta t^2}{12}\,\Big[\frac{1}{6}\Delta\big(2\,\mathrm{d}iv q\big) + \frac{1}{2}\big(\partial^2_x - \partial^2_y\big)\Big(\frac{2}{3}\Big(\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y}\Big)\Big) + 2\,\partial_x\partial_y\Big(\frac{1}{3}\Big(\frac{\partial q_x}{\partial y} + \frac{\partial q_x}{\partial y}\Big)\Big)\Big] + \mathrm{O}(\Delta t^4) \\ &= \frac{\Delta t^2}{12}\,\Big[\frac{2}{3}\Delta\Big(\frac{\partial q_x}{\partial x}\Big) + \frac{2}{3}\Delta\Big(\frac{\partial q_y}{\partial y}\Big)\Big] + \mathrm{O}(\Delta t^4)\end{aligned}$$

and the relation (4.73) is completely established. We observe now that by derivation of (4.72) relatively to time and taking into account the relations (4.74) and (4.75) 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 (4.41). We have

$$\Big(\sigma^2_\ell - \frac{1}{6}\Big)\Lambda^{\ell}_{\alpha\beta}\partial_t\partial_\beta\theta_\ell = \Big(\sigma^2_3 - \frac{1}{6}\Big)\Lambda^{3}_{\alpha\beta}\partial_\beta\big(\partial_t\theta_3\big) + \Big(\sigma^2_7 - \frac{1}{6}\Big)\Big[\Lambda^{7}_{\alpha\beta}\partial_\beta\big(\partial_t\theta_7\big) + \Lambda^{8}_{\alpha\beta}\partial_\beta\big(\partial_t\theta_8\big)\Big]$$

and for $\alpha = 1$,

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

and all the terms of equation (4.74) have been put in evidence. For $\alpha = 2$, we have

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

and all the terms of (4.75) have been found. We finally observe that the last term in relation (4.41), *i*d 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. □

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.

ANNEX

Tensor of momentum-velocity for D2Q9 lattice Boltzmann scheme.

We explicit matrices Λ_{kp}^{ℓ} for all indices α, β and ℓ in the range from 0 to 8. Recall that Λ_{kp}^{ℓ} is defined from matrix M according to (4.14) and for classical D2Q9 scheme, the matrix M follows (4.66). The result is just a tedious exercice of calculus. We obtain

$$\Lambda_{kp}^{0} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & \frac{2}{3}\lambda^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & \frac{2}{3}\lambda^2 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{4}{3} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{4}{3} & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{4}{9} & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{4}{9} \end{pmatrix},$$

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

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

$$\Lambda^3_{kp} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{6}\lambda^2 & 0 & 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{6}\lambda^2 & 0 & 0 & 0 & \frac{1}{3}\lambda & 0 & 0 \\ 1 & 0 & 0 & -1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -2 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{9} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{9} \end{pmatrix},$$

$$\Lambda^4_{kp} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3}\lambda & 0 & 0 \\ 0 & 0 & 0 & 2 & -2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & -\frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{2}{9} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{9} \end{pmatrix},$$

$$\Lambda^5_{kp} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda & \lambda & 0 & 0 & -\frac{1}{3}\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3}\lambda \\ 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & -\frac{1}{3}\lambda & 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 \end{pmatrix},$$

$$\Lambda^6_{kp} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3}\lambda \\ 0 & 0 & 0 & \lambda & \lambda & 0 & 0 & \frac{1}{3}\lambda & 0 \\ 0 & 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 & -\frac{2}{3} & 0 \\ 0 & 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & -\frac{2}{3} & 0 & 0 \\ 0 & \frac{1}{3}\lambda & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \end{pmatrix},$$

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

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

CHAPTER 5

INTRODUCTION TO BOUNDARY CONDITIONS

We first consider the so-called bounce-back and anti-bounce-back boundary conditions for a very simple mono-dimensional model. Then we extend this approach to the case of a uni-dimensional boundary located at an arbitrary place for the one-dimensionel mesh, and present the algorithm developed by Bouzidi, Firdaouss and Lallemand [17]. We extend this method to two space dimensions and describe briefly the genaral case of a regular boundary in two space dimensions. We refer also the reader to the original contributions of Ginzburg and Adler [65], He *et al.* [76], and Zou and He [136].

5.1 BOUNCE-BACK AND ANTI-BOUNCE-BACK FOR THE D1Q3 SCHEME

We consider to fix the ideas the D1Q3 fluid scheme as studied in section 1.2 of chapter 1. The equilibrium values of the particule distribution $f \equiv \big(f_0\,,\, f_+\,,\, f_-\big)$ satisfy

$$\begin{aligned} f_0^{\rm eq} + f_+^{\rm eq} + f_-^{\rm eq} &= \rho & (5.1)\\ f_+^{\rm eq} - f_-^{\rm eq} &= \frac{\rho\, u}{\lambda} & (5.2)\\ f_+^{\rm eq} + f_-^{\rm eq} &= \alpha\, \rho\,. & (5.3) \end{aligned}$$

We consider a “left” boundary, described on Figure 5.1: the node x is a vertex of the lattice but the node $x-\Delta x$ is outside the computational domain. The difficulty is to define the density value $f_+(x\,,\, t+\Delta t)$ of the incoming particles at the new time step. If we simply describe the internal lattice Boltzmann scheme, we have

$$f_+(x\,,\, t+\Delta t) \,=\, f_+^*(x-\Delta x\,,\, t)\,. \qquad (5.4)$$

The value $f_+^*(x-\Delta x\,,\, t)$ has now to be re-constructed from the values $f_0\,,\, f_+\,,\, f_-$ in the field and the knowledge of some physical data associated to the boundary condition.

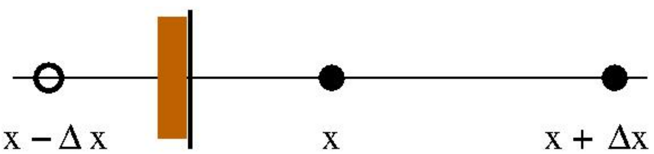

Figure 5.1 – *Left boundary for a D1Q3 lattice Boltzmann scheme.*

• **Bounce back**. We suppose to fix the ideas that the momentum $J_0 \equiv \rho_0 \, u_0$ is given at this left boundary. If we suppose that the node $x - \Delta x$ is an ordinary vertex of the lattice, we have, due to the equilibrium (5.2), the following calculus at a very poor precision of order zero:

$$\begin{aligned} f_+^*(x-\Delta x, t) - f_-^*(x, t) &= f_+^{\rm eq}(x-\Delta x, t) + {\rm O}(\Delta x) - \Big[f_-^{\rm eq}(x, t) + {\rm O}(\Delta x) \Big] \\ &= f_+^{\rm eq}(x, t) - f_-^{\rm eq}(x, t) + {\rm O}(\Delta x) \\ &= \frac{1}{\lambda} J_0 + {\rm O}(\Delta x) \,. \end{aligned}$$

With the so-called "bounce back" boundary condition, we neglect the ${\rm O}(\Delta x)$ error in the previous calculus (!) and we set:

$$f_+^*(x-\Delta x, t) = f_-^*(x, t) + \frac{1}{\lambda} \rho_0 \, u_0 \,. \tag{5.5}$$

We have reconstructed an incoming particle density $f_+^*(x-\Delta x, t)$ in the node outside the admissible mesh from a given value of the particle distribution and the momentum boundary condition. For the new time step, we mix the relations (5.4) and (5.5) and we avoid the "ghost nodes" introduced long time ago by Roache [116]:

$$f_+(x, t+\Delta t) = f_-^*(x, t) + \frac{1}{\lambda} \rho_0 \, u_0 \,. \tag{5.6}$$

• **Anti-bounce-back**. It the density ρ is given on the boundary with a value ρ_0 we use the relation (5.3):

$$\begin{aligned} f_+^*(x-\Delta x, t) + f_-^*(x, t) &= f_+^{\rm eq}(x-\Delta x, t) + {\rm O}(\Delta x) + \Big[f_-^{\rm eq}(x, t) + {\rm O}(\Delta x) \Big] \\ &= f_+^{\rm eq}(x, t) + f_-^{\rm eq}(x, t) + {\rm O}(\Delta x) \\ &= \alpha \, \rho_0 + {\rm O}(\Delta x) \,. \end{aligned}$$

With the so-called "anti-bounce-back" boundary condition, we neglect the term ${\rm O}(\Delta x)$ and we set:

$$f_+^*(x-\Delta x, t) = -f_-^*(x, t) + \alpha \, \rho_0 \,. \tag{5.7}$$

We have again reconstructed an incoming particle density $f_+^*(x-\Delta x, t)$ in the outside vertex from a given value, the value (1.48) of the equilibrium energy and the knowledge of the density ρ_0 on the boundary. Once again, the value $f_+(x, t+\Delta t)$ follows the relations (5.4) and (5.7). We have for anti-bounce-back:

$$f_+(x, t+\Delta t) = -f_-^*(x, t) + \alpha \, \rho_0 \,. \tag{5.8}$$

All these relations are operational if the boundary is located "between" two grid points, *id est* at a distance of $\frac{\Delta x}{2}$ from the last grid point, as illustrated on Figure 5.1.

5.2 BOUZIDI *et al.* BOUNDARY CONDITIONS FOR THE D1Q3 SCHEME

If the boundary is not located exactly between two grid points but at a distance $\xi\,\Delta x$ (with $0 < \xi < 1$) of the last grid point, as illustrated in Figure 5.2, we have two possibilities. On one hand, to neglect the exact value of the parameter $\xi \in]0,1[$ and replace its value by $\frac{1}{2}$. In this case, we have a staircase approximation of the boundary, studied *e.g.* in [103, 128]. On the other hand, we try to take into account the precise position of the boundary described by the parameter ξ. Our question here is to adapt the boudary conditions (5.6) and (5.8) to take into account explicitely the ξ value that parameterizes the precise location of the boundary. With the method proposed by Bouzidi, Firdaouss and Lallemand [17], we follow the particle trajectories. Two cases have to be considered, whreas the boundary is close to the last mesh point ($\xi < \frac{1}{2}$, first case) of "far" from the last mesh point ($\xi > \frac{1}{2}$, second case).

We first write in a synthetic form the bounce-back and anti-bounce-back relations under the form

$$f_+(x\,,\,t+\Delta t)\;\equiv\;f_+^*(x-\Delta x\,,\,t)\;=\;\epsilon\,f_-^*(x\,,\,t)+\Phi_0\,, \tag{5.9}$$

with $\epsilon = 1$ in the bounce-back case (5.5), $\epsilon = -1$ in the anti-bounce-back case (5.7), and Φ_0 equal to $\rho_0\,u_0\,/\,\lambda$ or to $\alpha\,\rho_0$ as appropriate.

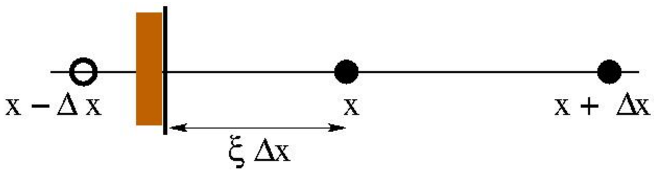

Figure 5.2 – *The left boundary is not located between two grid points.*

- **First case**: $0 < \xi \leqslant \frac{1}{2}$. In this case, we retro-propagate the trajectory of the particle that arrives exactly at the position x at time $t+\Delta t$, as illustrated in Figure 5.3. We introduce y the point between the vertices x and $x+\Delta x$ whose trajectory started (see the figure 5.3). We replace the boundary condition (5.9) by

$$f_+^*(x-\Delta x\,,\,t)\;=\;\epsilon\,f_-^*(y\,,\,t)+\Phi_0\,, \tag{5.10}$$

We now just have to evaluate with a good precision the particle density $f_-^*(y\,,\,t)$ at the point y. In one time step, the particle follows a trajectory of total length equal to Δx. We then have

$$2\xi\,\Delta x + y - x\;=\;\Delta x$$

and we can write the point y as an interpolate betwen the vertices x and $x+\Delta x$:

$$y\;=\;2\xi\,x + (1-2\xi)\,(x+\Delta x)\,.$$

We replace $f_-^*(y\,,\,t)$ by its affine interpolate between the values $f_+^*(x\,,\,t)$ and $f_+^*(x+\Delta x\,,\,t)$ and we have:

$$f_-^*(y\,,\,t)\;\simeq\;2\xi\,f_-^*(x\,,\,t)+(1-2\xi)\,f_-^*(x+\Delta x\,,\,t)\,.$$

The Bouzidi boundary condition can be written in that case:

$$f_+^*(x-\Delta x,\, t) \;=\; \epsilon\Big[2\xi\, f_-^*(x,\, t) + (1-2\xi)\, f_-^*(x+\Delta x,\, t)\Big] + \Phi_0\,, \qquad 0<\xi\leqslant\frac{1}{2}\,. \tag{5.11}$$

In coherence with the interior scheme (5.4), the condition may be formulated only with interior nodes:

$$f_+(x,\, t+\Delta t) \;=\; \epsilon\Big[2\xi\, f_-^*(x,\, t) + (1-2\xi)\, f_-^*(x+\Delta x,\, t)\Big] + \Phi_0\,, \qquad 0<\xi\leqslant\frac{1}{2}\,. \tag{5.12}$$

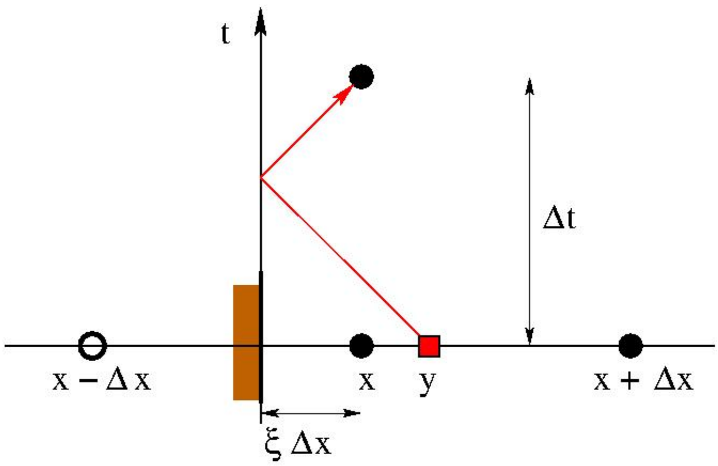

Figure 5.3 – *Bouzidi boundary conditions,* $0<\xi\leqslant\frac{1}{2}$.

- **Second case**: $\frac{1}{2}\leqslant\xi<1$. The previous method is inappropriate: the point y in Figure 5.4 is no longer between the vertices x and $x+\Delta x$ and the formula (5.11) is unstable because is is no longer an interpolate formula but an extrapolation. In this case, the Bouzidi method adopts an other point of view. We consider the two families of particles f_+ and f_- issued from the vertex x, as illustrated on Figure 5.4. The particle away from the border (going to the right direction) arrives exactly at the vertex $x+\Delta x$ at time $t+\Delta t$. In consequence, the general iteration (5.4) is correct and we write it as:

$$f_+(x+\Delta x,\, t+\Delta t) \;=\; f_+^*(x,\, t)\,. \tag{5.13}$$

The particle "minus" that goes to the border is reflected by the boundary and is finally located at the point z at time $t+\Delta t$, as illustrated on the figure 5.4. With this point z, the initial bounce-back or anti-bounce-back boundary condition (5.9) is naturally replaced by

$$f_+(z,\, t+\Delta t) \;=\; \epsilon\, f_-^*(x,\, t) + \Phi_0\,. \tag{5.14}$$

We just have now to consider the vertex x as an interpolate between the point z and the vertex $x+\Delta x$ and apply thereafter an affine interpolation. We say that in one time step, the particle travels a distance of Δx:

$$\xi\,\Delta x + z - (x-\xi\,\Delta x) \;=\; \Delta x\,,$$

id est $z = x + (1-2\xi)\,\Delta x$. We then write that the vertex x is an interpolate between z and $x+\Delta x$:

$$
\begin{aligned}
x &= \theta\, z + (1-\theta)\,(x+\Delta x) \\
&= \theta \Big[x + (1-2\xi\,\Delta x)\,\Delta x \Big] + (1-\theta)\,(x+\Delta x) \\
&= x + \big(1 - 2\theta\,\xi\big)\,\Delta x
\end{aligned}
$$

and we deduce that $\theta = \dfrac{1}{2\xi}$. In consequence,

$$
x = \frac{1}{2\xi}\, z + \Big(1 - \frac{1}{2\xi}\Big)\,(x+\Delta x)\,.
$$

To obtain the second case of the Bouzidi numerical boundary condition, we finally compute $f_+(x\,,\,t+\Delta t)$ by interpolation between the values $f_+(z\,,\,t+\Delta t)$ and $f_+(x+\Delta x\,,\,t+\Delta t)$ presented in (5.14) and (5.13) respectively, with the respective weighting $\frac{1}{2\xi}$ and $1-\frac{1}{2\xi}$:

$$
f_+(x\,,\,t+\Delta t) = \frac{1}{2\xi}\Big[\epsilon\, f_-^*(x\,,\,t) + \Phi_0\Big] + \Big(1-\frac{1}{2\xi}\Big)\, f_+^*(x\,,\,t)\,, \qquad \frac{1}{2} \leqslant \xi < 1\,. \tag{5.15}
$$

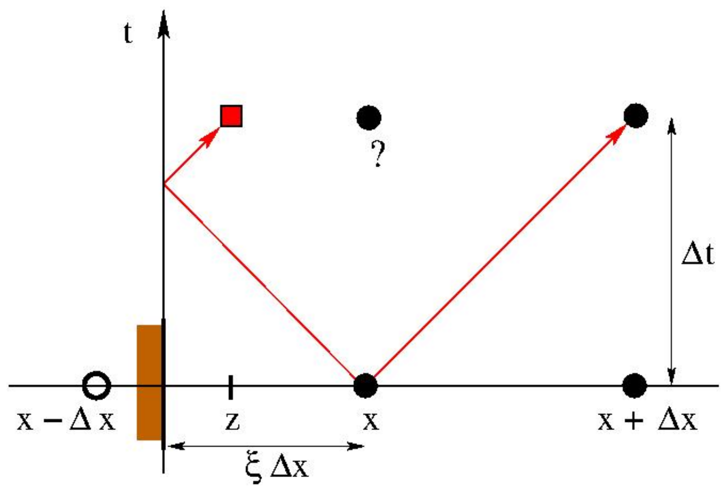

Figure 5.4 – *Bouzidi boundary conditions,* $\frac{1}{2} \leqslant \xi < 1$.

As in the bounce-back and anti-bounce-back approach, we have reconstructed an incoming particle density $f_+(x\,,\,t+\Delta t)$ at the new time step from given values in the internal field and physical data on the boundary. We observe also that in the particular case $\xi = 1/2$, the two relations (5.12) and (5.15) degenerate into the initial bounce-back and anti-bounce-back (5.9).

5.3 SOME EXAMPLES IN A TWO-DIMENSIONAL SPACE

The bounce-back and anti-bounce-back are generalized in two space dimensions without major difficulty. We consider to fix the ideas the D2Q9 lattice Boltzmann scheme studied in chapter 3. A basic problem is described in Figure 5.5. The vertex $x \equiv (x_1\,,\,x_2)$ is located inside the computational domain whereas the vertices translated by $-(0\,,\Delta x)$ are outside. We suppose in a first approach that the boundary is located between the two lines of grid points. The determination of the three incoming particle distributions f_2, f_5 and f_6 is a real problem. The internal iteration of the scheme

$$\begin{aligned} f_2(x_1\,,x_2\,,t+\Delta t) &= f_2^*(x_1\,,x_2-\Delta x\,,t) &(5.16)\\ f_5(x_1\,,x_2\,,t+\Delta t) &= f_5^*(x_1-\Delta x\,,x_2-\Delta x\,,t) &(5.17)\\ f_6(x_1\,,x_2\,,t+\Delta t) &= f_6^*(x_1+\Delta x\,,x_2-\Delta x\,,t) &(5.18)\end{aligned}$$

can not be implemented because the three vertices $(x_1\,,x_2-\Delta x)$, $(x_1-\Delta x\,,x_2-\Delta x)$ and $(x_1+\Delta x\,,x_2-\Delta x)$ are not inside the domain of physical interest.

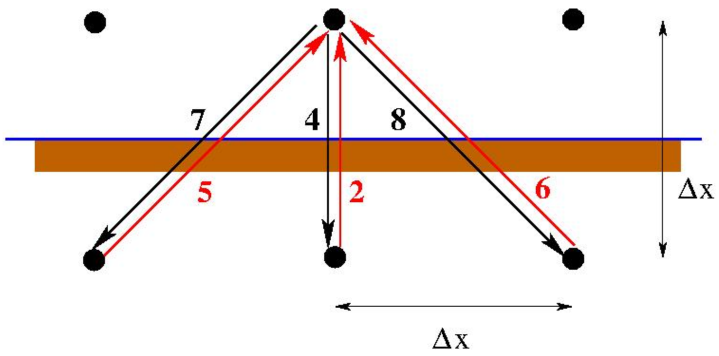

Figure 5.5 – *Simple boundary condition for the D2Q9 scheme. The incoming density of particles $f_2^*(x_1\,,x_2-\Delta x)$, $f_5^*(x_1-\Delta x\,,x_2-\Delta x)$ and $f_6^*(x_1+\Delta x\,,x_2-\Delta x)$ (in red) have to be determined. This is done using respectively the outgoing particle distributions $f_2^*(x_1\,,x_2)$, $f_7^*(x_1\,,x_2)$ and $f_8^*(x_1\,,x_2)$.*

We start from the D2Q9 equilibrium particle distribution (3.82) in a linearized approach:

$$f^{\rm eq} = \left\{ \begin{aligned} f_0^{\rm eq} &= \frac{4}{9}\rho + {\rm O}\big(|u|^2\big)\\ f_1^{\rm eq} &= \frac{1}{9}\rho + \frac{1}{3}\frac{\rho\,u_x}{\lambda} + {\rm O}\big(|u|^2\big)\\ f_2^{\rm eq} &= \frac{1}{9}\rho + \frac{1}{3}\frac{\rho\,u_y}{\lambda} + {\rm O}\big(|u|^2\big)\\ f_3^{\rm eq} &= \frac{1}{9}\rho - \frac{1}{3}\frac{\rho\,u_x}{\lambda} + {\rm O}\big(|u|^2\big)\\ f_4^{\rm eq} &= \frac{1}{9}\rho - \frac{1}{3}\frac{\rho\,u_y}{\lambda} + {\rm O}\big(|u|^2\big)\\ f_5^{\rm eq} &= \frac{1}{36}\rho + \frac{1}{12}\frac{\rho\,(u_x+u_y)}{\lambda} + {\rm O}\big(|u|^2\big)\\ f_6^{\rm eq} &= \frac{1}{36}\rho + \frac{1}{12}\frac{\rho\,(-u_x+u_y)}{\lambda} + {\rm O}\big(|u|^2\big)\\ f_7^{\rm eq} &= \frac{1}{36}\rho - \frac{1}{12}\frac{\rho\,(u_x+u_y)}{\lambda} + {\rm O}\big(|u|^2\big)\\ f_8^{\rm eq} &= \frac{1}{36}\rho + \frac{1}{12}\frac{\rho\,(u_x-u_y)}{\lambda} + {\rm O}\big(|u|^2\big). \end{aligned}\right. \tag{5.19}$$

In the following, we neglect the $O(|u|^2)$ terms. We first remark that we have on one hand

$$
\begin{aligned}
f_2^{eq} - f_4^{eq} &= \frac{2}{3\lambda}\,\rho\, u_y && (5.20)\\
f_5^{eq} - f_7^{eq} &= \frac{1}{6\lambda}\,\rho\,(u_x + u_y) && (5.21)\\
f_6^{eq} - f_8^{eq} &= \frac{1}{6\lambda}\,\rho\,(-u_x + u_y) && (5.22)
\end{aligned}
$$

and on the other hand

$$
\begin{aligned}
f_2^{eq} + f_4^{eq} &= \frac{2}{9}\,\rho && (5.23)\\
f_5^{eq} + f_7^{eq} &= \frac{1}{18}\,\rho && (5.24)\\
f_6^{eq} + f_8^{eq} &= \frac{1}{18}\,\rho\,. && (5.25)
\end{aligned}
$$

- At a boundary, we replace the values of density and velocity by the notations ρ_0, u_0 and v_0, to enforce the fact that these date are supposed to be (eventually!) known at the boundary. We have now a simple calculus analogous to the one done previously in the one-dimensional case:

$$
\begin{aligned}
f_2^*(x_1, x_2 - \Delta x, t) \;-\; f_4^*(x_1, x_2, t) &= f_2^{eq}(x_1, x_2 - \Delta x, t) + O(\Delta x) - \left[f_4^{eq}(x_1, x_2, t) + O(\Delta x) \right]\\
&= f_2^{eq}(x_1, x_2, t) - f_4^{eq}(x_1, x_2, t) + O(\Delta x) = \frac{2}{3\lambda}\,\rho_0\, v_0 + O(\Delta x)\,,
\end{aligned}
$$

$$
\begin{aligned}
f_5^*(x_1 - \Delta x, x_2 - \Delta x, t) \;-\; f_7^*(x_1, x_2, t) &= f_5^{eq}(x_1 - \Delta x, x_2 - \Delta x, t) - f_7^{eq}(x_1, x_2, t) + O(\Delta x)\\
&= f_5^{eq}(x_1, x_2, t) - f_7^{eq}(x_1, x_2, t) + O(\Delta x) = \frac{1}{6\lambda}\,\rho\,(u_0 + v_0) + O(\Delta x)\,,
\end{aligned}
$$

$$
\begin{aligned}
f_6^*(x_1 + \Delta x, x_2 - \Delta x, t) \;-\; f_8^*(x_1, x_2, t) &= f_6^{eq}(x_1 + \Delta x, x_2 - \Delta x, t) - f_8^{eq}(x_1, x_2, t) + O(\Delta x)\\
&= f_6^{eq}(x_1, x_2, t) - f_8^{eq}(x_1, x_2, t) + O(\Delta x) = \frac{1}{6\lambda}\,\rho\,(-u_0 + v_0) + O(\Delta x)\,.
\end{aligned}
$$

We can formulated the **bounce-back** boundary condition when the momentum $(\rho_0\, u_0, \rho_0\, v_0)$ is given at the boundary in the particular case described on the figure 5.5:

$$
\begin{aligned}
f_2(x_1, x_2, t + \Delta t) &= f_2^*(x_1, x_2 - \Delta x, t) = f_4^*(x_1, x_2, t) + \frac{2}{3\lambda}\,\rho_0\, v_0 && (5.26)\\
f_5(x_1, x_2, t + \Delta t) &= f_5^*(x_1 - \Delta x, x_2 - \Delta x, t) = f_7^*(x_1, x_2, t) + \frac{1}{6\lambda}\,\rho\,(u_0 + v_0) && (5.27)\\
f_6(x_1, x_2, t + \Delta t) &= f_6^*(x_1 + \Delta x, x_2 - \Delta x, t) = f_8^*(x_1, x_2, t) + \frac{1}{6\lambda}\,\rho\,(-u_0 + v_0)\,. && (5.28)
\end{aligned}
$$

- We have now a simple adaptation of the previous calculus by a simple change of some signs:

$$\begin{aligned} f_2^*(x_1\,,\,x_2-\Delta x\,,\,t) \quad + \quad f_4^*(x_1\,,\,x_2\,,\,t) &= f_2^{\rm eq}(x_1\,,\,x_2-\Delta x\,,\,t) + {\rm O}(\Delta x) + \Big[f_4^{\rm eq}(x_1\,,\,x_2\,,\,t) + {\rm O}(\Delta x) \Big] \\ &= f_2^{\rm eq}(x_1\,,\,x_2\,,\,t) + f_4^{\rm eq}(x_1\,,\,x_2\,,\,t) + {\rm O}(\Delta x) = \frac{2}{9}\,\rho_0 + {\rm O}(\Delta x)\,, \end{aligned}$$

$$\begin{aligned} f_5^*(x_1-\Delta x\,,\,x_2-\Delta x\,,\,t) \quad + \quad f_7^*(x_1\,,\,x_2\,,\,t) &= f_5^{\rm eq}(x_1-\Delta x\,,\,x_2-\Delta x\,,\,t) + f_7^{\rm eq}(x_1\,,\,x_2\,,\,t) + {\rm O}(\Delta x) \\ &= f_5^{\rm eq}(x_1\,,\,x_2\,,\,t) + f_7^{\rm eq}(x_1\,,\,x_2\,,\,t) + {\rm O}(\Delta x) = \frac{1}{18}\,\rho_0 + {\rm O}(\Delta x)\,, \end{aligned}$$

$$\begin{aligned} f_6^*(x_1+\Delta x\,,\,x_2-\Delta x\,,\,t) \quad + \quad f_8^*(x_1\,,\,x_2\,,\,t) &= f_6^{\rm eq}(x_1+\Delta x\,,\,x_2-\Delta x\,,\,t) + f_8^{\rm eq}(x_1\,,\,x_2\,,\,t) + {\rm O}(\Delta x) \\ &= f_6^{\rm eq}(x_1\,,\,x_2\,,\,t) + f_8^{\rm eq}(x_1\,,\,x_2\,,\,t) + {\rm O}(\Delta x) = \frac{1}{18}\,\rho_0 + {\rm O}(\Delta x)\,. \end{aligned}$$

The **anti-bounce-back** boundary condition for the D2Q9 scheme can be formulated as follows when the density ρ_0 (or the pressure $p_0 = c_0^2\,\rho_0$) is given at the boundary in the particular case of Figure 5.5:

$$f_2(x_1\,,\,x_2\,,\,t+\Delta t) = f_2^*(x_1\,,\,x_2-\Delta x\,,\,t) = -f_4^*(x_1\,,\,x_2\,,\,t) + \frac{2}{9}\,\rho_0 \tag{5.29}$$

$$f_5(x_1\,,\,x_2\,,\,t+\Delta t) = f_5^*(x_1-\Delta x\,,\,x_2-\Delta x\,,\,t) = -f_7^*(x_1\,,\,x_2\,,\,t) + \frac{1}{18}\,\rho_0 \tag{5.30}$$

$$f_6(x_1\,,\,x_2\,,\,t+\Delta t) = f_6^*(x_1+\Delta x\,,\,x_2-\Delta x\,,\,t) = -f_8^*(x_1\,,\,x_2\,,\,t) + \frac{1}{18}\,\rho_0\,. \tag{5.31}$$

The bounce-back relations (5.26), (5.27) and (5.28) must be adapted when the momentum is given in an other geometry that the one presented in Figure 5.5. We have the same remark for the anti-bounce-back (5.29), (5.30) and (5.28) conditions. To cover all the possible cases can be a true difficulty when implementing the lattice Boltzmann scheme in several space dimensions.

- The adaptation of the Bouzidi boundary conditions in two space dimensions does not set new fundamental problems. An example is presented in Figure 5.6. For a given direction of the lattice, the relations (5.11) and (5.15) are adapted: The "+−" duality of the D1Q3 scheme is replaced by the "24", "57" and "68" dualities for opposite directions. All is needed is a second mesh point in the mesh direction inside the computational domain. As observed in Figure 5.6, a curved discrete boundary is not composed by staircases steps. This fact explains why the Bouzidi boundary condition is precise from a geometric point of view.

Finally, we observe that the so-called "Bouzidi boundary condition" is intensively used for simulations with the lattice Boltzmann scheme. We refer to [1, 2, 34, 98] and the open-softwares "OpenLB" [1] or "pyLBM" [2] among others! More elaborated boundary conditions have been proposed among others by d'Humières and Ginzburg [82]. We refer also to the work of Tekitek *et al* [129] for absorbing boundary conditions, or to our previous work [51, 52] for the development of boundary quartic parameters in the multirelaxation time approach to enforce the precision of the lattice Boltzmann scheme.

[1] see http://optilb.com/openlb.
[2] used during this course!

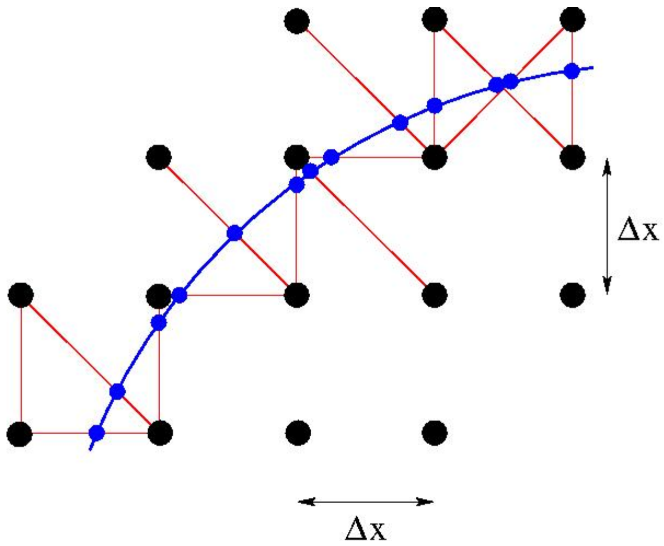

Figure 5.6 – *Curved two-dimensional boundary (in bue) discretized with the Bouzidi boundary condition. All the links in red are active for this boundary condition. Observe that the discrete boundary taken into account by the lattice Boltzmann scheme is composed by all blue points. The discrete boundary is not composed by staircases steps!*

CHAPTER 6

HIGHER ORDER FORMAL EXPANSION OF LINEAR LATTICE BOLTZMANN SCHEMES

We propose the derivation of acoustic-type isotropic partial differential equations that represent the truncation error of a linear lattice Boltzmann scheme. The corresponding linear equivalent partial differential equations are generated with the "Berliner version" of the Taylor expansion method [1]. The corresponding partial differential equations can be computed at an arbitrary order of accuracy.

6.1 Introduction

• The lattice Boltzmann scheme is a numerical method for simulation of a wide family of partial differential equations associated with conservation laws of physics. The principle is to mimic at a discrete level the dynamics of the Boltzmann equation. In this paradigm, the number $f(x,\,t)\,\mathrm{d}x\,\mathrm{d}v$ of particles at position x, time t and velocity v with an uncertainty of $\mathrm{d}x\,\mathrm{d}v$ follows the Boltzmann partial differential equation in the phase space (see *e.g.* Chapman and Cowling [26]):

$$\frac{\partial f}{\partial t} + v \bullet \nabla_x f = Q(f)\,. \tag{6.1}$$

Note that the left hand side is a simple advection equation whose solution is trivial through the method of characteristics:

$$f(x,\,v,\,t) = f(x - v\,t,\,v,\,0) \qquad \mathrm{i}f \quad Q(f) \equiv 0\,. \tag{6.2}$$

Remark also that the right hand side is a collision operator, local in space and integral relative to velocities:

$$Q(f)(x,\,v,\,t) = \int \mathscr{C}\big(f(x,\,w,\,t), x,\,v,\,t\big)\,\mathrm{d}w\,, \tag{6.3}$$

where $\mathscr{C}(\bullet)$ describes collisions at a microscopic level. Due to microscopic conservation of mass, momentum and energy, an equilibrium distribution $f^{\mathrm{e}q}(x,\,v,\,t)$ satisfy the nullity of first moments of the distribution of collisions:

$$\int Q(f^{\mathrm{e}q})(x,\,v,\,t) \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\,|v|^2 \end{pmatrix} \mathrm{d}v \;=\; 0\,.$$

Such an equilibrium distribution f^{eq} satisfies classically the Maxwell-Boltzmann distribution.

[1] This contribution has been originally published in [6].

• The lattice Boltzmann method follows all these physical recommandations with specific additional options. First, space x is supposed to live in a lattice $\mathcal{L}$ included in Euclidian space of dimension d. Second, velocity belongs to a finite set $\mathcal{V}$ composed by given velocities v_j $(0 \leqslant j \leqslant J)$ chosen in such a way that

$$x \in \mathcal{L} \text{ and } v_j \in \mathcal{V} \implies x + \Delta t \, v_j \in \mathcal{L},$$

where Δt is the time step of the numerical method. Then the distribution of particles, f, is denoted by $f_j(x, t)$ with $0 \leqslant j \leqslant J$, x in the lattice $\mathcal{L}$ and t an integer multiple of time step Δt.

• In the pioneering work of cellular automata introduced by Hardy, Pomeau and De Pazzis [73], Frisch, Hasslacher and Pomeau [59] and developed by d'Humières, Lallemand and Frisch [84], the distribution $f_j(x, t)$ was chosen as Boolean. Since the so-called lattice Boltzmann equation of Mac Namara and Zanetti [101], Higuera, Succi and Benzi [79], Chen, Chen and Matthaeus [27], Higuera and Jimenez [78] (see also Chen and Doolen [28]), the distribution $f_j(\bullet, \bullet)$ takes real values in a continuum and the collision process follows a linearized approach of Bhatnagar, Gross and Krook [9]. With Qian, d'Humières and Lallemand [113], the equilibrium distribution f^{eq} is determined with a polynomial in velocity. In the work of Karlin *et al* [91], the equilibrium state is obtained with a general methodology of entropy minimization.

• The asymptotic analysis of cellular automata (see *e.g.* Hénon [77]) provides evidence supporting asymptotic partial differential equations and viscosity coefficients related to the induced parameter defined by $\sigma_k \equiv \frac{1}{s_k} - \frac{1}{2}$. The lattice Boltzmann scheme has been analyzed by d'Humières [80] with a Chapman-Enskog method coming from statistical physics. Remark that the extension of the discrete Chapman-Enskog expansion to higher order already exists (Qian-Zhou [115], d'Humières [81]). But the calculation in the nonthermal case ($N > 1$) is quite delicate from an algebraic point of view and introduces noncommutative formal operators. Recently, Junk and Rheinländer [89] developed a Hilbert type expansion for the analysis of lattice Boltzmann schemes at high order of accuracy. We have proposed in previous works [42, 44] the Taylor expansion method which is an extension to the lattice Boltzmann scheme of the so-called equivalent partial differential equation method proposed independently by Lerat and Peyret [100] and by Warming and Hyett [133]. In this framework, the parameter Δt is considered as the only infinitesimal variable and we introduce a **constant** velocity ratio λ between space step and time step: $\lambda \equiv \frac{\Delta x}{\Delta t}$. The lattice Boltzmann scheme is classically considered as second-order accurate (see *e.g.* [95]). In fact, the viscosity coefficients μ relative to second-order terms are recovered according to a relation of the type $\mu = \zeta \lambda^2 \Delta t \sigma_k$ for a particular value of label k. The coefficient ζ is equal to $\frac{1}{3}$ for the simplest models that are considered hereafter.

• A natural question is to extend this accuracy to third or higher orders. In the case of single relaxation times (the BGK variant of d'Humières scheme), progresses in this direction have been proposed by Shan *et al* [123, 124] and Philippi *et al* [110] using Hermite polynomial methodology for the approximation of the Boltzmann equation. The price to pay is an extension of the stencil of the numerical scheme and the practical associated problems for the numerical treatment of boundary conditions. Note also the work of the Italian team (Sbragaglia *e*t al [120], Falcucci *et al* [57]) on application to multiphase flows. In the context of scheme with multiple relaxation times, Ginzburg, Verhaeghe and d'Humières have analyzed with the Chapman-Enskog method the "Two Relaxation Times" version of the scheme [66, 67]. A nonlinear extension of this scheme, the so-called "cascaded lattice Boltzmann method" has been proposed by Geier *et al* [63]. It gives also high order accuracy and the analysis is under development (see *e.g.* Asinari [5]). The general nonlinear extension of the Taylor expansion method to third-order of accuracy of d'Humières scheme is presented in [45]. It provides evidence of the importance of the so-called tensor of momentum-velocity defined by

$$\Lambda_{kp}^{\ell} \equiv \sum_{j=0}^{J} M_{kj}\, M_{pj}\, M_{j\ell}^{-1}\,, \qquad 0 \leqslant k,\, p,\, \ell \leqslant J\,. \tag{6.4}$$

Moreover, it shows also that for athermal Navier Stokes equations, the mass conservation equation contains a remaining term of third-order accuracy that cannot be set to zero by fitting relaxation parameters [45].

• Our motivation in this contribution is to show that it is possible to extend the order of accuracy of an existing *a priori* second-order accurate lattice Boltzmann scheme to higher orders. We use the Taylor expansion method [44] to determine the equivalent partial differential equation of the numerical scheme to higher orders of accuracy. Nevertheless, it is quite impossible to determine explicity the entire expansion in all generality in the nonlinear case. In consequence, we restrict here to a first step. We propose in the following a general methodology for deriving the equivalent equation of the d'Humières scheme at an arbitrary order when the equilibrium is **linear**.

• Each iteration of a lattice Boltzmann scheme is composed by two steps: relaxation and propagation. The relaxation is local in space: the particle distribution $f(x) \in \mathbb{R}^q$ for x a node of the lattice $\mathscr{L}$, is transformed into a "relaxed"' distribution $f^*(x)$ that is non linear in general. In this contribution, we restrict to linear functions $\mathbb{R}^q \ni f \longmapsto f^* \in \mathbb{R}^q$. As usual with the d'Humières scheme [80], we introduce an invertible matrix M with q lines and q columns. The moments m are obtained from the particle distribution thanks to the associated transformation

$$m_k = \sum_{j=0}^{q-1} M_{kj}\, f_j\,, \qquad 0 \leqslant k \leqslant q-1\,. \tag{6.5}$$

Then we consider the conserved moments $W \in \mathbb{R}^N$:

$$W_i = m_i\,, \qquad 0 \leqslant i \leqslant N-1\,. \tag{6.6}$$

For the usual acoustic equations for d space dimensions, we have $N = d+1$. The first moment is the density and the next ones are composed by the d components of the physical momentum. Then we define a conserved value $m_k^{\mathrm{e}q}$ for the non-equilibrium moments m_k for $k \geqslant N$. With the help of "Gaussian" functions $G_k(\bullet)$, we obtain:

$$m_k^{\mathrm{e}q} = G_k(W)\,, \qquad N \leqslant k \leqslant q-1\,. \tag{6.7}$$

In the present contribution, we suppose that this equilibrium value is a linear function of the conserved variables. In other terms, the Gaussian functions are linear:

$$G_{N+\ell}(W) = \sum_{i=1}^{n-1} E_{\ell i}\, W_i\,, \qquad \ell \geqslant 0 \tag{6.8}$$

for some equilibrium coefficients $E_{\ell i}$ for $\ell \geqslant 0$ and $0 \leqslant i \leqslant N-1$.

- The relaxed moments m_k^* are linear functions of m_k and m_k^{eq} :

$$m_k^* = m_k + s_k \left(m_k^{eq} - m_k\right), \qquad k \geqslant N. \tag{6.9}$$

For a stable scheme, we have

$$0 < s_k < 2. \tag{6.10}$$

We remark that if $s_k = 0$, the corresponding moment is conserved. In some particular cases, the value $s_k = 2$ can also be used (see *e.g.* see Chapter 1 and [47]). The conserved moments are not affected by the relaxation:

$$m_i^* = m_i = W_i, \qquad 0 \leqslant i \leqslant N-1.$$

From the moments m_ℓ^* for $0 \leqslant \ell \leqslant q-1$ we deduce the particle distribution f_j^* by resolution of the linear system

$$M f^* = m^*.$$

- The propagation step couples the node $x \in \mathscr{L}$ with his neighbours $x - v_j \Delta t$ for $0 \leqslant j \leqslant q-1$. The time iteration of the scheme can be written as

$$f_j(x, t + \Delta t) = f_j^*(x - v_j \Delta t, t), \qquad 0 \leqslant j \leqslant q-1, \quad x \in \mathscr{L}. \tag{6.11}$$

- From the knowledge of the previous algorithm, it is possible to derive a set of equivalent partial differential equations for the conserved variables. If the Gaussian functions G_k are linear, this set of equations takes the form

$$\frac{\partial W}{\partial t} - \alpha_1 W - \Delta t \, \alpha_2 W - \cdots - \Delta t^{j-1} \alpha_j W - \cdots - = 0, \tag{6.12}$$

where α_j is for $j \geqslant 1$ is a space derivation operator of order j. We refer the reader to [44] for the presentation of our approach in the general case. In this contribution, we have developed an explicit algebraic linear version of the algorithm detailed in Appendix 1. Moreover, we consider that the lattice Boltzmann scheme is invariant by rotation at order ℓ if the equivalent partial differential equation

$$\frac{\partial W}{\partial t} - \sum_{j=1}^{\ell} \Delta t^{j-1} \alpha_j W = 0 \tag{6.13}$$

obtained from (6.12) by truncation at the order ℓ is invariant by rotation. In the following, we determine the equivalent partial differential equations for classical lattice Bolzmann schemes in the general linear case. Then we fit the equilibrium and relaxation parameters of the scheme in order to enforce rotational invariances at all orders between 1 and 4.

6.2 A FORMAL EXPANSION IN THE LINEAR CASE

• We present in this Section the "Berliner version" [46] of the algorithm proposed in all generality in our contribution [50]. We suppose having defined a lattice Boltzmann scheme "DdQq" with d space dimensions and q discrete velocities at each vertex. The invertible matrix M between the particules and the moments is given:

$$m_k = \sum_{j=0}^{q-1} M_{kj}\, f_j \equiv \big(M \bullet f\big)_k\,, \quad 0 \leqslant k \leqslant q-1\,. \tag{6.14}$$

The lattice Boltzmann scheme generates N conservation laws: the first moments

$$m_k \equiv W_k\,, \qquad 0 \leqslant k \leqslant N-1$$

are conserved during the collision step :

$$m^* = m_k = W_k\,. \tag{6.15}$$

The $q-N$ "slave" moments Y with

$$Y_\ell \equiv m_{N+\ell}\,, \qquad 0 \leqslant \ell \leqslant q-N-1 \tag{6.16}$$

relax towards an equilibrium value $Y_\ell^{\rm eq}$. This equilibrium value is supposed to be a **linear** function of the state W. We introduce a constant rectangular matrix E with $N-q$ lines and N columns to represent this linear function:

$$Y_\ell^{\rm eq} = \sum_{k=0}^{N-1} E_{\ell k}\, W_k\,, \qquad 0 \leqslant \ell \leqslant q-N-1\,. \tag{6.17}$$

The relaxation step is obtained through the usual algorithm [80] that decouples the moments:

$$Y_\ell^* = Y_\ell + s_\ell\,(Y_\ell^{\rm eq} - Y_\ell)\,,\ s_\ell > 0\,, \qquad 0 \leqslant \ell \leqslant q-N-1\,. \tag{6.18}$$

Observe that the numbering of the "s" coefficients used in (6.18) differ just a little from the one used for the equation (6.9) and the four examples considered previously. With a matricial notation, the relaxation can be written as:

$$m^* = J_0 \bullet m \tag{6.19}$$

with a matrix J_0 of order q decomposed by blocks according to

$$J_0 = \begin{pmatrix} \mathrm{I}_N & 0 \\ S\bullet E & \mathrm{I}_{q-N} - S \end{pmatrix} \tag{6.20}$$

and a diagonal matrix S of order $q-N$ defined by $S \equiv \mathrm{d}iag\big(s_0\,, s_1\,, \ldots\,, s_{q-N-1}\big)$. The discrete advection step follows the method of characteristics:

$$f_j(x, t+\Delta t) = f_j^*(x - v_j \Delta t, t)\,, \qquad 0 \leqslant j \leqslant q-1\,. \tag{6.21}$$

• With the d'Humières's lattice Boltzmann scheme [80] previously defined, we can proceed to a formal Taylor expansion:

$$\begin{aligned} m_k(t+\Delta t) &= \sum_j M_{kj}\, f_j^*(x-v_j\Delta t) = \sum_{j\ell} M_{kj}\, M^{-1}_{j\ell}\, m^*_\ell(x-v_j\Delta t) \\ &= \sum_{j\ell} M_{kj}\, M^{-1}_{j\ell} \sum_{n=0}^{\infty} \frac{\Delta t^n}{n!} \Big(-\sum_{\alpha=1}^{d} v_j^\alpha\, \partial_\alpha \Big)^n m^*_\ell \\ &= \sum_{n=0}^{\infty} \frac{\Delta t^n}{n!} \sum_{j\ell p} M_{kj}\, M^{-1}_{j\ell} \Big(-\sum_{\alpha=1}^{d} v_j^\alpha\, \partial_\alpha \Big)^n (J_0)_{\ell p}\, m_p\,. \end{aligned}$$

We introduce a derivation matrix of order $n \geqslant 0$, defined by blocks of space differential operators of order n:

$$\begin{pmatrix} A_n & B_n \\ C_n & D_n \end{pmatrix}_{kp} \equiv \frac{1}{n!} \sum_{j\ell} M_{kj} \left(M^{-1}\right)_{j\ell} \Big(-\sum_{\alpha=1}^{d} v_j^\alpha\, \partial_\alpha \Big)^n (J_0)_{\ell p}\,, \quad n \geqslant 0\,. \tag{6.22}$$

We observe that in the relation (6.22), the blocks A_n and D_n are square matrices of order N and $q-N$ respectively. The matrices B_n and C_n are rectangular of order $N\times(q-N)$ and $(q-N)\times N$ respectively. We remark also that at order zero, the matrices A_0, B_0, C_0 and D_0 are known:

$$\begin{pmatrix} A_0 & B_0 \\ C_0 & D_0 \end{pmatrix} = J_0 = \begin{pmatrix} \mathrm{I}_N & 0 \\ S\bullet E & \mathrm{I}_{q-N} - S \end{pmatrix}. \tag{6.23}$$

The previous Taylor expansion can now be written under a matricial form:

$$\begin{pmatrix} W \\ Y \end{pmatrix}(x,\, t+\Delta t) = \sum_{n=0}^{\infty} \Delta t^n \begin{pmatrix} A_n & B_n \\ C_n & D_n \end{pmatrix} \bullet \begin{pmatrix} W \\ Y \end{pmatrix}(x,\, t)\,. \tag{6.24}$$

- At order zero relative to Δt we have:

$$\begin{pmatrix} W \\ Y \end{pmatrix}(x,\, t) + \mathrm{O}(\Delta t) = J_0 \bullet \begin{pmatrix} W \\ Y \end{pmatrix} + \mathrm{O}(\Delta t) = \begin{pmatrix} W \\ S\bullet E\bullet W + (\mathrm{I}-S)\bullet Y \end{pmatrix} + \mathrm{O}(\Delta t)$$

and the non-conserved moments are close to the equilibrium:

$$Y(x,\, t) = E\bullet W(x,\, t) + \mathrm{O}(\Delta t)\,. \tag{6.25}$$

- We make now the hypothesis of a **general form for the expansion of the nonconserved moments**:

$$Y(x,\, t) = \Big(E + \sum_{n\geqslant 1} \Delta t^n\, \beta_n \Big) \bullet W(x,\, t) \tag{6.26}$$

and the hypothesis of a formal linear partial differential system of arbitrary order for the conserved variables W:

$$\frac{\partial W}{\partial t} = \Big(\sum_{\ell\geqslant 0} \Delta t^\ell\, \alpha_{\ell+1} \Big) \bullet W(x,\, t)\,, \tag{6.27}$$

where α_ℓ and β_n are space differential operators of order ℓ and n respectively. We develop the first equation of (6.24) up to first order:

$$W + \Delta t \frac{\partial W}{\partial t} + \mathrm{O}(\Delta t^2) = W + \Delta t \big(A_1 W + B_1 Y\big) + \mathrm{O}(\Delta t^2)$$
$$= W + \Delta t \big(A_1 W + B_1 E W\big) + \mathrm{O}(\Delta t^2)$$

due to (6.25). Then

$$\frac{\partial W}{\partial t} = \big(A_1 + B_1 E\big) \bullet W + \mathrm{O}(\Delta t) \tag{6.28}$$

and the relation (6.27) is satisfied at order one, with

$$\alpha_1 = A_1 + B_1 E . \tag{6.29}$$

The "Euler equations" are emerging ! We have an analogous calculus for the second equation of (6.24) :

$$Y + \Delta t \frac{\partial Y}{\partial t} + \mathrm{O}(\Delta t^2) = S E W + (\mathrm{I} - S) Y + \Delta t \big(C_1 W + D_1 E W\big) + \mathrm{O}(\Delta t^2) .$$

We clarify the time derivative $\partial_t Y$ at order zero by differentiating (formally !) the relation (6.25) relative to time:

$$\frac{\partial Y}{\partial t} = E \frac{\partial W}{\partial t} + \mathrm{O}(\Delta t) = E \alpha_1 W + \mathrm{O}(\Delta t) .$$

We introduce this expression inside the previous calculus. Then:

$$S Y + \Delta t E \alpha_1 W + \mathrm{O}(\Delta t^2) = S E W + \Delta t \big(C_1 W + D_1 E W\big) + \mathrm{O}(\Delta t^2) .$$

Consequently we have established the expansion of the nonconserved moments at order one:

$$Y = E W + \Delta t S^{-1} \big(C_1 + D_1 E - E \alpha_1\big) W + \mathrm{O}(\Delta t^2) \tag{6.30}$$

with

$$\beta_1 = S^{-1} \big(C_1 + D_1 E - E \alpha_1\big) . \tag{6.31}$$

Now, we have formally

$$\frac{\partial^2 W}{\partial t^2} = \frac{\partial}{\partial t}\big(\alpha_1 W + \mathrm{O}(\Delta t)\big) = \alpha_1 \frac{\partial W}{\partial t} + \mathrm{O}(\Delta t) = \alpha_1 \big(\alpha_1 W\big) + \mathrm{O}(\Delta t) = \alpha_1^2 W + \mathrm{O}(\Delta t)$$

and we recognize the "wave equation"

$$\frac{\partial^2 W}{\partial t^2} - \alpha_1^2 W = \mathrm{O}(\Delta t) . \tag{6.32}$$

- We can derive a **formal expansion at order two**. We go one step further in the Taylor expansion of equation (6.24) :

$$W + \Delta t \frac{\partial W}{\partial t} + \frac{1}{2} \Delta t^2 \alpha_1^2 W + \mathrm{O}(\Delta t^3) =$$
$$= W + \Delta t \big(A_1 W + B_1 Y\big) + \Delta t^2 \big(A_2 W + B_2 Y\big) + \mathrm{O}(\Delta t^3)$$
$$= W + \Delta t \big(A_1 W + B_1 (E W + \Delta t \beta_1 W)\big) + \Delta t^2 \big(A_2 W + B_2 E W\big) + \mathrm{O}(\Delta t^3)$$

and dividing by Δt, we obtain a "Navier-Stokes type" second order equivalent equation:

$$\frac{\partial W}{\partial t} = \alpha_1 W + \Delta t \Big(B_1 \beta_1 + A_2 + B_2 E - \frac{1}{2} \alpha_1^2 \Big) W + \mathrm{O}(\Delta t^2) .$$

With the notations introduced in (6.27), we have made explicit the partial differential equations for the conserved variables at the order two:

$$\frac{\partial W}{\partial t} = \alpha_1 W + \Delta t \, \alpha_2 W + \mathrm{O}(\Delta t^2)$$

with

$$\alpha_2 = A_2 + B_2 E + B_1 \beta_1 - \frac{1}{2} \alpha_1^2 . \tag{6.33}$$

We remark that this Taylor expansion method can be viewed as a "numerical Chapman Enskog expansion" relative to a specific numerical parameter Δt instead of a small physical relaxation time step. For the moments Y out of equilibrium, we expand the first order derivative of Y relative to time with a formal derivation of the relation (6.30):

$$\begin{aligned} \frac{\partial Y}{\partial t} &= \frac{\partial}{\partial t} \Big(E W + \Delta t \, \beta_1 W \Big) + \mathrm{O}(\Delta t^2) \\ &= E \big(\alpha_1 W + \Delta t \, \alpha_2 W \big) + \Delta t \, \beta_1 \alpha_1 W + \mathrm{O}(\Delta t^2) \\ &= \Big(E \alpha_1 + \Delta t \big(E \alpha_2 + \beta_1 \alpha_1 \big) \Big) W + \mathrm{O}(\Delta t^2) . \end{aligned}$$

Then

$$\frac{\partial Y}{\partial t} = \Big(E \alpha_1 + \Delta t \big(E \alpha_2 + \beta_1 \alpha_1 \big) \Big) W + \mathrm{O}(\Delta t^2) . \tag{6.34}$$

Analogously for the second order time derivative:

$$\frac{\partial^2 Y}{\partial t^2} = E \alpha_1^2 W + \mathrm{O}(\Delta t) . \tag{6.35}$$

We re-write the second line of the expansion of the equation (6.24) at second order accuracy:

$$\begin{aligned} & Y + \Delta t \frac{\partial Y}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 Y}{\partial t^2} + \mathrm{O}(\Delta t^3) = \\ & \qquad = S E W + (\mathrm{I} - S) Y + \Delta t \big(C_1 W + D_1 Y \big) + \Delta t^2 \big(C_2 W + D_2 Y \big) + \mathrm{O}(\Delta t^3) \end{aligned}$$

and we get

$$\begin{aligned} S Y &= S E W - \Delta t \big(E \alpha_1 + \Delta t (E \alpha_2 + \beta_1 \alpha_1) \big) W - \frac{\Delta t^2}{2} E \alpha_1^2 W \\ & \quad + \Delta t \Big(C_1 W + D_1 \big(E + \Delta t \beta_1 \big) W \Big) + \Delta t^2 \big(C_2 W + D_2 E W \big) + \mathrm{O}(\Delta t^3) \\ Y &= E W + \Delta t \, S^{-1} \big(C_1 + D_1 E - E \alpha_1 \big) W \\ & \quad + \Delta t^2 \, S^{-1} \Big(C_2 + D_2 E + D_1 \beta_1 - E \alpha_2 - \beta_1 \alpha_1 - \frac{1}{2} E \alpha_1^2 \Big) W + \mathrm{O}(\Delta t^3) . \end{aligned}$$

It is exactly the expansion (6.27) at second order :

$$Y \,=\, E\,W + \Delta t\,\beta_1\,W + \Delta t^2\,\beta_2\,W + \mathrm{O}(\Delta t^2)$$

with

$$\beta_2 = S^{-1}\Big[\,C_2 + D_2\,E + D_1\,\beta_1 - E\,\alpha_2 - \,\beta_1\,\alpha_1 - \frac{1}{2}\,E\,\alpha_1^2\Big] \tag{6.36}$$

• For the **general case**, we proceed by induction. We suppose that the developments (6.26) and (6.27) are correct up to the order k, that is:

$$\left\{ \begin{array}{rcl} \dfrac{\partial W}{\partial t} &=& \Big(\alpha_1 + \Delta t\,\alpha_2 + \ldots\,\Delta t^{k-1}\,\alpha_k\Big)\,W + \mathrm{O}(\Delta t^k) \\ Y &=& \Big(E + \Delta t\,\beta_1 + \Delta t^2\,\beta_2 + \ldots\,\Delta t^k\,\beta_k\Big)\,W + \mathrm{O}(\Delta t^{k+1})\,. \end{array} \right. \tag{6.37}$$

We expand the relation (6.24) at order $k+2$, we eliminate the zeroth order term and divide by Δt. We obtain

$$\frac{\partial W}{\partial t} + \sum_{j=2}^{k+1} \frac{\Delta t^{j-1}}{j!}\,\big(\partial_t^j W\big) + \mathrm{O}(\Delta t^{k+1}) = \sum_{j=1}^{k+1} \Delta t^{j-1}\,\big(A_j\,W + B_j\,Y\big) + \mathrm{O}(\Delta t^{k+1})\,. \tag{6.38}$$

The term $\partial_t^j W \,=\, \big(\sum_{\ell=1}^{\infty} \Delta t^{\ell-1}\,\alpha_\ell\big)^j$ on the left hand side of (6.38) can be evaluated by taking the formal power of the equation (6.27) at the order j. We define the coefficients Γ_m^j according to:

$$\Big(\sum_{\ell=1}^{\infty} \Delta t^{\ell-1}\,\alpha_\ell\Big)^j \equiv \sum_{\ell=0}^{\infty} \Delta t^\ell\,\Gamma_{j+\ell}^j\,, \qquad j \geq 0\,. \tag{6.39}$$

They can be evaluated without difficulty from the coefficients α_ℓ, taking care of the non-commutativity of the product of two matrices. We report the corresponding terms and we identify the coefficients in factor of Δt^k between the two sides of the equation (6.38), with the help of the induction hypothesis (6.37). We deduce:

$$\alpha_{k+1} \,=\, A_{k+1} + \sum_{j=1}^{k+1} B_j\,\beta_{k+1-j} - \sum_{j=2}^{k+1} \frac{1}{j!}\,\Gamma_{k+1}^j\,. \tag{6.40}$$

We do the same operation with the second relation of (6.24) :

$$Y + \sum_{j=1}^{k+1} \frac{\Delta t^j}{j!}\,\big(\partial_t^j Y\big) + \mathrm{O}(\Delta t^{k+2}) = S\,E\,W + (\mathrm{I}-S)\,Y + \sum_{j=1}^{k+1} \Delta t^j\,\big(C_j\,W + D_j\,Y\big) + \mathrm{O}(\Delta t^{k+2})\,. \tag{6.41}$$

As in the previous case, we suppose that we have evaluated formally the temporal derivative

$$\begin{aligned} \partial_t^j Y &= \partial_t^j \Big[\big(E + \Delta t\,\beta_1 + \Delta t^2\,\beta_2 + \ldots + \Delta t^k\,\beta_k + \ldots\big)\,W\Big] \\ &= \big(E + \Delta t\,\beta_1 + \Delta t^2\,\beta_2 + \ldots + \Delta t^k\,\beta_k + \ldots\big)\,\big(\partial_t^j W\big) \\ &= \big(E + \Delta t\,\beta_1 + \Delta t^2\,\beta_2 + \ldots + \Delta t^k\,\beta_k + \ldots\big)\,\big(\alpha_1 + \Delta t\,\alpha_2 + \cdots + \Delta t^\ell\,\alpha_\ell + \ldots\big)^j\,W \end{aligned}$$

relatively to the space derivatives. Then with the help of the induction hypothesis

$$\Big(E + \sum_{m=1}^{\infty} \Delta t^m\,\beta_m\Big)\Big(\sum_{p=1}^{\infty} \Delta t^{p-1}\,\alpha_p\Big)^j \equiv \sum_{\ell=0}^{\infty} \Delta t^\ell\,K_{j+\ell}^j\,, \quad j \geq 0\,, \tag{6.42}$$

we identify the two expressions of the coefficient of Δt^{k+1} issued from the equation (6.41):

$$S\beta_{k+1} = C_{k+1} + \sum_{j=1}^{k+1} D_j\, \beta_{k+1-j} - \sum_{j=1}^{k+1} \frac{1}{j!} K_{k+1}^{j} . \tag{6.43}$$

- The explicitation of the coefficients $\Gamma_{j+\ell}^{j}$ and K_{k+1}^{j} of the matricial formal series is now easy, due to the relations (6.39) and (6.42). We specify the coefficients $\Gamma_{j+\ell}^{\ell}$ obtained in the matricial formal series (6.39). For $j = 0$, the power in relation (6.39) is the identity. Then

$$\Gamma_0^0 = \mathrm{I}, \qquad \Gamma_\ell^0 = 0, \quad \ell \geqslant 1 . \tag{6.44}$$

When $j = 1$, the initial series is not changed. Then

$$\Gamma_\ell^1 = \alpha_\ell , \qquad \ell \geqslant 1 . \tag{6.45}$$

For $j = 2$, we have to compute the square of the initial series, paying attention that the matrix operators α_ℓ do not commute. Observe that with the formal Chapman-Enskog method used *e.g.* in [80], non-commutation relations have also to be taken into consideration for higher order terms in the case of several conserved moments. We have

$$\Big(\sum_{\ell=1}^{\infty} \Delta t^\ell\, \alpha_{\ell+1}\Big)\Big(\sum_{j=1}^{\infty} \Delta t^j\, \alpha_{j+1}\Big) = \sum_{p=0}^{\infty} \Delta t^p \sum_{\ell+j=p} \alpha_{\ell+1}\, \alpha_{j+1}$$

and we have in particular

$$\Gamma_2^2 = \alpha_1^2, \quad \Gamma_3^2 = \alpha_1\,\alpha_2 + \alpha_2\,\alpha_1, \quad \Gamma_4^2 = \alpha_1\,\alpha_3 + \alpha_2^2 + \alpha_3\,\alpha_1 . \tag{6.46}$$

In the general case, we have

$$\Big(\sum_{\ell=0}^{\infty} \Delta t^\ell\, \alpha_{\ell+1}\Big)^j = \sum_{\ell=0}^{\infty} \Delta t^p \sum_{\ell_1+\cdots+\ell_j=p} \alpha_{\ell_1+1} \ldots \alpha_{\ell_j+1}$$

and in consequence

$$\Gamma_{p+j}^{j} = \sum_{\ell_1+\cdots+\ell_j=p} \alpha_{\ell_1+1} \ldots \alpha_{\ell_j+1} . \tag{6.47}$$

We have in particular for $j = 3$ and $j = 4$:

$$\Gamma_3^3 = \alpha_1^3, \qquad \Gamma_4^3 = \alpha_1^2\,\alpha_2 + \alpha_1\,\alpha_2\,\alpha_1 + \alpha_2\,\alpha_1^2, \qquad \Gamma_4^4 = \alpha_1^4 . \tag{6.48}$$

For the explicitation of the coefficients K_{k+1}^{j}, we can replace the power of the formal series of the relation (6.39) in the relation (6.42). We obtain, with the notation $\beta_0 \equiv E$,

$$\Big(\sum_{m=0}^{\infty} \Delta t^m\, \beta_m\Big)\Big(\sum_{\ell=0}^{\infty} \Delta t^\ell\, \Gamma_{j+\ell}^{j}\Big) \equiv \sum_{p=0}^{\infty} \Delta t^p\, K_{j+p}^{j}$$

then we have by induction

$$K_{j+p}^{j} = \sum_{m+\ell=p} \beta_m\, \Gamma_{j+\ell}^{j} . \tag{6.49}$$

For $j = 0$, we deduce

$$K_0^0 = E\,, \qquad K_p^0 = 0\,, \quad p \geqslant 1 \tag{6.50}$$

and for $j = 1$, we have a simple product of two formal series:

$$K_p^1 = E\,\alpha_p + \beta_1\,\alpha_{p-1} + \ldots + \beta_{p-1}\,\alpha_1\,, \quad p \geqslant 1\,. \tag{6.51}$$

We specify some particular values of the coefficients K_{j+p}^j when $j = 2$, $j = 3$ and for $j = 4$:

$$\left\{ \begin{array}{lll} K_2^2 = E\,\Gamma_2^2\,, & K_3^2 = E\,\Gamma_3^2 + \beta_1\,\Gamma_2^2\,, & K_4^2 = E\,\Gamma_4^2 + \beta_1\,\Gamma_3^2 + \beta_2\,\Gamma_2^2\,, \\ K_3^3 = E\,\Gamma_3^3\,, & K_4^3 = E\,\Gamma_4^3 + \beta_1\,\Gamma_3^3\,, & K_4^4 = E\,\Gamma_4^4\,. \end{array} \right. \tag{6.52}$$

- It is now possible to make explicit up to **fourth order** to fix the ideas the matricial coefficients of the expansion (6.26) of the nonconserved moments and of the associated partial differential equation (6.27). We have, following the natural order of the algorithm:

$$\left\{ \begin{array}{lll} \beta_0 & = & E \\ \alpha_1 & = & A_1 + B_1\,E \\ \beta_1 & = & S^{-1}\big(C_1 + D_1\,E - K_1^1\big) \\ \alpha_2 & = & A_2 + B_2\,E + B_1\,\beta_1 - \frac{1}{2}\,\Gamma_2^2 \\ \beta_2 & = & S^{-1}\Big[\,C_2 + D_2\,E + D_1\,\beta_1 - K_2^1 - \frac{1}{2}\,K_2^2\,\Big] \\ \alpha_3 & = & A_3 + B_1\,\beta_2 + B_2\,\beta_1 + B_3\,E - \frac{1}{2}\,\Gamma_3^2 - \frac{1}{6}\,\Gamma_3^3 \\ \beta_3 & = & S^{-1}\Big[\,C_3 + D_1\,\beta_2 + D_2\,\beta_1 + D_3\,E - K_3^1 - \frac{1}{2}\,K_3^2 - \frac{1}{6}\,K_3^3\,\Big] \\ \alpha_4 & = & A_4 + B_1\,\beta_3 + B_2\,\beta_2 + B_3\,\beta_1 + B_4\,E - \frac{1}{2}\,\Gamma_4^2 - \frac{1}{6}\,\Gamma_4^3 - \frac{1}{24}\,\Gamma_4^4\,. \end{array} \right. \tag{6.53}$$

Observe that with the explicit relations (6.53), the computer time for deriving formally the equivalent partial equation like (6.37) at fourth order of accuracy has been reduced by three orders of magnitude (!) in comparison with the algorithm presented in the contribution [50].

CHAPTER 7

INTRODUCTION TO THE STABILITY OF LATTICE BOLTZMANN SCHEMES

We introduce [1]. the idea of monotonic stability to enforce the positivity of the partcle distribution of a lattice Boltzmann scheme. This framework is applied in one space dimension for the thermic D1Q3 and the fluid D1Q3 schemes.

7.1 MONOTONIC STABILITY

Let us consider a $DdQq$ lattice Boltzmann scheme on the cartesian lattice $\mathcal{L}$ in $\mathbb{R}^d$.

- The idea is to control the total mass

$$m(t) \equiv \sum_{x\in\mathcal{L}} \sum_{j=0}^{q-1} f_j(x,\, t) = \sum_{x\in\mathcal{L}} \rho(x,\, t) \tag{7.1}$$

for any time. We suppose that the initial distributions of particles is nonnegative:

$$f_j(x, 0) \geqslant 0\,, \qquad x \in \mathcal{L}\,, \quad 0 \leqslant j \leq q-1 \tag{7.2}$$

and that the initial total mass $m(0)$ is bounded:

$$\exists M > 0\,, \qquad m(0) \leqslant M\,. \tag{7.3}$$

We wish to have the same conditions at time t:

$$f_j(x,\, t) \geqslant 0\,, \qquad x \in \mathcal{L}\,,\, 0 \leqslant j \leq q\,,\, \forall \text{ discrete } t \tag{7.4}$$

$$m(t) \leqslant M\,, \qquad \forall \text{ discrete } t\,. \tag{7.5}$$

If it is the case, we say here that the scheme has the property of **monotonic stability**.

- The lattice Boltzmann scheme is given by the condition

$$f_j(x,\, t+\Delta t) = f_j^*(x - v_j\,\Delta t\,,\, t)\,, \qquad 0 \leqslant j \leqslant q-1\,, \quad \forall \text{ discrete } t \tag{7.6}$$

and the nonlinear relaxation is always a **local** functional in space:

$$\exists \mathcal{R} : \mathbb{R}^q \longrightarrow \mathbb{R}^q\,, \quad f_j^*(x\,,\, t) = \mathcal{R}_j\Big(\big\{f_i(x\,,\, t), 0 \leqslant i \leqslant q-1\big\}\Big)\,, \qquad 0 \leqslant j \leqslant q-1\,, \quad x \in \mathcal{L}\,. \tag{7.7}$$

[1] This ideas presented in this chapter have been proposed previously in [49].

The previous relation (7.7) can also be written in a simpler form:

$$\exists \mathscr{R} : \mathbb{R}^q \longrightarrow \mathbb{R}^q , \quad f^* = \mathscr{R}\big(f\big) . \tag{7.8}$$

We suppose that the nonlinear relaxation $\mathscr{R}$ is positive: all the components of the vector $f^* \in \mathbb{R}^q$ are positive if it is the case for all the components of $f \in \mathbb{R}^q$:

$$\big(f \geqslant 0\big) \Longrightarrow \big(\mathscr{R}(f) \geqslant 0\big) . \tag{7.9}$$

We suppose also (for technical reasons) that the lattive $\mathscr{L}$ is periodic *id est* the boundary conditions are periodic). Then for each index j, we have

$$\sum_{x \in \mathscr{L}} f_j^*(x - v_j \, \Delta t , \, t) = \sum_{x \in \mathscr{L}} f_j^*(x , \, t) , \qquad j = 0, \ldots q-1 . \tag{7.10}$$

- We have the following property.

Proposition 1. L^1 monotonic stability.
We suppose that the previous framework of periodicity (7.10) and positivity (7.9) of the relaxation operator $\mathscr{R}$ is satisfied. Then if the total mass is conserved by the microscopic collisions, *id est* if we have

$$\sum_j f_j^*(x , \, t) \equiv \rho^* = \rho \equiv \sum_j f_j(x , \, t) , \tag{7.11}$$

the lattice Boltzmann scheme is L^1 stable at the following sence: if the conditions (7.2) and (7.3) are realized at time $t = 0$, then the inequalities (7.4) and (7.5) are satisfied for each discrete time.

Proof of Proposition 1.
The proof is be done by induction. The positivity of the vector f^* is a direct consequence of the positivity (7.9) of the relaxation operator $\mathscr{R}$. Then the entire vector $f(\bullet, \, t + \Delta t)$ is positive at the new discrete time due to the iteration (7.6). Moreover, if the relation (7.5) is satisfied for a discrete time t, we have

$$\begin{aligned} m(t+\Delta t) &= \sum_{x \in \mathscr{L}} \sum_{j=0}^{q-1} f_j(x, \, t+\Delta t) = \sum_{x \in \mathscr{L}} \sum_{j=0}^{q-1} f_j^*(x - v_j \, \Delta t , \, t) \qquad \text{due to (7.6)} \\ &= \sum_{j=0}^{q-1} \sum_{x \in \mathscr{L}} f_j^*(x - v_j \, \Delta t , \, t) = \sum_{j=0}^{q-1} \sum_{x \in \mathscr{L}} f_j^*(x , \, t) \qquad \text{due to (7.10)} \\ &= \sum_{j=0}^{q-1} \sum_{x \in \mathscr{L}} f_j(x , \, t) \qquad \text{due to (7.11)} \\ &= m(t) \end{aligned}$$

and the relation (7.5) is satisfied for time step $t + \Delta t$. □

- In practice, the monotonic stability of a lattice Boltzmann scheme that conserves the mass can be reduced to the sufficient condition of positivity (7.9) of the relaxation operator $\mathscr{R}$. If the operator $\mathscr{R}$ is **linear**, we can write

$$f_j^* = \big(\mathscr{R} f\big)_j \equiv \sum_{k=0}^{q-1} L_{jk} \, f_k . \tag{7.12}$$

The positivity (7.9) is equivalent to the positivity of all the coefficients L_{jk}:

$$L_{jk} \geqslant 0 , \qquad 0 \leqslant j , \, k \leqslant q-1 . \tag{7.13}$$

We look now to this condition for two very elementary examples.

7.2 MONOTONIC STABILITY OF THE THERMAL D1Q3 SCHEME

The D1Q3 scheme is defined by three particle distributions f_0, f_+ and f_-. The momenta are defined as in (4.46) and (4.47):

$$\left\{ \begin{array}{lcl} \rho &=& f_0 + f_+ + f_- \\ J &=& \lambda\,(f_+ - f_-) \\ \varepsilon &=& \frac{\lambda^2}{2}\,(f_+ + f_-)\,. \end{array} \right. \tag{7.14}$$

The discrete evolution associated with the relaxation step can be formulated as

$$\left\{ \begin{array}{lcll} \rho^* &=& \rho & \\ J^* &=& J + s\,(J^{\text{eq}} - J)\,, & J^{\text{eq}} = \lambda\,u\,\rho \\ \varepsilon^* &=& \varepsilon + s'\,(\varepsilon^{\text{eq}} - \varepsilon)\,, & \varepsilon^{\text{eq}} = \frac{\lambda^2}{2}\,\zeta\,\rho \end{array} \right. \tag{7.15}$$

Proposition 2. Relaxation operator $\mathscr{R}$ for the D1Q3 scheme.
If we set

$$f \equiv \big(f_0\,,\, f_+\,,\, f_-\big)^{\text{t}}, \tag{7.16}$$

the matrix L introduced in (7.12) can be explicited as

$$L = \begin{pmatrix} 1-\zeta\,s' & (1-\zeta)\,s' & (1-\zeta)\,s' \\ \frac{1}{2}\,(u\,s+\zeta\,s') & \frac{1}{2}\,(2-s-s'+u\,s+\zeta\,s') & \frac{1}{2}\,(u\,s+\zeta\,s'+s-s') \\ \frac{1}{2}\,(-u\,s+\zeta\,s') & \frac{1}{2}\,(s-u\,s+\zeta\,s'-s') & \frac{1}{2}\,(2-s-s'-u\,s+\zeta\,s') \end{pmatrix}. \tag{7.17}$$

Proof of Proposition 2.
We first explicit the two moments J^* and ε^* as a function of the particle distribution:

$$\begin{aligned} J^* &= (1-s)\,J + s\,J^{\text{eq}} = (1-s)\,\lambda\,(f_+ - f_-) + s\,\lambda\,u\,\rho \\ &= (1-s)\,\lambda\,(f_+ - f_-) + s\,\lambda\,u\,(f_0 + f_+ + f_-) = \lambda\big(u\,s\,f_0 + (1-s+u\,s)\,f_+ + (u\,s-1+s)\,f_-\big), \end{aligned}$$

and

$$\begin{aligned} \varepsilon^* &= (1-s')\,\varepsilon + s'\,\varepsilon^{\text{eq}} = (1-s')\,\frac{\lambda^2}{2}\,(f_+ + f_-) + s'\,\frac{\lambda^2}{2}\,\zeta\,\rho \\ &= \frac{\lambda^2}{2}\Big((1-s')\,(f_+ + f_-) + s'\,\zeta\,(f_0 + f_+ + f_-)\Big) = \frac{\lambda^2}{2}\Big(s'\,\zeta\,f_0 + (\zeta\,s' + 1 - s')\,(f_+ + f_-)\Big). \end{aligned}$$

Then

$$\left\{ \begin{array}{lcl} J^* &=& \lambda\big(u\,s\,f_0 + (1-s+u\,s)\,f_+ + (u\,s-1+s)\,f_-\big) \\ \varepsilon^* &=& \frac{\lambda^2}{2}\Big(s'\,\zeta\,f_0 + (\zeta\,s' + 1 - s')\,(f_+ + f_-)\Big). \end{array} \right. \tag{7.18}$$

We invert now the relation (7.14):

$$\left\{ \begin{array}{lcl} f_0^* &=& \rho^* - \frac{2}{\lambda^2}\varepsilon^* \\ f_+^* &=& \frac{1}{2\lambda}\,J^* + \frac{1}{\lambda^2}\,\varepsilon^* \\ f_-^* &=& -\frac{1}{2\lambda}\,J^* + \frac{1}{\lambda^2}\,\varepsilon^* \end{array} \right. \tag{7.19}$$

and we have, due to the first relation of (7.15):

$$f_0^* = \rho - \frac{2}{\lambda^2}\varepsilon^* = f_0 + f_+ + f_- - \frac{2}{\lambda^2}\,\frac{\lambda^2}{2}\Big(s'\,\zeta\,f_0 + (\zeta\,s' + 1 - s')\,(f_+ + f_-)\Big) = (1-\zeta\,s')\,f_0 + s'\,(1-\zeta)\,(f_+ + f_-)$$

$$f_+^* = \frac{1}{2\lambda} J^* + \frac{1}{\lambda^2} \varepsilon^* = \frac{1}{2\lambda} \lambda \big(u\, s\, f_0 + (1-s+u\, s)\, f_+ + (u\, s-1+s)\, f_-\big) + \frac{1}{\lambda^2} \frac{\lambda^2}{2} \Big(s' \zeta\, f_0 + (\zeta\, s' + 1 - s')\,(f_+ + f_-)\Big)$$
$$= \frac{1}{2} \big((u\, s + \zeta\, s')\, f_0 + (2 - s - s' + u\, s + \zeta\, s')\, f_+ + (u\, s + \zeta\, s' + s - s')\, f_-\big)$$

$$f_-^* = -\frac{1}{2\lambda} J^* + \frac{1}{\lambda^2} \varepsilon^* = -\frac{1}{2} \big(u\, s\, f_0 + (1-s+u\, s)\, f_+ + (u\, s-1+s)\, f_-\big) + \frac{1}{2} \Big(s' \zeta\, f_0 + (\zeta\, s' + 1 - s')\,(f_+ + f_-)\Big)$$
$$= \frac{1}{2} \big((-u\, s + \zeta\, s')\, f_0 + (s - u\, s + \zeta\, s' - s')\, f_+ + (2 - s - s' - u\, s + \zeta\, s')\, f_-\big),$$

and the relation (7.17) is clear. □

- We express now the positivity of the operator $\mathscr{R}$. In other terms, all the coefficients of the matrix L proposed in (7.17) must be non-negative. We have

Proposition 3. Monotonic stability of the thermal D1Q3 scheme.
Consider the D1Q3 scheme for advection-diffusion defined in (7.14) and (7.15). We set

$$s'' = (1-\zeta)\, s'. \tag{7.20}$$

A necessary condition for this scheme to be monotically stable is to satisfy the following two inequalities:

$$0 \leqslant s'' \leqslant s, \qquad s + s'' \leqslant 2. \tag{7.21}$$

When the inequalities are satisfied, the scheme (7.14) (7.15) is monotically stable if and only if

$$|\,u\,| \leqslant \min\Big(\zeta\, \frac{s'}{s},\ \frac{1}{s}(2 - s - s''),\ 1 - \frac{s''}{s}\Big). \tag{7.22}$$

The inequalities (7.21) are illustrated in Figure 1.

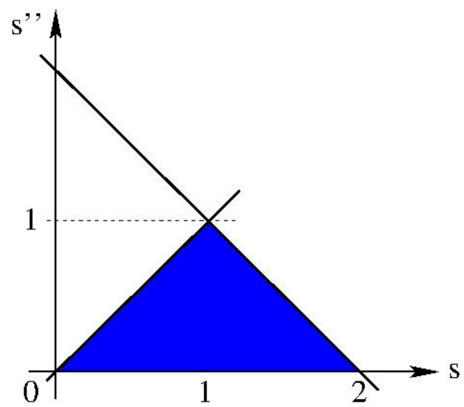

Figure 1. Stability zone for monotony (7.21) in dark.

Proof of Proposition 3.

We express that all the coefficients of the matrix L in (7.17) are non-negative:

$$\begin{cases} 1-\zeta\, s' & \geqslant & 0 \\ s'(1-\zeta) & \geqslant & 0 \\ u\, s+\zeta\, s' & \geqslant & 0 \\ -u\, s+\zeta\, s' & \geqslant & 0 \\ 2-s-s'+u\, s+\zeta\, s' & \geqslant & 0 \\ 2-s-s'-u\, s+\zeta\, s' & \geqslant & 0 \\ u\, s+\zeta\, s'+s-s' & \geqslant & 0 \\ -u\, s+\zeta\, s'+s-s' & \geqslant & 0\,. \end{cases}$$

In other terms,

$$\zeta\, s' \leqslant 1 \qquad (7.23)$$

$$s' \geqslant \zeta\, s' \qquad (7.24)$$

$$|\, u\, s\,| \leqslant \zeta\, s' \qquad (7.25)$$

$$|\, u\, s\,| \leqslant 2-s-s'+\zeta\, s' \qquad (7.26)$$

$$|\, u\, s\,| \leqslant \zeta\, s'+s-s'\,. \qquad (7.27)$$

We deduce from (7.24) and (7.25): $0 \leqslant |\, u\, s\,| \leqslant \zeta\, s' \leqslant s'$ and

$$s' \geqslant 0\,. \qquad (7.28)$$

Then $\zeta\, s' \geqslant 0$ and $(1-\zeta)\, s' \geqslant 0$ and we deduce

$$0 \leqslant \zeta \leqslant 1 \qquad (7.29)$$

because $s' \neq 0$ by construction; the third moment ε is not at equilibrium for this particular lattice Boltzmann scheme.

- We have now from (7.27) $s \geqslant (1-\zeta)\, s' \geqslant 0$ and

$$s \geqslant 0\,. \qquad (7.30)$$

With the notation s'' introduced in (7.20), we have $s \geqslant s'' \geqslant 0$ from (7.27) and $s+s'' \leqslant 2$ from (7.26). The inequalities (7.21) are established. The parameter s is in fact strictly positive because the second momentum J is not at equilibrium. Then the relation (7.22) is a direct consequence of the inequalities (7.25) (7.26) (7.27). The proposition 3 is established. □

7.3 NON MONOTONIC STABILITY OF THE FLUID D1Q3 SCHEME

We suppose now that the D1Q3 lattice Boltzmann scheme is used for a fluid simulation. Instead of one partial differential equation, we enforce the momenta conservations of ρ and J. We can simulate a fluid system with mass and momentum conservation. Technically speaking, the difference with the previous section (7.2) is very small. The second momentum J is at equilibrium, we enforce $J^* = J$ and this condition is obtained by taking $s = 0$ in the relations (7.15). The relaxation follows now the relations

$$\begin{cases} \rho^* & = & \rho \\ J^* & = & J \\ \varepsilon^* & = & \varepsilon + s'\,(\varepsilon^{eq}-\varepsilon)\,, \qquad \varepsilon^{eq} = \frac{\lambda^2}{2}\,\zeta\,\rho\,. \end{cases} \qquad (7.31)$$

We observe here that the monotonic stability is strongly impacted by the change of parameters. We have the

Proposition 4. Non-monotonic stability of the fluid D1Q3 scheme.
With the above notations, the relaxation operator $\mathscr{R}$ associated to the fluid D1Q3 lattice Boltzmann scheme (7.14) (7.31) is associated to the following matrix

$$L = \begin{pmatrix} 1-\zeta\, s' & (1-\zeta)\, s' & (1-\zeta)\, s' \\ \frac{1}{2}\zeta\, s' & \frac{1}{2}(2-s'+\zeta\, s') & \frac{1}{2}(\zeta\, s'-s') \\ \frac{1}{2}\zeta\, s' & \frac{1}{2}(\zeta\, s'-s') & \frac{1}{2}(2-s'+\zeta\, s')\,. \end{pmatrix} \tag{7.32}$$

The monotonic stability conditions $L_{jk} \geqslant 0$ take now the form

$$0 \leqslant s' = \zeta\, s' \leqslant 1 \tag{7.33}$$

and because $s' \neq 0$ by construction, the condition (7.33) implies $\zeta = 1$.

Proof of Proposition 4.
The expression (7.32) is nothing else than the matrix (7.17) in the particular case $s = 0$. We express now that all its coefficients are non-negative:

$$\left\{ \begin{array}{lcl} 1-\zeta\, s' & \geqslant & 0 \\ s'\,(1-\zeta) & \geqslant & 0 \\ \zeta\, s' & \geqslant & 0 \\ 2-s'+\zeta\, s' & \geqslant & 0 \\ \zeta\, s'-s' & \geqslant & 0\,. \end{array} \right.$$

Then $s'\,(1-\zeta) = 0$ because it is both positive and negative. The end of the proposition is clear. □

CHAPTER 8

A DUAL ENTROPY APPROACH FOR MONODIMENSIONAL NONLINEAR WAVES

In this chapter [1] we follow the mathematical framework proposed by Bouchut [14] and present in this contribution a dual entropy approach for determining equilibrium states of a lattice Boltzmann scheme. This method is expressed in terms of the dual of the mathematical entropy relative to the underlying conservation law. It appears as a good mathematical framework for establishing a "H-theorem" for the system of equations with discrete velocities. The dual entropy approach is used with D1Q3 lattice Boltzmann schemes for the Burgers equation. It conducts to the explicitation of three different equilibrium distributions of particles and induces naturally a nonlinear stability condition. Satisfactory numerical results for strong nonlinear shocks and rarefactions are presented. We prove also that the dual entropy approach can be applied with a D1Q3 lattice Boltzmann scheme for systems of linear and nonlinear acoustics and we present a numerical result with strong nonlinear waves for nonlinear acoustics. We establish also a negative result: with the present framework, the dual entropy approach cannot be used for the shallow water equations.

8.1 Introduction

An hyperbolic partial differential equation like the Burgers equation

$$\partial_t u + \partial_x\big(F(u)\big) = 0, \quad F(u) \equiv \frac{u^2}{2} \tag{8.1}$$

exhibits shock waves (see *e.g.* [69]), *id est* discontinuities propagating with finite velocity. In order to select the physically relevant weak solution, it is necessary to enforce the so-called entropy condition

$$\partial_t\big(\eta(u)\big) + \partial_x\big(\zeta(u)\big) \leqslant 0 \tag{8.2}$$

as suggested by Godunov [71] and Friedrichs and Lax [58]. In the relation (8.2), $\eta(\bullet)$ is a strictly convex function and $\zeta(\bullet)$ the associated entropy flux (see *e.g.* [69], [39] or [97]). For the Burgers equation, the quadratic entropy is usually considered

$$\eta(u) \equiv \frac{u^2}{2}, \qquad \zeta(u) \equiv \frac{u^3}{3}. \tag{8.3}$$

Remark that the entropy condition (8.2) is just one of at least three possible criteria for selecting the physically relevant weak solution. One may also consider the vanishing viscosity limit, or the Lax entropy criterion (see *e.g.* [69] or [97]).

[1] This contribution has been originally published in [47] .

• The computation of discrete shock waves with lattice Boltzmann approaches began with viscous Burgers approximations in the framework of lattice gaz automata (see Boghosian and Levermore [10], Elton [53], Elton *et al.* [54]). With the lattice Boltzmann methods described *e.g.* by Lallemand and Luo [95], first tentatives were proposed by d'Humières [80], Alexander *et al.* [3], Qian and Zhou [114]. The study of nonlinear scalar equation with the help of the lattice Boltzmann scheme has been emphasized by Buick *at al.* [21] for nonlinear acoustics. The approximation of the Burgers equation with a quantum variant of the method has been presented by Yepez [135]. A D1Q2 entropic scheme for the one-dimensional viscous Burgers equation has been developed by Boghosian *et al.* [11] and we refer to Duan and Liu [41] for the approximation of two-dimensional Burgers equation. The extension for gas dynamics equations and in particular shock tubes problems is under study with *e.g.* the works of Philippi *et al.*, [111], Brownlee *et al.* [20], Nie, Shan and Chen [106], Karlin and Asinari [90], Chikatamarla and Karlin [33].

• In this contribution, we experiment the ability of lattice Boltzmann schemes to approach weak entropic solutions of hyperbolic equations. In such situations, the scheme exhibits some kind of vanishing viscosity limit. We start from the mathematical framework developed by Bouchut [14] making the link between the finite volume method and kinetic models in the framework of the BGK [9] approximation. The key notion is the representation of the dual entropy with the help of convex functions associated with the discrete velocities of the lattice. We call "dual entropy approach" the set of associated constraints for the equilibrium distribution. In section 2, we recall this framework with emphasis on the one-dimensional case and prove a continuous version of the "H-theorem". In section 3 we derive three equilibria for a D1Q3 kinetic distribution associated with the lattice Boltzmann method applied to the Burgers equation. In section 4, we precise our numerical D1Q3 scheme and make a simple link with the finite volume approach. We present numerical experiments with nonlinear Burgers waves in section 5. In section 6, we study the ability of the dual entropy approach to determine D1Q3 equilibria for systems of linear and nonlinear acoustics. We study the system of shallow water equations in Section 7.

8.2 KINETIC REPRESENTATION OF THE DUAL ENTROPY

The Legendre-Fenchel-Moreau duality is a classic notion defined when we consider a convex function $\eta(\bullet)$ of several variables. We can apply the duality transform that suggests that convex function $\eta(\bullet)$ is parametrized by the slopes of the tangent planes. In other terms,

$$\eta^*(\varphi) = \sup_W \Big(\varphi \bullet W - \eta(W)\Big). \tag{8.4}$$

The upper bound in the right hand side of relation (8.4) is obtained (when it is not on the boundary of the domain of variation of the state W) by solving the equation of unknown W:

$$\eta'(W) = \varphi. \tag{8.5}$$

A first example is simply $\eta(w) \equiv \mathrm{e}^w$ at one space dimension. Then $\mathrm{e}^w = \varphi$, $\eta^*(\varphi) = \varphi \log\varphi - \varphi$ and we recover in this way the fundamental tool to define the so-called "Shannon entropy" [125].

• We can derive the dual function : if $\mathrm{d}\eta(W) \equiv \varphi \bullet \mathrm{d}W$ then

$$\mathrm{d}\eta^*(\varphi) = \mathrm{d}\varphi \bullet W \tag{8.6}$$

and the "physical state" W is the Jacobian of the dual entropy. In an analogous way, we can introduce (see *e.g.* [69], [39] or [97]) in the context of hyperbolic conservation laws

$$\partial_t W + \partial_x\big(F(W)\big) = 0 \tag{8.7}$$

the so-called "dual entropy flux" $\zeta^*(\varphi)$. It is defined with the help of the "physical flux" $F(\bullet)$ according to

$$\zeta^*(\varphi) = \varphi \bullet F(W) - \zeta(W),$$

with the condition (8.5) as previously. Then $\mathrm{d}\zeta^*(\varphi) = \mathrm{d}\varphi \bullet F(W)$ and the physical flux $F(W)$ is the Jacobian of the dual entropy flux. In other terms, all the physics associated with the conservation laws (8.7) can be expressed in terms of the dual entropy η^* and of the dual entropy flux ζ^*. The example of Burgers equation (8.1) with the quadratic entropy and associated flux gives without difficulty

$$\eta^*(\varphi) = \frac{\varphi^2}{2}\,, \quad \zeta^*(\varphi) = \frac{\varphi^3}{6}\,. \tag{8.8}$$

- Independently of the framework relative to hyperbolic conservation laws, the Boltzmann equation with discrete velocities has been studied by Broadwell [18] (see also Gatignol [61] and Cabannes [23]). In this contribution, we write this model for $(J+1)$ velocities in one space dimension :

$$\partial_t f_j + v_j\,\partial_x f_j = Q_j(f)\,, \quad 0 \leqslant j \leqslant J. \tag{8.9}$$

The unknown quantity $f_j(x,\, t)$ is the density of particles at point x and time t with a discrete velocity v_j. We have for example $J=2$ for the D1Q3 lattice Boltzmann scheme (presented in section 4). The equation (8.9) admits N microscopic collision invariants M_{kj} :

$$\sum_j M_{kj}\, Q_j(f) = 0\,, \qquad 1 \leqslant k \leqslant N$$

and $N = 1$ for a scalar (*e.g.* Burgers) equation. The N first conserved moments :

$$W_k \equiv \sum_j M_{kj}\, f_j\,, \quad 1 \leqslant k \leqslant N \tag{8.10}$$

satisfy a system of conservation laws :

$$\partial_t W_k + \partial_x\Big(\sum_j M_{kj}\, v_j\, f_j\Big) = 0\,, \quad 1 \leqslant k \leqslant N. \tag{8.11}$$

Of course, we make the hypothesis that this system admits a mathematical entropy $\eta(W)$ with an associated entropy flux $\zeta(W)$. We denote by φ the derivative of the entropy (*id est* $\mathrm{d}\eta = \varphi \bullet \mathrm{d}W$) and by $M_j \in \mathbb{R}^N$ the vector of components M_{kj} (with k running from 1 to N). Then the following scalar expression :

$$\varphi \bullet M_j \equiv \sum_{k=1}^{N} \varphi_k\, M_{kj}\,, \quad 0 \leqslant j \leqslant J\,, \tag{8.12}$$

is well defined. In some sense, the vector $\varphi \in \mathbb{R}^N$ can be split into $J+1$ (with $J \geqslant N$) **s**calar contributions $\varphi \bullet M_j$ associated with the particle distribution of the Boltzmann method. In the following, we denote this contribution as the "j^{o} particle component of the entropy variables".

• The link between the Boltzmann models and the entropy variables has been first proposed by Perthame [109]. We follow here the approach developed by Bouchut [14]. We say that the "dual entropy approach" is satisfied if we suppose that there exists J **c**onvex scalar functions h_j^* such that

$$\sum_j h_j^*\big(\varphi \bullet M_j\big) \equiv \eta^*(\varphi)\,, \quad \sum_j v_j\, h_j^*\big(\varphi \bullet M_j\big) \equiv \zeta^*(\varphi)\,, \quad \forall \varphi. \tag{8.13}$$

We introduce $h_j(f_j) \equiv \sup_y \big(y\, f_j - h_j^*(y)\big)$ the Legendre dual of the convex function $h_j^*(\bullet)$. The function $h_j(\bullet)$ is a real scalar convex function and we can write here the relation (8.5) making for each j the link between f_j and $\varphi \bullet M_j$ under the scalar form

$$h_j'\big(f_j\big) = \varphi \bullet M_j\,, \quad 0 \leqslant j \leqslant J\,. \tag{8.14}$$

The so-called microscopic entropy

$$H(f) \equiv \sum_j h_j(f_j)$$

is a convex function in the domain where the h_j's are convex. When the hypothesis (8.13) is satisfied, we can prove a discrete version of the Boltzmann H-theorem. If

$$\sum_j h_j'(f_j)\, Q_j(f) \leqslant 0, \tag{8.15}$$

we have dissipation of the microscopic entropy :

$$\partial_t H(f) + \partial_x \Big(\sum_j v_j\, h_j(f_j)\Big) \leqslant 0 \tag{8.16}$$

and this function is a natural Lyapunov function. The equilibrium distribution $f_j^{eq}(W)$ is then defined by

$$f_j^{eq}(W) \equiv \big(h_j^*\big)'\big(\varphi \bullet M_j\big)\,, \quad 0 \leqslant j \leqslant J \tag{8.17}$$

because the relation (8.6) holds. Then we recover the Karlin *et al* [91] minimization property : $H(f) \geqslant H(f^{eq})$ for each f such that $\sum_j M_{kj}\, f_j = \sum_j M_{kj}\, f_j^{eq} \equiv W_k$ with $1 \leqslant k \leqslant N$.

• By differentiation of the relations (8.13) relative to the entropy variable φ and taking into account the previous relations (8.17), we have the necessary equilibrium conditions $\sum_j M_j\, f_j^{eq} = W$ and $\sum_j v_j\, M_j\, f_j^{eq} = F(W)$. In other terms, the conserved variables are given by the relations (8.17)(8.10) and the macroscopic fluxes by

$$F_k(W) \equiv \sum_j M_{kj}\, v_j\, f_j^{eq}\,, \ 1 \leqslant k \leqslant N\,.$$

The macroscopic entropy and associated entropy fluxes satisfy

$$\eta(W) = \sum_j h_j\big(f_j^{eq}\big)\,, \quad \zeta(W) = \sum_j v_j\, h_j\big(f_j^{eq}\big)\,.$$

When the Boltzmann equation with discrete velocities satisfies the so-called BGK hypothesis [9], *id est*

$$Q_j(f) = \frac{1}{\tau}\big(f_j^{eq} - f_j\big)\,, \quad 0 \leqslant j \leqslant J \tag{8.18}$$

for some constant $\tau > 0$, the Boltzmann H-theorem is satisfied. We give the proof for completeness : we first have the following convexity inequality

$$\Big(h'_j(f_j^{\rm eq}) - h'_j(f_j)\Big)\,\Big(f_j^{\rm eq} - f_j\Big) \geq 0\,, \quad 0 \leq j \leq J\,.$$

If the BGK hypothesis (8.18) occurs, we have by summation over j,

$$\tau \sum_j h'_j(f_j)\, Q_j(f) = \sum_j h'_j(f_j)\,\Big(f_j^{eq} - f_j\Big) \leq \sum_j h'_j(f_j^{eq})\,\Big(f_j^{eq} - f_j\Big) =$$

$$= \sum_j (\varphi \bullet M_j)\,\Big(f_j^{eq} - f_j\Big) = \varphi \bullet \sum_j M_j\,\Big(f_j^{eq} - f_j\Big) = 0$$

and due to (8.14), the hypothesis (8.15) is satisfied. In consequence the H-theorem is established in this case.

- As a summary of this mathematical section, we explicit the dual entropy approach in the case of the Burgers equation (8.1) equipped with a quadratic entropy. If there exists **c**onvex functions $h_j^*(\varphi)$ of the entropy variable φ such that

$$\sum_j h_j^*(\varphi) \equiv \eta^*(\varphi) = \frac{\varphi^2}{2}\,, \quad \sum_j v_j\, h_j^*(\varphi) \equiv \zeta^*(\varphi) = \frac{\varphi^3}{6} \tag{8.19}$$

then the equilibrium $f_j^{eq}(u) \equiv \frac{{\rm d}h_j^*}{{\rm d}\varphi}$ defines a **s**table approximation in a sense detailed in Chen *et al* [29] and extended by Bouchut [13, 15].

8.3 PARTICLE DECOMPOSITIONS FOR THE BURGERS EQUATION

We propose in this contribution to construct kinetic decompositions of a scalar variable in order to solve the Burgers equation in cases where weak solutions can occur, *id est* when shock waves can be developed. We consider only the simple D1Q3 stencil with three discrete velocities $-\lambda$, 0 and λ. Recall that the scalar $\lambda \equiv \frac{\Delta x}{\Delta t}$ is a fundamental numerical parameter that is very often taken equal to unity by lattice Boltzmann scheme users (see *e.g.* [95]). For the Burgers equation (8.1) a possible mathematical entropy is the quadratic one (8.3). The dual entropy $\eta^*(\varphi)$ and the associated dual entropy flux $\zeta^*(\varphi)$ are given according to the relations (8.8). Due to the framework of dual entropy approach proposed in the previous section, we search three convex functions $h_+^*(\varphi)$, $h_0^*(\varphi)$ and $h_-^*(\varphi)$ such that (8.19) holds, *id est* for D1Q3 :

$$h_+^*(\varphi) + h_0^*(\varphi) + h_-^*(\varphi) \equiv \frac{\varphi^2}{2}\,, \quad \lambda\,\Big(h_+^*(\varphi) - h_-^*(\varphi)\Big) \equiv \frac{\varphi^3}{6}\,. \tag{8.20}$$

- A first possible solution of the previous system consists in introducing some parameter α such that $0 < \alpha \leq 1$. Then we consider the particular function

$$h_0^*(\varphi) = (1-\alpha)\,\frac{\varphi^2}{2}\,. \tag{8.21}$$

Of course, if $\alpha = 1$, this function $h_0^*(\bullet)$ is singular. In this case, we switch from D1Q3 to D1Q2 scheme, as presented in the following of this contribution. Due to (8.20), the two other dual functions $h_+^*(\varphi)$ and $h_-^*(\varphi)$ are determined :

$$h_+^* = \alpha\,\frac{\varphi^2}{4} + \frac{\varphi^3}{12\,\lambda}\,, \quad h_-^* = \alpha\,\frac{\varphi^2}{4} - \frac{\varphi^3}{12\,\lambda}\,. \tag{8.22}$$

The associated dual functions can be written explicitly without particular difficulty :

$$\left\{ \begin{array}{rcl} h_+(f_+) &=& \dfrac{\lambda^2}{6}\left[\left(\alpha^2+4\,\dfrac{f_+}{\lambda}\right)^{3/2}-6\,\alpha\,\dfrac{f_+}{\lambda}-\alpha^3\right] \\ h_0(f_0) &=& \dfrac{1}{2\,(1-\alpha)}\,f_0^2 \\ h_-(f_-) &=& \dfrac{\lambda^2}{6}\left[\left(\alpha^2-4\,\dfrac{f_-}{\lambda}\right)^{3/2}+6\,\alpha\,\dfrac{f_-}{\lambda}-\alpha^3\right]. \end{array}\right. \tag{8.23}$$

The three functions h_j^* introduced in (8.21) and (8.22) are convex when

$$|\varphi| \leqslant \alpha\,\lambda \tag{8.24}$$

and the relation (8.24) can be interpreted as a Courant-Friedrichs-Lewy stability condition :

$$\Delta t \leqslant \frac{\alpha}{|u|}\,\Delta x.$$

The dual entropy approach contains in particular the numerical stability condition (8.24). The stability is in fact defined as the domain of convexity of the dual functions h_j^* presented algebraically by relations (8.21) (8.22) and illustrated in Figure 1. The explicit determination of the equilibrium distribution is then a consequence of the relation (8.17) taking also into account that $\varphi \equiv u$ for the quadratic entropy. We have

$$f_+^{\mathrm{eq}}(u) = \frac{\alpha}{2}\,u + \frac{u^2}{4\,\lambda}\,,\quad f_0^{\mathrm{eq}} = (1-\alpha)\,u\,,\quad f_-^{\mathrm{eq}} = \frac{\alpha}{2}\,u - \frac{u^2}{4\,\lambda}\,. \tag{8.25}$$

- Another solution of the previous system (8.20) can be obtained as follows. Derive the two relations in (8.20) two times. Then

$$\left(h_+^*\right)''(\varphi) = \left(h_-^*\right)''(\varphi) + \frac{\varphi}{\lambda}\,,\quad \left(h_0^*\right)''(\varphi) + 2\left(h_-^*\right)''(\varphi) = 1 - \frac{\varphi}{\lambda}\,.$$

In order to have a better stability property than the condition (8.24) obtained previously, we try to enforce the convexity condition $\left(h_j^*\right)''(\varphi) \geqslant 0$ if $|\varphi| \leqslant \lambda$ instead of (8.24). For $\varphi \leqslant 0$, we propose to replace the inequality $\left(h_+^*\right)''(\varphi) \equiv \left(h_-^*\right)''(\varphi) + \frac{\varphi}{\lambda} \geqslant 0$ by an equality. Then $\left(h_-^*\right)''(\varphi) = -\frac{\varphi}{\lambda}$ if $\varphi \leqslant 0$. We deduce $\left(h_+^*\right)''(\varphi) = 0$ and $\left(h_0^*\right)''(\varphi) = 1 + \frac{\varphi}{\lambda}$ if $\varphi \leqslant 0$. With analogous arguments, we obtain $\left(h_+^*\right)''(\varphi) = \frac{\varphi}{\lambda}$, $\left(h_0^*\right)''(\varphi) = 1 - \frac{\varphi}{\lambda}$ and $\left(h_-^*\right)''(\varphi) = 0$ when $\varphi \geqslant \lambda$. We construct in this way an "upwind" distribution for the decomposition of the dual entropy:

$$h_+^*(\varphi) = \left\{ \begin{array}{l} \dfrac{\varphi^3}{6\,\lambda} \\ \\ 0 \end{array}\right.,\quad h_0^*(\varphi) = \left\{ \begin{array}{l} \dfrac{\varphi^2}{2} - \dfrac{\varphi^3}{6\,\lambda} \\ \\ \dfrac{\varphi^2}{2} + \dfrac{\varphi^3}{6\,\lambda} \end{array}\right.,\quad h_-^*(\varphi) = \left\{ \begin{array}{ll} 0, & \varphi \geqslant 0 \\ \\ -\dfrac{\varphi^3}{6\,\lambda}, & \varphi \leqslant 0. \end{array}\right. \tag{8.26}$$

It is presented in Figure 2. The associated equilibrium distribution (8.17) takes the form

$$f_+^{\mathrm{eq}}(u) = \left\{ \begin{array}{l} \dfrac{u^2}{2\,\lambda} \\ \\ 0 \end{array}\right.,\quad f_0^{\mathrm{eq}}(u) = \left\{ \begin{array}{l} u - \dfrac{u^2}{2\,\lambda} \\ \\ u + \dfrac{u^2}{2\,\lambda} \end{array}\right.,\quad f_-^{\mathrm{eq}}(u) = \left\{ \begin{array}{ll} 0, & u \geqslant 0 \\ \\ -\dfrac{u^2}{2\,\lambda}, & u \leqslant 0\,. \end{array}\right. \tag{8.27}$$

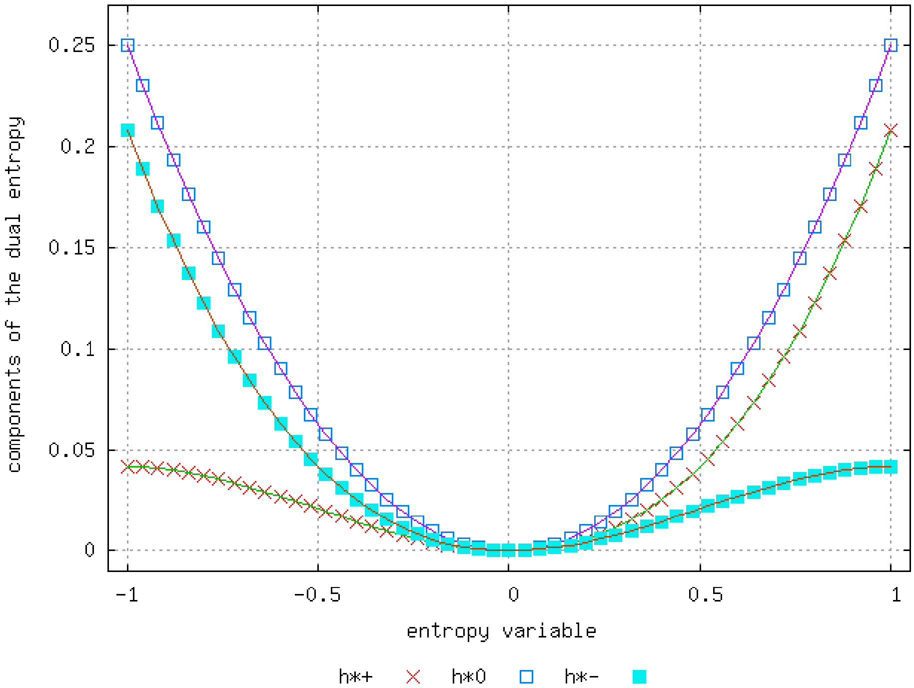

Figure 8.1 – *Kinetic decomposition (8.21) (8.22) of the dual entropy for the Burgers equation with a "centered" D1Q3 scheme ($\alpha = \frac{1}{2}$).*

By considering the Legendre duals of the relations (8.26), we have

$$\begin{cases} h_+(f_+) &= \dfrac{2}{3} f_+ \sqrt{2\,\lambda\, f_+} & \text{with } f_+ \geq 0 \\ h_0(f_0) &= \dfrac{\lambda^2}{3} \left[\left(1 - 2\dfrac{|f_0|}{\lambda}\right)^{3/2} + 3\dfrac{|f_0|}{\lambda} - 1 \right] & \text{with } f_0 \in \mathbb{R} \\ h_-(f_-) &= -\dfrac{2}{3} f_- \sqrt{-2\,\lambda\, f_-} & \text{with } f_- \leq 0 . \end{cases} \tag{8.28}$$

- We observe that if $\alpha = 1$ for the "centered" equilibrium for D1Q3 Burgers scheme, the null velocity does not contribute to the equilibrium because $h_0(\varphi) \equiv 0$; this vertex of null velocity is no more active. In that case, we obtain a D1Q2 centered lattice Boltzmann scheme for Burgers equation. Then

$$h^*_+(\varphi) = \frac{\varphi^2}{4} + \frac{\varphi^3}{12\,\lambda}, \quad h^*_- = \frac{\varphi^2}{4} - \frac{\varphi^3}{12\,\lambda}. \tag{8.29}$$

These two functions represented in Figure 3 are convex if

$$|\varphi| \leq \lambda \tag{8.30}$$

and the associated Courant-Friedrichs-Lewy stability condition states as follows

$$\Delta t \leq \frac{1}{|u|} \Delta x .$$

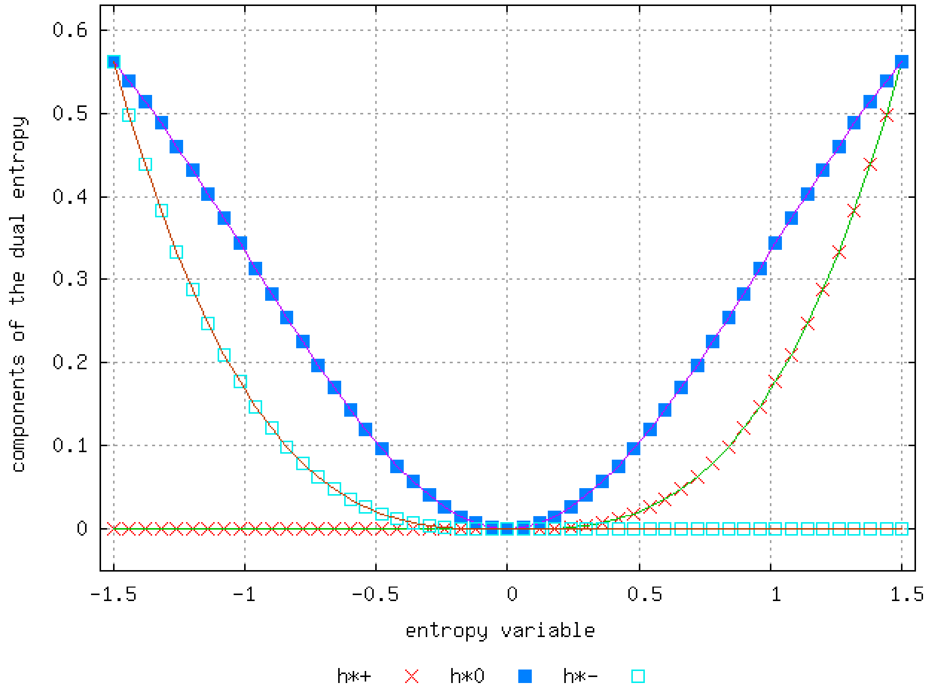

Figure 8.2 – *Kinetic decomposition for Burgers equation, equilibria (8.26) for the lattice Boltzmann upwind scheme D1Q3.*

The dual equilibrium entropy function defined at relations (8.29) are represented on Figure 3. The associated components $h_+(f_+)$ and $h_-(f_-)$ of the microscopic entropy follow from (8.23) in the particular case $\alpha = 1$. Observe that $h_0(f_0)$ is no more defined which is coherent with a choice of a “D1Q2” lattice Boltzmann scheme. The associated equilibrium particle distribution is obtained according to

$$f_+^{eq}(u) = \frac{1}{2}\,u + \frac{u^2}{4\,\lambda}\,, \quad f_-^{eq} = \frac{1}{2}\,u - \frac{u^2}{4\,\lambda}\,. \tag{8.31}$$

8.4 D1Q3 LATTICE BOLTZMANN SCHEME

As developed in the preceding section, we here consider three examples of stable equilibria in the context of the lattice Boltzmann scheme. More precisely, following the approach proposed by d’Humières [80], we discretize in space and time the Boltzmann equation with discrete velocities (8.9) in the following way. We introduce a matrix M that links particle densities f_j $(j = -, 0, +)$ and moments m_k. For the simple D1Q3 lattice Boltzmann scheme, we obtain

$$m \equiv M \bullet f\,, \quad M = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \lambda^2 & 0 & \lambda^2 \end{pmatrix}, \quad u \equiv f_{-1} + f_0 + f_1 = m_1\,. \tag{8.32}$$

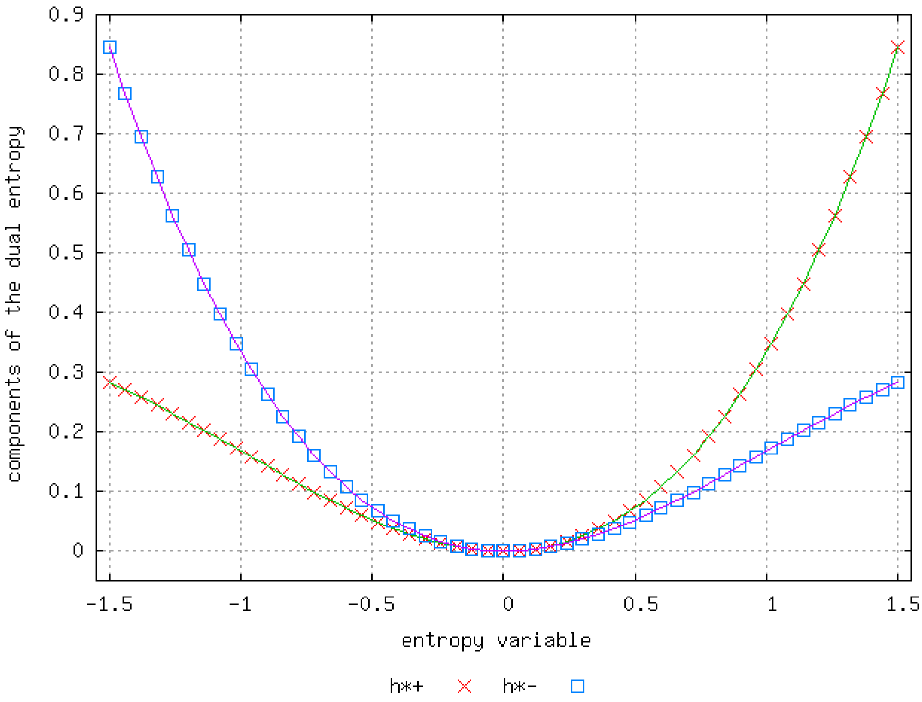

Figure 8.3 – *Kinetic decomposition for Burgers ; D1Q2 centered scheme.*

- The first equilibrium (8.25) can be translated in terms of moments under the form

$$m^{\mathrm{eq},1} \equiv \Big(u\,,\,\frac{u^2}{2}\,,\,\alpha\,\lambda^2\,u\Big)^t\,.$$

When using the "upwind" equilibrium (8.27), we obtain an other possible value for moments at equilibrium :

$$m^{\mathrm{eq},2} \equiv \Big(u\,,\,\frac{u^2}{2}\,,\,\lambda\,\mathrm{sgn}(u)\,\frac{u^2}{2}\Big)^t\,.$$

The simpler scheme D1Q2 corresponds to the first equilibrium (8.25) with the particular value $\alpha = 1$ as proposed in relations (8.31). We have only two components in this case :

$$m^{\mathrm{eq},3} \equiv \Big(u\,,\,\frac{u^2}{2}\Big)^t\,.$$

- The relaxation step is nonlinear and local in space :

$$m_1^* = m_1^{eq} = u\,, \quad m_k^* = m_k + s_k\,(m_k^{eq} - m_k) \text{ for } k \geqslant 2, \tag{8.33}$$

with $s_2 = s_3 = 1.7$ in our simulations unless otherwise stated. For nonlinear hyperbolic systems (8.7) of two conservation laws in one space dimension, the moments m_1 and m_2 are at equilibrium and the relation (8.33) is written in this case

$$m_1^* = m_1^{eq} = W_1\,, \quad m_2^* = m_2^{eq} = W_2\,, \quad m_3^* = m_3 + s_3\,(m_3^{eq} - m_3)\,. \tag{8.34}$$

The particle distribution f_j^* after relaxation is obtained by inversion of relation (8.32) : $f^* = M^{-1} \bullet m^*$. The time iteration of the scheme follows the characteristic directions of velocity v_j :

$$f_j(x,\, t+\Delta t) = f_j^*(x - v_j\,\Delta t,\, t)\,.$$

This advection step is linear and associates the node x with its neighbors.

• In [44] we have observed that a one-dimensional lattice Boltzmann scheme can be interpreted with the help of finite volumes. In the case considered here, we have

$$\frac{1}{\Delta t}\Big(u(x,\, t+\Delta t) - u(x,\, t)\Big) + \frac{1}{\Delta x}\Big[\psi\Big(x + \frac{\Delta x}{2},\, t\Big) - \psi\Big(x - \frac{\Delta x}{2},\, t\Big)\Big] = 0$$

with a numerical flux $\psi\big(x + \frac{\Delta x}{2},\, t\big)$ at the interface between the vertices x and $x + \Delta x$ defined according to

$$\psi\Big(x + \frac{\Delta x}{2},\, t\Big) = \lambda\,\Big(f_+^*(x,\, t) - f_-^*(x + \Delta x,\, t)\Big)\,. \tag{8.35}$$

We observe that the resulting lattice Boltzmann scheme is **n**ot a traditional finite volume scheme (in the sense proposed *e.g.* in [39]) if $(s_2,\, s_3) \neq (1,\, 1)$ because the distribution of particles after collision f^* is also a function of the two (or one in the D1Q2 scheme) other nonconserved moments m_2 and m_3 as described in relations (8.33). On the contrary, the lattice Boltzmann method is mainly a particle method with given velocities, as analyzed *e.g.* in Junk *al.* [88] with an asymptotic expansion technique. Nevertheless, if $s_2 = s_3 = 1$, we can give an interpretation of the associated flux (8.35) because in this case, $f_j^* \equiv f_j^{\mathrm{e}q}$ for all j.

• We observe that we can also decompose the "physical" flux $F(\bullet)$ (see the relation (8.1) or (8.7) in all generality) under the form $F(u) \equiv F_+(u) + F_-(u)$ with

$$F_+(u) = \lambda\, f_+^{\mathrm{e}q}(u)\,, \quad F_-(u) = -\lambda\, f_-^{\mathrm{e}q}(u)\,. \tag{8.36}$$

We have $F_+\big(u(x,\, t)\big) + F_-\big(u(x+\Delta x,\, t)\big) = \lambda\,\big(f_+^{\mathrm{e}q}\big(u(x,\, t)\big) - f_+^{\mathrm{e}q}\big(u(x+\Delta x,\, t)\big)\big)$ and when $s_2 = s_3 = 1$ the numerical flux ψ introduced in (8.35) admits the classical so-called flux splitting form :

$$\psi\Big(x + \frac{\Delta x}{2},\, t\Big) = F_+\big(u(x,\, t)\big) + F_-\big(u(x+\Delta x,\, t)\big)\,. \tag{8.37}$$

With this above link between fluxes and particle distributions (8.37) it is natural to re-interpret, with classical flux decompositions as (8.36), those proposed in this contribution at relations (8.25), (8.27) and (8.31). As remarked by Bouchut [16], the relations (8.25) and (8.31) are associated with two variants of the Lax-Friedrichs scheme (see *e.g.* Lax [97]) whereas the upwind scheme (8.27) corresponds exactly to the Engquist-Osher [56] scheme !

8.5 TEST CASES FOR BURGERS NONLINEAR WAVES

We test the previous numerical schemes for two classical problems : a converging shock wave and the Riemann problem. We use the three variants (8.25), (8.27) and (8.31) of the lattice Boltzmann scheme for each problem.

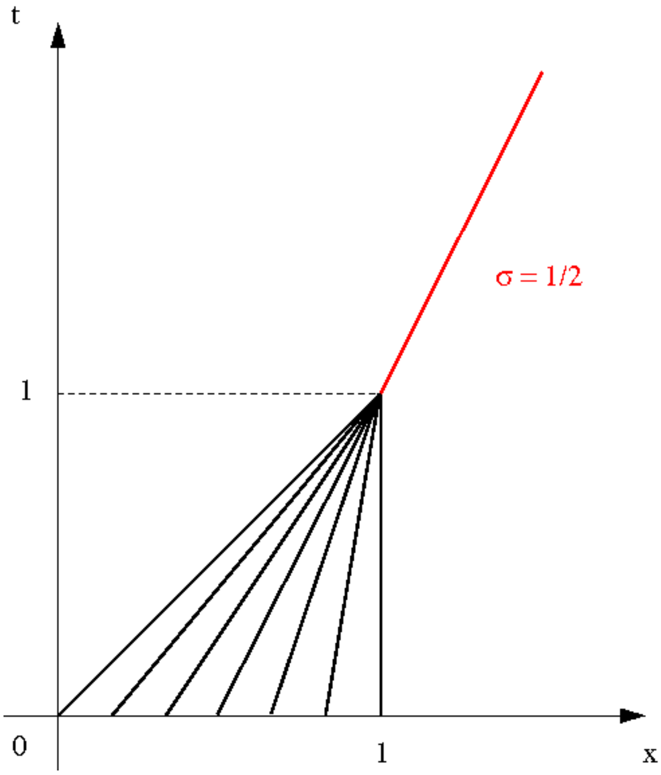

Figure 8.4 – *A converging shock wave for the Burgers equation. The decreasing profile (8.38) at $t = 0$ leads to an admissible discontinuity at $t = 1$.*

Then a shock wave with velocity $\sigma = \frac{1}{2}$ develops.

- The first test case concerns a converging shock wave and is displayed in Figure 4. At time $t = 0$ the initial profile $u_0(x)$ is given according to

$$u_0(x) = \begin{cases} 1 & if \quad x \leqslant 0 \\ 1 - x & if \quad 0 \leqslant x \leqslant 1 \\ 0 & if \quad x \geqslant 1\,. \end{cases} \tag{8.38}$$

When $t < 1$ the profile $u(x, t)$ remains a continuous function of space x but when $t > 1$ a shock wave with velocity $\sigma = \frac{1}{2}$ is present (see *e.g.* [69], [39] or [97]). It is a challenge if a lattice Boltzmann scheme is able to capture in a systematic way such a discontinuous solution.

- The first experiment (see Figure 5) concerns the first centered scheme (8.25) and the choice $\alpha = \frac{1}{2}$ and $\lambda = 1.8$ for the numerical parameters. The result is catastrophic, as depicted on Figure 5. The scheme is unstable and diverges within a very little time after the solution becomes discontinuous. The reason is simple *a posteriori*. Observe that for the previous test case $\alpha = \frac{1}{2}$ and particular values $u(x, t) \geqslant 1$ have to be considered. But the convexity-stability condition (8.24) reads as $|\,u\,| \leqslant \frac{\lambda}{2}$ and is incompatible with the chosen numerical values because we take $\lambda = 1.8$ in the numerical simulation. We observe that under conditions that violate the inequality (8.24), the lattice Boltzmann scheme is unstable in this strongly nonlinear situation, even if we respect the linear stability condition

$$0 < s_j < 2 \tag{8.39}$$

proposed initially by Hénon [77].

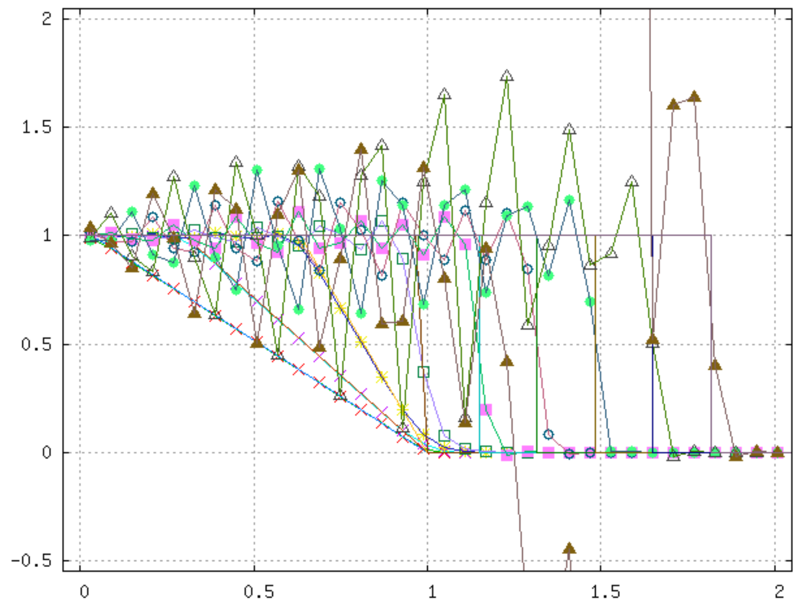

Figure 8.5 – *Burgers equation. Instable D1Q3 lattice Boltzmann simulation for a converging shock with equilibrium (8.25) associated to the parameters* $\alpha = \frac{1}{2}$, $s_2 = s_3 = 1.7$ *and* $\lambda = 1.8$. *Computed values are displayed every 10 time steps.*

- We repeat the same numerical experiment with a smaller time step. We take $\lambda = 3$ in a second experiment. The condition (8.24) is now satisfied and the scheme is stable. The results are correct and are presented in Figure 6. The shock is spread on 4 to 5 mesh points and we observe simply an overshoot at the location of the shock wave. With the extreme set of values $s_2 = s_3 = 2$ (if we refer to relation (8.39)), the numerical experiment does not give correct results because no entropy is dissipated. But the scheme remains stable; the numerical values remain inside an interval $[-0.4, 1.7]$ relatively close to the set $[0, 1]$ of correct values for this particular problem. The nonlinear stability condition enters into competition with the linear stability condition (8.39).

- With the same initial condition (8.38), we use the D1Q3 upwind version (8.27) of the lattice Boltzmann scheme. Now the stability condition is not as severe as in the previous case and we take $\lambda = 1.1$. The results, presented in Figure 7, are qualitatively analogous to the previous one (see Figure 6). We observe on Figure 7 an alternance of monotonic and over or undershooting discrete shock profiles.

- With the same decreasing initial condition (8.38), using the D1Q2 version (8.31) leads to results presented on Figure 8. We observe only an over-shooting at the discrete shock profile without any under-overshooting.

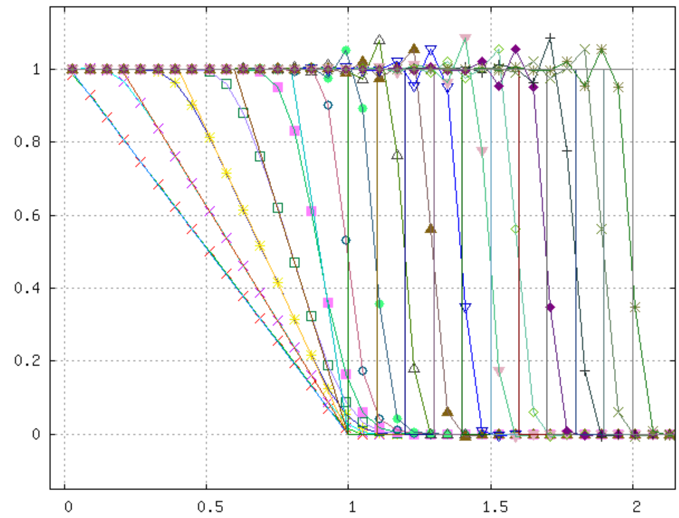

Figure 8.6 – *Burgers equation. Stable D1Q3 lattice Boltzmann simulation for a converging shock with equilibrium (8.25) associated to the parameters* $\alpha = \frac{1}{2}$, $\lambda = 3$ *and* $s_2 = s_3 = 1.7$. *Computed values are displayed every 10 time steps.*

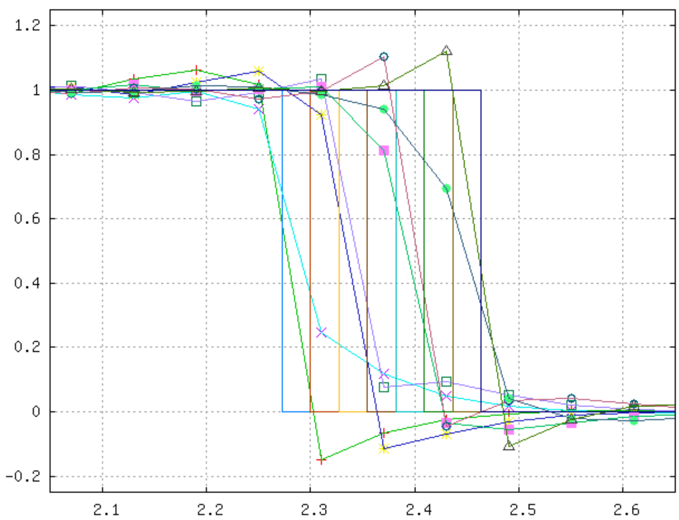

Figure 8.7 – *Burgers equation. Stable D1Q3 lattice Boltzmann simulation for a converging shock with upwind equilibrium (8.27) with* $\lambda = 1.1$ *and* $s_2 = s_3 = 1.7$. *Eight consecutive discrete time steps.*

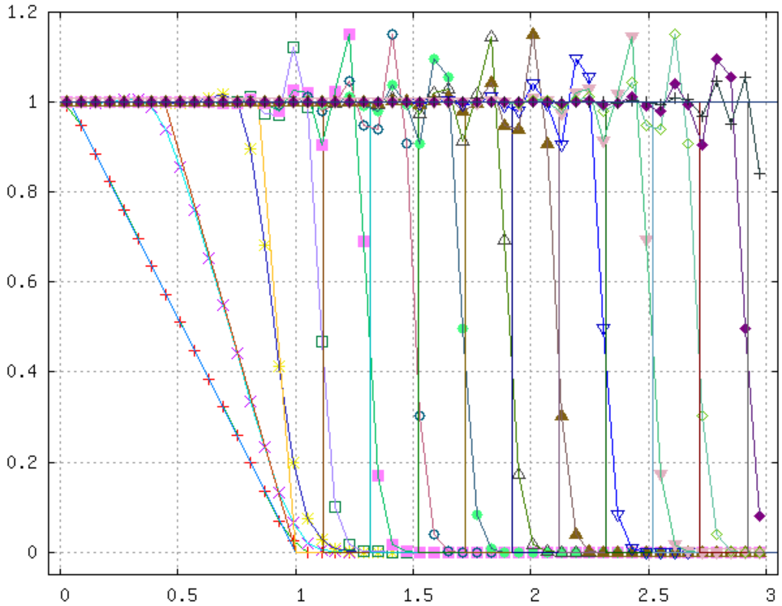

Figure 8.8 – *Burgers equation. Stable D1Q2 lattice Boltzmann simulation for a converging shock with equilibrium (8.31),* $\lambda = 1.5$ *and* $s_2 = 1.7$*. Computed values are displayed every 10 time steps.*

- In a second set of experiments, we use the very simple "two steps" or "Riemann" initial condition. The first one is simply

$$u_0(x) = \begin{cases} 1 & \text{if} \quad x < 0.2 \\ 0 & \text{if} \quad x > 0.2\,. \end{cases} \tag{8.40}$$

The entropic solution of this Riemann problem composed by the Burgers equation (8.1) associated with the initial condition (8.40) is a discontinuity propagating at the velocity $\sigma = \frac{1}{2}$ (see *e.g.* [69], [39] or [97]). With the numerical schemes introduced previously, this entropy satisfying solution is captured with a precision comparable to finite-volume type methods except that for a moving shock, a total variation diminishing scheme would not show oscillations ahead and behind the shock. The results are presented on Figure 9 for numerical schemes (8.25), (8.27) and (8.31). On Figure 10, a zoom of the previous data shows that this moving shock is captured by a stencil of four to five mesh points.

- We reverse the values 0 and 1 in the initial condition (8.40) and obtain in this way a new initial condition :

$$u_0(x) = \begin{cases} 0 & \text{if} \quad x < 0.2 \\ 1 & \text{if} \quad x > 0.2\,. \end{cases} \tag{8.41}$$

The entropic solution of (8.1)(8.41) is a rarefaction wave : a continuous solution with two constant states and a self-similar component as detailed *e.g.* [69], [39] or [97]. Without any modification of the scheme, the numerical solution with the three previous variants are presented on Figure 11. At the tricky zones of the foot (Figure 12) and the top (Figure 13) of the rarefaction, the slope is

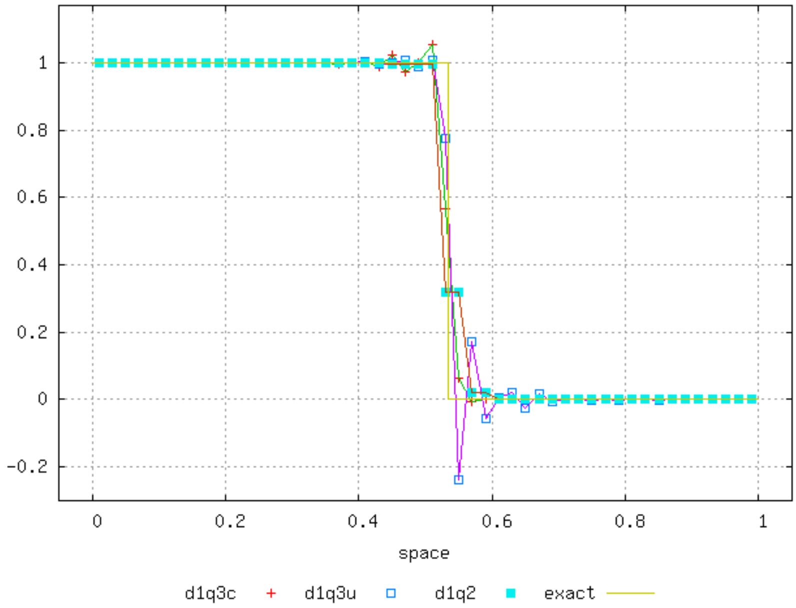

Figure 8.9 – *The Riemann problem for the Burgers equation associated with the initial condition (8.40) develops a shock wave. The figures shows the numerical solutions with the three variants of the scheme after 100 discrete time steps and parameters* $\lambda = 3$ *and* $s_2 = s_3 = 1.7$.

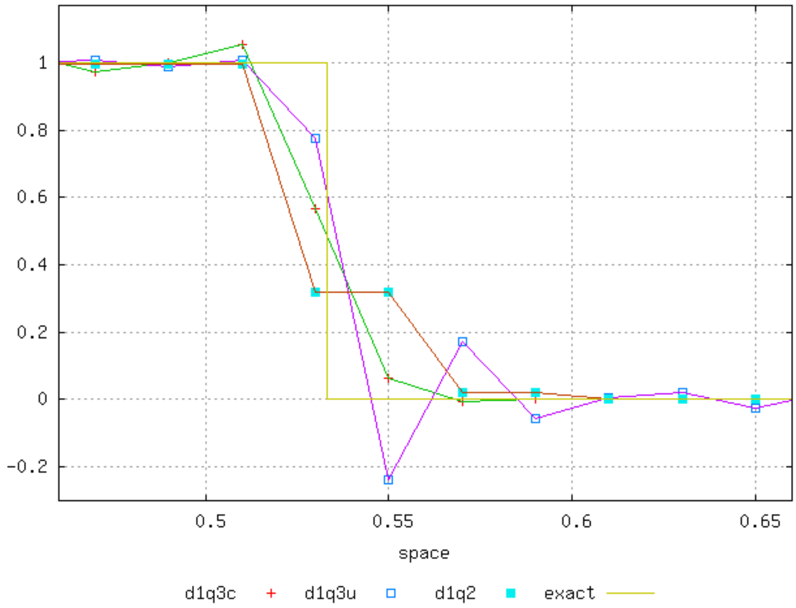

Figure 8.10 – *Zoom of Figure 10 around the location of the shock wave.*

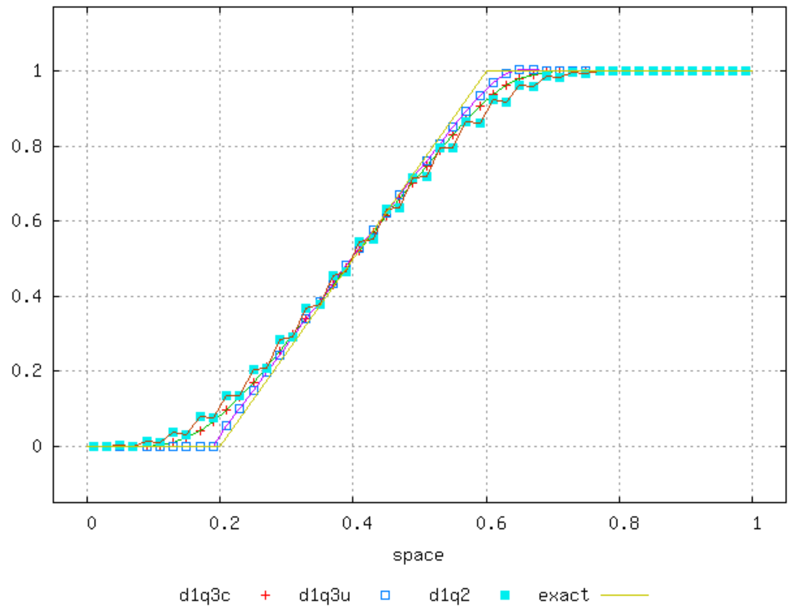

Figure 8.11 – *The Riemann problem for the Burgers equation associated with the initial condition (8.41) develops a rarefaction wave. Numerical solutions with the three variants of the lattice Boltzmann scheme after 100 discrete time steps and parameters* $\lambda = 3, \; s_2 = s_3 = 1.7$.

discontinuous and the solution of the problem (8.1)(8.41) is just continuous. We observe that the “D1Q2” version of the lattice Boltzmann scheme exhibits a two point discrete structure ; in some sense the little number of mesh points of this version (8.31) induces some rigidity in the discrete approximation.

• In this section relative to test cases for unstationary solutions of the Burgers equation, we have observed two facts. First, if the dual entropy approach is achieved, the resulting scheme is naturally stable even in circumstance where the classic linear analysis is *a priori* in defect. A precise analysis of the competition between nonlinear equilibrium and over-relaxation step (8.33) can be found the work of Brownlee *et al.* [20] with a totally different point of view. Second, under the convexity condition of the h_j^* functions of the particle decomposition (8.20), we observe that the entropy condition is automatically enforced. No so-called rarefaction shock has never been observed with the initial condition (8.41).

8.6 LINEAR AND NONLINEAR ACOUSTICS

The extension of the previous ideas from scalar equation to hyperbolic systems is a difficult task. We study in this section the first order systems of linear and nonlinear acoustics.

• Consider the example of one-dimensional linear acoustics with D1Q3 lattice Boltzmann scheme to fix the ideas. We recall that we can write this physical model as a hyperbolic system of first order :

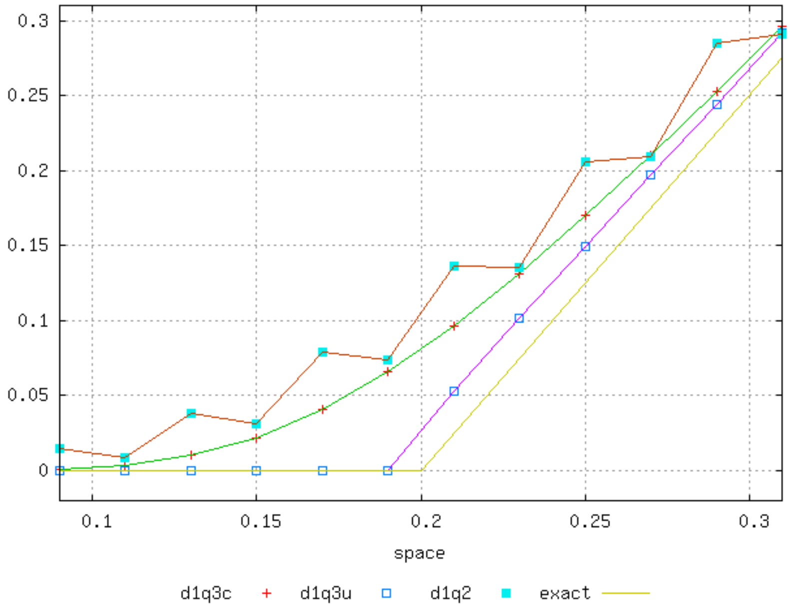

Figure 8.12 – *Zoom of Figure 12 at the foot of the rarefaction.*

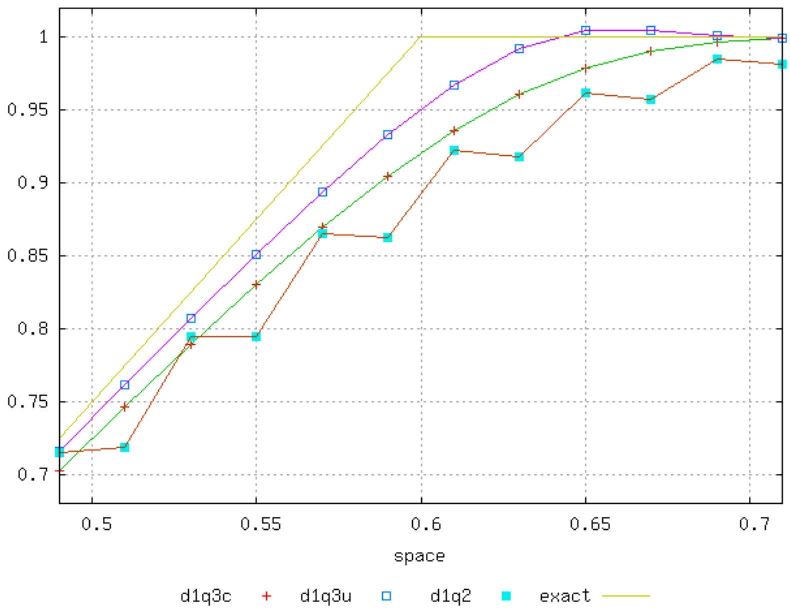

Figure 8.13 – *Zoom of Figure 12 at the top of the rarefaction.*

$$\partial_t \begin{pmatrix} \rho \\ q \end{pmatrix} + \partial_x \begin{pmatrix} q \\ c_0^2 \, \rho \end{pmatrix} = 0 \,. \tag{8.42}$$

Then a mathematical entropy is simply a quadratic form that corresponds to the physical energy :

$$\eta(W) \equiv \frac{\rho^2}{2} + \frac{q^2}{2\, c_0^2} \,. \tag{8.43}$$

The entropy variables are the gradients of the entropy (8.43) relative to the conserved variables (ρ, q) and we have

$$\varphi = \Big(\rho \,, \frac{q}{c_0^2} \Big) \,. \tag{8.44}$$

The associated entropy flux $\zeta(W)$ is easy to determine and $\zeta(W) = \rho\, q$. The dual entropy $\eta^*(\varphi) \equiv \varphi \bullet W - \eta(W)$ and the dual entropy flux $\zeta^*(\varphi) \equiv \varphi \bullet F(W) - \zeta(W)$ can be evaluated without difficulty and we obtain

$$\eta^*(\varphi) = \eta(W) \,, \quad \zeta^*(\varphi) = \zeta(W) \,; \tag{8.45}$$

all is quadratic in this system !

- We approach the system (8.42) with a D1Q3 lattice Boltzmann scheme. We use the moments m associated with the same matrix M used for the Burgers equation (see (8.32)). The associated particle components of the entropy variables $\varphi \bullet M_j$ introduced in (8.12) are given according to

$$\varphi \bullet M_+ \equiv \rho + \frac{\lambda\, q}{c_0^2} \,, \quad \varphi \bullet M_0 \equiv \rho \,, \quad \varphi \bullet M_- \equiv \rho - \frac{\lambda\, q}{c_0^2} \,. \tag{8.46}$$

The identities (8.13) take now the form

$$\left\{ \begin{array}{ll} h_+^* \big(\varphi \bullet M_+ \big) + h_0^* \big(\varphi \bullet M_0 \big) + h_-^* \big(\varphi \bullet M_- \big) & \equiv \eta^*(\varphi) \\ \lambda \, h_+^* \big(\varphi \bullet M_+ \big) - \lambda \, h_-^* \big(\varphi \bullet M_- \big) & \equiv \zeta^*(\varphi) \,. \end{array} \right. \tag{8.47}$$

We search a possible solution of system (8.47) with simple quadratic functions : $h_0^*(y) \equiv a\, y^2$ and $h_+^*(y) = h_-^*(y) \equiv b\, y^2$. After some lines of algebra, the previous representation and the above conditions (8.47) leads to

$$\left\{ \begin{array}{ll} h_+^* \Big(\rho + \dfrac{\lambda\, q}{c_0^2} \Big) & = \dfrac{c_0^2}{4\, \lambda^2} \Big(\rho + \dfrac{\lambda\, q}{c_0^2} \Big)^2 \\ h_0^*(\rho) & = \dfrac{1}{2} \Big(1 - \dfrac{c_0^2}{\lambda^2} \Big) \rho^2 \\ h_-^* \Big(\rho - \dfrac{\lambda\, q}{c_0^2} \Big) & = \dfrac{c_0^2}{4\, \lambda^2} \Big(\rho - \dfrac{\lambda\, q}{c_0^2} \Big)^2 . \end{array} \right. \tag{8.48}$$

The functions proposed in (8.48) are convex under the stability condition :

$$| c_0 | \leq \lambda \,. \tag{8.49}$$

This inequality means that the numerical waves go faster than the physical ones, a familiar interpretation of the Courant-Friedrichs-Lewy condition (see *e.g.* [97]). A microscopic entropy $H(f) = h_+(f_+) + h_0(f_0) + h_-(f_-)$ can be easily derived from (8.48) with the following contributors :

$$h_+(f_+) = \frac{\lambda^2}{c_0^2} f_+^2, \quad h_0(f_0) = \frac{1}{2\left(1 - \frac{c_0^2}{\lambda^2}\right)} f_0^2, \quad h_-(f_-) = \frac{\lambda^2}{c_0^2} f_-^2 .$$

The particle distribution f_j^{eq} at equilibrium is a direct consequence of relations (8.17) and (8.48) and we have

$$f_+^{eq} = \frac{c_0^2}{2\lambda^2}\Big(\rho + \frac{\lambda q}{c_0^2}\Big), \quad f_0^{eq} = \frac{1}{2}\Big(1 - \frac{c_0^2}{\lambda^2}\Big)\rho, \quad f_-^{eq} = \frac{c_0^2}{2\lambda^2}\Big(\rho - \frac{\lambda q}{c_0^2}\Big). \tag{8.50}$$

In terms of moments, the relations (8.50) reduce to $m_3^{eq} = c_0^2\,\rho$ as proposed in Qian *et al.* [113]. Observe that the equilibrium (8.50) for acoustics satisfies the dual entropy approach if the CFL condition (8.49) is satisfied.

• We propose now to introduce a system of nonlinear acoustics obtained by replacing the linear pressure law in (8.42) by a nonlinear one. We consider to fix the ideas the particular example of barotropic pressure law $p(\rho)$ given according to

$$p(\rho) = \frac{1}{\gamma}\,\rho_0\, c_0^2 \Big(\frac{\rho}{\rho_0}\Big)^{\gamma}, \tag{8.51}$$

with $\gamma > 1$. The corresponding nonlinear system of equations is quite similar to the so-called *p-system.* It can be written as

$$\partial_t \rho + \partial_x q = 0, \quad \partial_t q + \partial_x\big(p(\rho)\big) = 0. \tag{8.52}$$

It admits a mathematical entropy η and an associated entropy flux ζ satisfying

$$\eta(W) = \Phi(\rho) + \frac{q^2}{2}, \quad \zeta(W) = p(\rho)\, q, \tag{8.53}$$

where $\Phi(\bullet)$ is a primitive of the function $p(\bullet)$ introduced at the relation (8.51). In consequence of (8.53), the entropy variables $\varphi \equiv (\alpha, \beta)$ take the form

$$\alpha = p(\rho), \quad \beta = q. \tag{8.54}$$

The dual entropy $\eta^*(\bullet)$ and dual entropy flux $\zeta^*(\bullet)$ admit the expressions

$$\left\{ \begin{array}{ll} \eta^*(\alpha,\beta) & = \dfrac{\rho_0^2\, c_0^2}{\gamma+1}\Big(\dfrac{\gamma\,\alpha}{\rho_0\, c_0^2}\Big)^{\frac{\gamma+1}{\gamma}} + \dfrac{\beta^2}{2} \equiv \dfrac{\rho_0^2\, c_0^2}{\gamma+1}\Big(\dfrac{\rho}{\rho_0}\Big)^{\gamma+1} + \dfrac{\beta^2}{2} \\ \zeta^*(\alpha,\beta) & = \alpha\,\beta \equiv \zeta(\rho, q). \end{array} \right. \tag{8.55}$$

• With the matrix M introduced at relation (8.32), we denote by φ_+, φ_0 and φ_- the particle components of the entropy variables $\varphi \bullet M_j$ and we have

$$\varphi_+ = \alpha + \lambda\,\beta, \quad \varphi_0 = \alpha, \quad \varphi_- = \alpha - \lambda\,\beta. \tag{8.56}$$

It is possible to find nonlinear convex functions satisfying (8.47) with the new entropy data (8.55). By differentiating the relations (8.55) relative to the two entropy variables (8.54), the equilibrium functions $f_+^{\rm eq}$, $f_0^{\rm eq}$ and $f_-^{\rm eq}$ must satisfy the relations

$$\left\{ \begin{array}{ll} f_+^{\rm eq}(\alpha+\lambda\,\beta) + f_0^{\rm eq}(\alpha) + f_-^{\rm eq}(\alpha-\lambda\,\beta) & = \rho \\ \lambda\, f_+^{\rm eq}(\alpha+\lambda\,\beta) - \lambda\, f_-^{\rm eq}(\alpha-\lambda\,\beta) & = q \equiv \beta \\ \lambda^2\, f_+^{\rm eq}(\alpha+\lambda\,\beta) + \lambda^2\, f_-^{\rm eq}(\alpha-\lambda\,\beta) & = p(\rho) \equiv \alpha\,. \end{array} \right. \tag{8.57}$$

Then

$$f_+^{\rm eq}(\alpha+\lambda\,\beta) = \frac{1}{2\,\lambda^2}\,(\alpha+\lambda\,\beta)\,,\ f_0^{\rm eq}(\alpha) = \rho - \frac{\alpha}{\lambda^2}\,,\ f_-^{\rm eq}(\alpha-\lambda\,\beta) = \frac{1}{2\,\lambda^2}\,(\alpha-\lambda\,\beta) \tag{8.58}$$

and by integration of (8.17) and (8.58), we deduce that the relations (8.48) have to be replaced by

$$h_+^*(\alpha) = h_-^*(\alpha) = \frac{1}{4\,\lambda^2}\,\alpha^2\,,\quad h_0^*(\alpha) = \frac{\rho_0^2\,c_0^2}{\gamma+1}\Big(\frac{\gamma\,\alpha}{\rho_0\,c_0^2}\Big)^{\frac{\gamma+1}{\gamma}} - \frac{\alpha^2}{2\,\lambda^2}\,. \tag{8.59}$$

The function $h_+^*(\bullet) \equiv h_-^*(\bullet)$ is clearly convex and it is also the case for the function $h_0^*(\bullet)$ if its second derivative relative to α is positive, *id est* if and only if the following "dual stability condition" is satisfied:

$$\Big(\frac{\rho}{\rho_0}\Big)^{\gamma-1}\Big(\frac{c_0}{\lambda}\Big)^2 \leqslant 1\,. \tag{8.60}$$

• We have tested the system of nonlinear acoustics (8.51) (8.52) with a D1Q3 lattice Boltzmann scheme for a Riemann problem. The initial condition is a discontinuity at $x = 0$:

$$(\rho(x,0)\,,\,q(x,0)) = \left\{ \begin{array}{ll} (\rho_\ell\,,\,q_\ell) & if\ x<0 \\ (\rho_r\,,\,q_r) & if\ x>0\,. \end{array} \right. \tag{8.61}$$

We have chosen the physical and numerical parameters as follows:

$$\gamma = 2\,,\quad \frac{\rho_\ell}{\rho_0} = 0.5\,,\quad \frac{\rho_r}{\rho_0} = 0.15\,,\quad q_\ell = q_r = 0\,,\quad \frac{\lambda}{c_0} = 1.2\,,\quad s_3 = 1.7\,. \tag{8.62}$$

The exact solution of the nonlinear hyperbolic system (8.52) (8.61) can be obtained without difficulty with the general methods presented in [39] or [69]. In the case of initial data (8.61) (8.62) a rarefaction wave propagates with a negative velocity and a shock wave propagates with a positive velocity $\sigma = 0.416\,c_0$. An intermediate state with $\rho^* = 0.348\,\rho_0$ and $q^* = 0.0824\,\rho_0\,c_0$ separates these two nonlinear waves. With the parameters (8.62), the condition (8.60) is realized: $\big(\frac{\rho}{\rho_0}\big)^{\gamma-1}\big(\frac{c_0}{\lambda}\big)^2 \leqslant 0.347$. The numerical results are presented at Figure 14. The rarefaction wave and the shock wave are correctly captured as in the case of the Burgers equation (see figures 9 and 10). When the dual stability condition (8.60) is not satisfied, the lattice Boltzmann scheme replaces the rarefaction by a spurious shock wave and becomes completely unusable for higher values of the parameter defined by the left hand side of (8.60).

• As a summary of this section, the generalization of what have been done in this contribution for the Burgers equation with the D1Q3 lattice Boltzmann scheme is essentially nontrivial. It is possible to simulate specific nonlinear systems of conservation laws and we have experimented with the case of nonlinear acoustics.

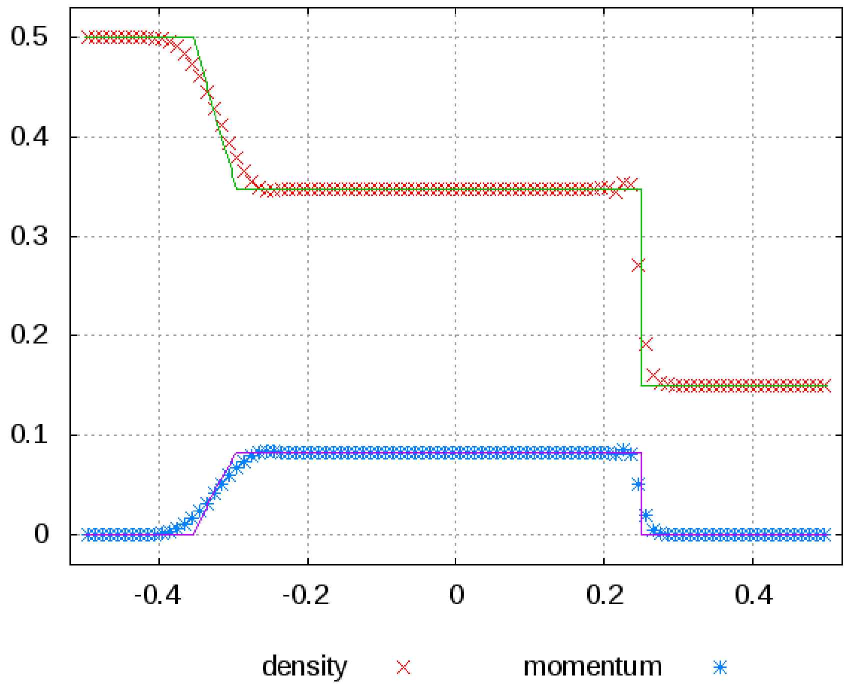

Figure 8.14 – *Riemann problem (8.52) (8.61) for the system of nonlinear acoustics. The numerical data are precised at the relations (8.62). A rarefaction wave is propagating from right to left and a shock wave from left to right. Exact (dotted lines) and approximated (discrete symbols) profiles of density (top) and momentum (bottom) for 100 mesh points and 60 time steps.*

8.7 THE CASE OF SHALLOW WATER EQUATIONS

The case of shallow water equations has been considered with the lattice Boltzmann scheme by Salmon [119] for oceanography applications. In the case of one space dimension we can apply the program presented above for linear and nonlinear acoustic models and try to represent the dual entropy with the help of a D1Q3 particle distribution. We will see in the following the kind of difficulties that we encounter with the dual entropy approach with the present choice of a single particle distribution.

• More precisely, we consider the one-dimensional system of conservation laws due to Barré de Saint Venant :

$$\partial_t \rho + \partial_x q = 0 \,, \qquad \partial_t q + \partial_x \Big(\frac{q^2}{\rho} + k \, \rho^\gamma \Big) = 0 \,, \tag{8.63}$$

where $k > 0$ and $\gamma \geqslant 1$ are given positive constants. We detail in the following the case $\gamma > 1$; the case $\gamma = 1$ is presented in the annex and conducts to analogous conclusions. We introduce velocity u, pressure p and sound velocity $c > 0$ according to the relations

$$u \equiv \frac{q}{\rho} \,, \quad p \equiv k \, \rho^\gamma \,, \quad c^2 \equiv \frac{\gamma \, p}{\rho} = \gamma \, k \, \rho^{\gamma - 1} \,. \tag{8.64}$$

Then the entropy η and the entropy flux ζ satisfy

$$\eta = \frac{1}{2}\rho\, u^2 + \frac{p}{\gamma - 1}\,, \quad \zeta = \eta\, u + p\, u\,; \tag{8.65}$$

the entropy variables $\varphi = \big(\partial_\rho \eta, \partial_q \eta\big) \equiv (\alpha, \beta)$ can be evaluated without difficulty :

$$\alpha = \frac{c^2}{\gamma - 1} - \frac{u^2}{2}\,, \quad \beta = u\,.$$

The dual entropy η^* and the dual entropy flux ζ^* can be expressed as functions of the entropy variables :

$$\eta^* = K\Big(\alpha + \frac{\beta^2}{2}\Big)^{\frac{\gamma}{\gamma-1}}\,, \quad \zeta^* = K\Big(\alpha + \frac{\beta^2}{2}\Big)^{\frac{\gamma}{\gamma-1}} \beta\,, \quad K = k\Big(\frac{\gamma - 1}{\gamma\, k}\Big)^{\frac{\gamma}{\gamma-1}}\,. \tag{8.66}$$

We remark that this dual entropy η^* explicited in (8.66) is no longer the sum of two functions of only one entropy variable as in (8.45) and (8.55) for linear and nonlinear acoustics respectively. The particle components of the entropy variables φ_+, φ_0 and φ_- are still given by the relations (8.56). The unknown **c**onvex functions h_j^* satisfy the identities (8.47) and take now the form

$$\left\{ \begin{array}{ll} h_+^*(\varphi_+) + h_0^*(\varphi_0) + h_-^*(\varphi_-) & = K\Big(\alpha + \frac{\beta^2}{2}\Big)^{\frac{\gamma}{\gamma-1}} \\ \lambda\, h_+^*(\varphi_+) - \lambda\, h_-^*(\varphi_-) & = K\Big(\alpha + \frac{\beta^2}{2}\Big)^{\frac{\gamma}{\gamma-1}} \beta\,. \end{array} \right. \tag{8.67}$$

• We prove in the following that the system of equations (8.67) where the unknowns are the convex functions h_+^*, h_0^* and h_-^* of a single real variable, has no solution. In order to establish this property, we introduce the equilibrium distributions f_j^{eq} according to (8.17). We differentiate the relations (8.67) relatively to α and β. We obtain relations very similar to (8.57):

$$\left\{ \begin{array}{ll} f_+^{eq}(\alpha + \lambda\,\beta) + f_0^{eq}(\alpha) + f_-^{eq}(\alpha - \lambda\,\beta) & = \rho \\ \lambda\, f_+^{eq}(\alpha + \lambda\,\beta) - \lambda\, f_-^{eq}(\alpha - \lambda\,\beta) & = \rho\, u \\ \lambda^2\, f_+^{eq}(\alpha + \lambda\,\beta) + \lambda^2\, f_-^{eq}(\alpha - \lambda\,\beta) & = \rho\, u^2 + p\,. \end{array} \right. \tag{8.68}$$

We are supposed to determine an increasing function f_0^{eq} of **o**nly one real variable α such that

$$f_0^{eq}\Big(\frac{c^2}{\gamma - 1} - \frac{u^2}{2}\Big) \equiv \rho - \frac{1}{\lambda^2}\big(\rho\, u^2 + p\big)\,. \tag{8.69}$$

Due to the elementary calculus $\frac{\mathrm{d}c^2}{\mathrm{d}\rho} = \gamma\, k\,(\gamma - 1)\rho^{\gamma - 2} = (\gamma - 1)\frac{c^2}{\rho}$, we differentiate the relation (8.69) relative to ρ and independently relatively to u. We obtain

$$\frac{c^2}{\rho}\,\big(f_0^{eq}\big)'(\alpha) + \frac{1}{\lambda^2}\big(u^2 + c^2\big) = 1\,, \quad -u\big(f_0^{eq}\big)'(\alpha) + \frac{2\rho\, u}{\lambda^2} = 0\,. \tag{8.70}$$

We extract the derivative $(f_0^{eq})'(\alpha)$ from the second equation of (8.70) and report the result in the first equation. We deduce

$$u^2 + 3\, c^2 = \lambda^2 \tag{8.71}$$

and this relation can be correct only for exceptional values of velocity and sound velocity ! This impossibility is mathematically natural : it is in general not possible to represent a function of two variables (the right hand side of relation (8.69)) by a simple function of only one variable.

CONCLUSION AND PERSPECTIVES

We first propose a summary of the algebraic work that a "user" has to do in order to determine in which domain a given lattice Boltzmann scheme satisfies the dual stability condition initially proposed by Bouchut [14]. If very interesting results are computed with a very good lattice Boltzmann scheme in the framework proposed by d'Humières [80], the procedure follows five steps. Suppose that the conserved variables

$$W_k \equiv \sum_j M_{kj}\, f_j$$

are determined. Then the convective fluxes follow the relation

$$F_{\alpha k}(W) \equiv \sum_j M_{kj}\, v_j^\alpha\, f_j^{\mathrm{eq}}.$$

First it is necessary to have a kinetic decomposition of the entropy and the associated entropy flux of the type

$$\eta(W) = \sum_j h_j(f_j^{\mathrm{eq}})\,, \qquad \zeta_\alpha(W) = \sum_j v_j^\alpha\, h_j(f_j^{\mathrm{eq}}).$$

Second determine the entropy variables

$$\varphi = \nabla_W \eta(W)$$

and the one to one mapping between W and φ. Third evaluate the Legendre-Fenchel-Moreau duals

$$h_j^*(y) \equiv \sup_f \, (y\, f - h_j(f))$$

of the scalar functions $h_j(\bullet)$. Fourth determine in which domain all the functions

$$\varphi \longmapsto h_j^*\big(\varphi \bullet M_j\big)$$

are convex. Fifth report this domain in the f space...

• Second, we recall that in this contribution, we have studied the role of Bouchut stability and convex decomposition of the dual entropy to develop stable lattice Boltzmann schemes in case of simulation of shock and rarefaction waves. We have applied the above procedure to the Burgers equation, a fundamental nonlinear scalar equation. Then nonlinear stability does not reduce to a simple criterion on the relaxation time parameters of the lattice Boltzmann scheme. A lattice Boltzmann scheme is in general not a finite volume scheme and the correct capture of shock waves presented in this contribution is mathematically absolutely non trivial. It remains open for us to understand why the discrete results with the lattice Boltzmann scheme are so well interpreted in terms of Bouchut's theory. Moreover, it is a natural question to know why the entropy condition is naturally enforced in the context of nonlinearly stable lattice Boltzmann schemes.

• Third we have observed that the situation for general nonlinear systems is not satisfactory. Even if all the methodology can be used for a simple nonlinear system as nonlinear acoustics, it is mathematically impossible to extend this algebraic construction to the familiar nonlinear system of Saint-Venant equations one space dimension. One idea is to keep the approach as a possible approximation of systems of conservation laws. Progress could also result from the use of a **v**ectorial particle distribution as initially proposed by Khobalatte and Perthame in [92] and developed by Bouchut [13] for the kinetic finite volume approach. Observe that this idea has been also recognized as very useful in the lattice Boltzmann community for the approximation of thermal fluids and magneto-hydrodynamics as suggested respectively by He, Chen and Doolen [75] and Dellar [36] and used by Peng, Shu and Chew [108] among others.

ANNEX. ON SHALLOW WATER EQUATIONS WITH $\gamma = 1$.

If $\gamma = 1$, we introduce a reference velocity c_* and replace the pressure law in (8.64) by $p = c_*^2\,\rho$. Then we introduce a reference density ρ_* to express in a physically consistent manner the algebraic expression a mathematical entropy:

$$\eta = \frac{q^2}{2\rho} + c_*^2\,\rho\,\log\frac{\rho}{\rho_*}\,.$$

Then

$$\alpha = \frac{\partial\eta}{\partial\rho} = c_*^2\Big(1+\log\frac{\rho}{\rho_*}\Big) - \frac{u^2}{2}\,,\quad \beta = \frac{\partial\eta}{\partial q} = u\,.$$

The entropy flux ζ is still obtained according to the relation (8.65): $\zeta = \eta\,u + p\,u$. After some lines of algebra, the dual entropy $\eta^* \equiv \alpha\,\rho + \beta\,q - \eta$ is equal to

$$\eta^* = c_*^2\,\rho = p = \rho_*\,c_*^2\,\exp\Big(\frac{\alpha+\beta^2/2}{c_*^2} - 1\Big)$$

and the dual flux $\zeta^* \equiv \alpha\,q + \beta\,(\rho\,u^2 + p) - \zeta$ is equal to $\eta^*\,\beta$ as in the case $\gamma > 1$. Then the relations (8.67) are generalized without difficulty and the identity (8.69) can be now written

$$f_0^{eq}\Big(c_*^2\,(1+\log\frac{\rho}{\rho_*}) - \frac{u^2}{2}\Big) \equiv \rho - \frac{1}{\lambda^2}\big(\rho\,u^2 + p\big)\,.$$

By derivation relative to density and velocity, we get respectively

$$\frac{c_*^2}{\rho}\,\big(f_0^{eq}\big)'(\alpha) + \frac{1}{\lambda^2}\big(u^2 + c_*^2\big) = 1\,,\quad -u\,\big(f_0^{eq}\big)'(\alpha) + \frac{2\,\rho\,u}{\lambda^2} = 0\,.$$

We deduce a necessary relation $u^2 + 3\,c_*^2 = \lambda^2$, very close to (8.71). This relation is satisfied only for exceptional values of velocity as in the case $\gamma > 1$.

CHAPTER 9

APPROXIMATION OF HYPERBOLIC SYSTEMS BY VECTORIAL LATTICE BOLTZMANN SCHEMES

We focus on mono-dimensional hyperbolic systems approximated by a particular lattice Boltzmann scheme. The scheme is described in the framework of the multiple relaxation times method and stability conditions are given. An analysis is done to link the scheme with an explicit finite differences approximation of the relaxation method proposed by Jin and Xin. Several numerical illustrations are given for the transport equation, Burger's equation, the p-system, and full compressible Euler's system[1].

9.1 INTRODUCTION

The strength of the lattice Boltzmann schemes lies in their effectivity. They are intensively used in academic and industrial contexts for numerical simulations of fluid dynamics. Their links with the mesoscopic physics and in particular with the Boltzmann equation make that these schemes are especially well adapted to simulate fluid phenomenas obtained by asymptotic limits from the kinetic theory. However, it is sometimes awkward to fix the several parameters of a lattice Boltzmann scheme in order to simulate a given equation, even if this equation is written into a conservative form: the conservation of the energy is classically a difficulty that can involve to use two different schemes coupled by a source term [132]. Other very particular schemes were proposed and investigated in order to simulate the full compressible Euler system, with substantial works on the equilibria [37, 38, 31, 32, 134].

In this contribution, a new lattice Boltzmann scheme is introduced in order to approximate any mono-dimensional hyperbolic conservative system, the intended target being the various equations of the fluid dynamics: many systems are written as conservation laws and the propagation of the waves is an essential property. In particular, the equations obtained by the kinetic theory of gases (as Euler's equations) are of that type [68]. The followed methodology is to treat separately the equations of the system by leaving aside the Boltzmann equation as much as possible. Usually, in order to increase the dimension of the system—that is the number of conservation equations—densities with larger velocities are introduced with two consequences: first, the lattice of the velocities is extended with the obvious difficulties concerning the boundary conditions; second, added new velocities deeply modifies the scheme so that all previous investigations have to be redone. The proposed scheme denoted by $\mathsf{D}_1\mathsf{Q}_2^n$ is built by duplicating for each of the n conserved moments the well-known and simplest lattice Boltzmann scheme: the $\mathsf{D}_1\mathsf{Q}_2$ (one spatial dimension and two discrete velocities). Therefore, the results on the scalar equation can easily be extended to the system of n equations. Moreover, as the boundary conditions are written on the densities in the framework

[1] This contribution has been originally published in [**?**]

of the lattice Boltzmann schemes, the decoupling of the density functions extremely simplifies the choices of the incoming densities on the boundaries to fit the boundary conditions on the moments.

In [85], Jin and Xin introduced the relaxation method to replace a non linear hyperbolic system of dimension n by a linear hyperbolic system of dimension $2n$ with a stiff source term—called a relaxation term as it enforces the added moment to relax to the flux of the initial system. The convergence of this method when the relaxation term becomes dominant was investigated in [4, 105]. Many publications deal then with numerical relaxation schemes [7, 8, 107]. Otherwise, Junk reinterprets the lattice Boltzmann method—in particular the $\mathsf{D}_2\mathsf{Q}_9$—as an explicit finite differences discretization of a relaxation formulation for the incompressible Navier-Stokes equation in the diffusive scaling [87]. In this paper, the proposed $\mathsf{D}_1\mathsf{Q}_2^n$ scheme is related to a particular discretization of the relaxation method: a splitting between the linear hyperbolic part treated with an explicit finite differences discretization (Lax-Friedrichs discretization) and the relaxation part treated with an explicit Euler solver.

The first section of this paper is devoted to the scalar case: the $\mathsf{D}_1\mathsf{Q}_2$ scheme is written into the framework of d'Humières [80]; the equivalent equations are given up to the second order by using the Taylor expansion method [42, 43]; the description of the scheme as a discretization of the relaxation method is then done and stability conditions are given; finally numerical illustrations for the transport equation and for Burger's equation are performed. In the second section, we consider the case of n-dimensional hyperbolic systems: the $\mathsf{D}_1\mathsf{Q}_2^n$ scheme is introduced and described; the Taylor expansion method is then used to obtain the second order equivalent equations and the link with the discretization of the relaxation method is done; finally numerical illustrations for the p-system and for the full compressible Euler equation are performed.

9.2 THE $\mathsf{D}_1\mathsf{Q}_2$ SCHEME FOR THE $1-D$ SCALAR EQUATION

In this section, we consider the following mono-dimensional hyperbolic equation

$$\partial_t \mathrm{u}(t,x) + \partial_x \varphi(\mathrm{u})(t,x) = 0, \qquad t>0,\ x\in\mathbb{R}, \tag{9.1}$$

where the flux φ is a smooth function on $\mathbb{R}$. A two-velocities lattice Boltzmann scheme is used to approximate the solution of this equation.

9.2.1 DESCRIPTION OF THE SCHEME

We use the notation proposed by d'Humières in [80] by considering $\mathscr{L}$, a regular lattice in one dimension of space with typical mesh size Δx. The time step Δt is determined after the specification of the velocity scale λ by the relation:

$$\Delta t = \frac{\Delta x}{\lambda}. \tag{9.2}$$

For the scheme denoted by $\mathsf{D}_1\mathsf{Q}_2$, we introduce $\mathcal{V} = (-\lambda, \lambda)$ the set of the two velocities and we assume that for each node x of $\mathscr{L}$, and each v_j in $\mathcal{V}$, the point $x + v_j\Delta t$ is also a node of the lattice $\mathscr{L}$. The aim of the $\mathsf{D}_1\mathsf{Q}_2$ scheme is to compute a particles distribution vector $\boldsymbol{f} = (f_0, f_1)^{\mathrm{T}}$ on the lattice $\mathscr{L}$ at discrete values of time: it is a numerical scheme to approximately solve the PDEs

$$\partial_t f_j + v_j \cdot \nabla f_j = -\frac{1}{\tau_j}(f_j - f_j^{\mathrm{eq}}), \qquad 0 \leqslant j \leqslant 1,$$

on a grid in space and time where f_j^{eq} describes the distribution f_j at the equilibrium and τ_j is the relaxation time (applied to f_j). The scheme splits into two phases for each time iteration: first, the relaxation phase that is local in space, and second, the transport phase for which an exact characteristic method is used.

The framework proposed by d'Humières [80] reduced here to the two moments denoted by $\mathbf{m} = (\mathrm{u},\mathrm{v})^{\mathrm{T}}$ and defined for each space point $x \in \mathscr{L}$ and for each time t by

$$\mathrm{u} = f_0 + f_1, \qquad \mathrm{v} = \lambda\left(-f_0 + f_1\right). \tag{9.3}$$

The matrix of the moments $\boldsymbol{M}$ such that $\mathbf{m} = \boldsymbol{M}\boldsymbol{f}$ satisfies

$$\boldsymbol{M} = \begin{pmatrix} 1 & 1 \\ -\lambda & \lambda \end{pmatrix}, \qquad \boldsymbol{M}^{-1} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2\lambda} \\ \frac{1}{2} & \frac{1}{2\lambda} \end{pmatrix}. \tag{9.4}$$

Let us now describe one time step of the scheme. The start point is the density vector $\boldsymbol{f}(x,t)$ in $x \in \mathscr{L}$ at time t, the moments are computed by

$$\mathbf{m}(x,t) = \boldsymbol{M}\boldsymbol{f}(x,t). \tag{9.5}$$

The relaxation phase then reads

$$\mathrm{u}^\star(x,t) = \mathrm{u}(x,t), \qquad \mathrm{v}^\star(x,t) = \mathrm{v}(x,t) + s(\mathrm{v}^{\text{eq}}(x,t) - \mathrm{v}(x,t)), \tag{9.6}$$

where s is the relaxation parameter and v^{eq} the second moment at equilibrium that is a function of u. As a consequence, the first moment u is conserved during the relaxation phase. The densities are then computed after the relaxation phase by

$$\boldsymbol{f}^\star(x,t) = \boldsymbol{M}^{-1}\mathbf{m}^\star(x,t). \tag{9.7}$$

The transport phase finally reads

$$f_j(x,t+\Delta t) = f_j^\star(x - v_j\Delta t, t), \qquad 0 \leqslant j \leqslant 1. \tag{9.8}$$

9.2.2 ASYMPTOTIC ANALYSIS : THE TAYLOR EXPANSION METHOD

The aim of this section is to find the equivalent equations of the scheme and in particular to fix the equilibrium value v^{eq} as a function of u in order to ensure that the scheme is consistent with (9.1). This reasoning consists in a formal development of the distribution functions $\boldsymbol{f}(x,t)$ at small Δt and Δx, assuming that these functions are regular enough to use the Taylor formula. The results of this section are particular cases of the general expansion of Dubois [42, 43]. The interested reader can find proofs in 9.A.

Proposition 9.2.1 (zeroth order)**.** *Defining the vectors* $\mathbf{m}^{\text{eq}} = (\mathrm{u},\mathrm{v}^{\text{eq}})^{\mathrm{T}}$ *and* $\boldsymbol{f}^{\text{eq}} = \boldsymbol{M}^{-1}\mathbf{m}^{\text{eq}}$*, we have*

$$f_j = f_j^{\text{eq}} + \mathcal{O}(\Delta t), \qquad f_j^\star = f_j^{\text{eq}} + \mathcal{O}(\Delta t), \qquad 0 \leqslant j \leqslant 1. \tag{9.9}$$

Proposition 9.2.2 (First order macroscopic equation)**.** *The first moment* u *satisfies the partial differential equation*

$$\partial_t \mathrm{u} + \partial_x \mathrm{v}^{\text{eq}} = \mathcal{O}(\Delta t). \tag{9.10}$$

The choice $\mathrm{v}^{\text{eq}} = \varphi(\mathrm{u})$ *is then done so that* u *satisfies* (9.1) *at order 1.*

We then define the equilibrium default θ by using the particular derivatives $\mathrm{d}_t^j = \partial_t + v_j \partial_x$, $0 \leqslant j \leqslant 1$,

$$\theta = \sum_{j=0}^{1} v_j \, \mathrm{d}_t^j f_j^{\mathrm{eq}}.$$

The equilibrium default θ can then be rewritten into the form

$$\theta = \partial_t \mathrm{v}^{\mathrm{eq}} + \lambda^2 \partial_x \mathrm{u}. \tag{9.11}$$

Lemma 9.2.3 (Transition lemma)**.** *The second moment* v *satisfies*

$$\mathrm{v} = \mathrm{v}^{\mathrm{eq}} - \frac{\Delta t}{s}\theta + \mathcal{O}(\Delta t^2), \qquad \mathrm{v}^{\star} = \mathrm{v}^{\mathrm{eq}} + \Delta t\Big(1 - \frac{1}{s}\Big)\theta + \mathcal{O}(\Delta t^2). \tag{9.12}$$

Moreover, we have

$$f_j^{\star} - f_j = \Delta t \, \mathrm{d}_t^j f_j^{\mathrm{eq}} + \mathcal{O}(\Delta t^2), \quad 0 \leqslant j \leqslant 1.$$

Proposition 9.2.4 (Second order macroscopic equation)**.** *The first moment* u *satisfies the second-order partial differential equation*

$$\partial_t \mathrm{u} + \partial_x \varphi(\mathrm{u}) = \Delta t \, \sigma \, \partial_x \Big(\big(\lambda^2 - (\varphi'(\mathrm{u}))^2 \big) \partial_x \mathrm{u} \Big) + \mathcal{O}(\Delta t^2), \tag{9.13}$$

with $\sigma = 1/s - 1/2$.

Let us remark that this second-order macroscopic equation (9.13) then contains a diffusion term with a regularization effect if $\sigma > 0$ (that is $s < 2$) and $|\varphi'(\mathrm{u})| < \lambda$. These conditions are indeed compatible with the stability conditions of the section 9.2.4. In order to simulate the hyperbolic equation (9.1), the relaxation parameter s could be taken equal to 2. But this term has a stabilization effect and it could be sometime useful to choose s smaller to minimize the oscillations around the discontinuities.

9.2.3 LINK WITH THE RELAXATION METHOD

The relaxation method introduced by Jin and Xin [85] to solve the conservation equation (9.1) consists in forming a linear hyperbolic system with a stiff source term:

$$\begin{cases} \partial_t \mathrm{u}^{\epsilon} + \quad \partial_x \mathrm{v}^{\epsilon} = 0, \\ \partial_t \mathrm{v}^{\epsilon} + a \partial_x \mathrm{u}^{\epsilon} = -\dfrac{1}{\epsilon}(\mathrm{v}^{\epsilon} - \varphi(\mathrm{u}^{\epsilon})), \end{cases} \tag{9.14}$$

where ϵ is a small positive parameter. This kind of approximation was proposed in the general setting of the quasilinear systems of hyperbolic conservation laws and possesses some very interesting features. Natalini proves in [4, 105] that u^{ϵ} and v^{ϵ} converge to u and $\varphi(\mathrm{u})$ when ϵ goes to zero under some technical assumptions where u is the unique entropy solution in the sense of Kružkov [93].

In this section we write the $\mathsf{D}_1\mathsf{Q}_2$ scheme as a discretization of the relaxation system. Indeed, denoting $\mathrm{u}_i^n = \mathrm{u}(x_i, t^n)$, $\mathrm{v}_i^n = \mathrm{v}(x_i, t^n)$, $x_i \in \mathscr{L}$ and $t^n = n\Delta t$, we have

$$\mathrm{v}_i^{n\star} = \mathrm{v}_i^n - s(\mathrm{v}_i^n - \varphi(\mathrm{u}_i^n)), \tag{9.15}$$
$$\mathrm{u}_i^{n+1} = \tfrac{1}{2}(\mathrm{u}_{i+1}^n + \mathrm{u}_{i-1}^n) - \tfrac{\Delta t}{2\Delta x}(\mathrm{v}_{i+1}^{n\star} - \mathrm{v}_{i-1}^{n\star}), \tag{9.16}$$
$$\mathrm{v}_i^{n+1} = \tfrac{1}{2}(\mathrm{v}_{i+1}^{n\star} + \mathrm{v}_{i-1}^{n\star}) - \lambda^2 \tfrac{\Delta t}{2\Delta x}(\mathrm{u}_{i+1}^n - \mathrm{u}_{i-1}^n). \tag{9.17}$$

We then reinterpret the scheme as a splitting of the relaxation system (9.14) between the relaxation part (9.15) and the hyperbolic part (9.16,9.17). The relaxation part is treated by the explicit Euler method with $\epsilon = \Delta t/s$, and the hyperbolic part by the Lax-Friedrichs method with $a = \lambda^2$.

Moreover, we observe that the transport phase of the lattice Boltzmann scheme corresponds exactly to the hyperbolic part in the base of the eigenvectors. Indeed, writting the hyperbolic part of Eq. (9.14) as

$$\partial_t U + \boldsymbol{A}\partial_x U = 0, \qquad \text{with} \quad \boldsymbol{A} = \begin{pmatrix} 0 & 1 \\ \lambda^2 & 0 \end{pmatrix},$$

we have

$$\boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{M} = \begin{pmatrix} -\lambda & 0 \\ 0 & \lambda \end{pmatrix}.$$

The D_1Q_2 scheme then treats the hyperbolic part of the relaxation system by an upwind method in the base of the eigenvectors.

9.2.4 STABILITY

In this section, we are interested in the stability of the D_1Q_2 scheme. We first investigate the L^2-stability for the linear scheme, that is if $\varphi(u) = cu$ with c a real constant. We then give a property of L^∞-stability in the general case but with a more restrictive condition.

In the case where $\varphi(u) = cu$, $c \in \mathbb{R}$, the amplification matrix of the linear D_1Q_2 scheme is given by

$$G(\Delta x, \xi) = \begin{pmatrix} \left(1 - \frac{s}{2}(1+\frac{c}{\lambda})\right) e^{-i\Delta x \xi} & \frac{s}{2}(1-\frac{c}{\lambda}) e^{-i\Delta x\xi} \\ \frac{s}{2}(1+\frac{c}{\lambda}) e^{i\Delta x \xi} & \left(1 - \frac{s}{2}(1-\frac{c}{\lambda})\right) e^{i\Delta x \xi} \end{pmatrix}.$$

Proposition 9.2.5. *The linear D_1Q_2 scheme is stable for the L^2-norm if, and only if, $\lambda \geqslant |c|$ and $s \in [0,2]$.*

Proof. Considering the two discs of Gershgorin of the matrix $G(\Delta x, \xi)$, the condition $|c| \leqslant \lambda$ and $s \in [0,2]$ immediately implies that the two eigenvalues of G have a modulus smaller than 1. The reciprocal property is trivially true taking $\xi = 0$. □

Proposition 9.2.6 (maximum principle)**.** *Let M be a positive constant and φ a smooth flux function such that $|\varphi'(\mathrm{u})| \leqslant K$ for u in the compact $[0, M]$. Considering the D_1Q_2 scheme where*

- *the initial distribution functions are nonnegative $f_j(x,0) \geqslant 0$, for $0 \leqslant j \leqslant 1$, $x \in \mathscr{L}$,*
- *the initial global mass $\mathrm{u}^{\mathrm{tot}} = \sum_{x\in\mathscr{L}} (f_0 + f_1)$ satisfies $\mathrm{u}^{\mathrm{tot}} \leqslant M$,*
- *the relaxation parameter s verifies $s \in [0,1]$,*
- *the velocity of the scheme is such that $\lambda \geqslant K$,*

then we have

$$0 \leqslant f_j(x, t^n) \leqslant M, \qquad \text{for } 0 \leqslant j \leqslant 1,\ x \in \mathscr{L},\ n \in \mathbb{N}. \tag{9.18}$$

As a consequence, the first moment u remains bounded and nonnegative.

Proof. As the transport phase (9.8) just exchanges the data, we prove that $f_j \geqslant 0$ implies $f_j^\star \geqslant 0$. The problem being invariant by adding a constant to the flux function φ, we assume that $\varphi(0) = 0$. We have for each discrete point $x \in \mathscr{L}$ and each discrete time $t^n = n\Delta t$

$$
\begin{aligned}
f_0^\star &= \Big(1 - \frac{s}{2}\Big) f_0 + \frac{s}{2} f_1 - \frac{s}{2\lambda}\varphi(f_0 + f_1),\\
f_1^\star &= \frac{s}{2} f_0 + \Big(1 - \frac{s}{2}\Big) f_1 + \frac{s}{2\lambda}\varphi(f_0 + f_1).
\end{aligned}
$$

Writting $\varphi(f_0 + f_1) = \varphi'(\xi)(f_0 + f_1)$ for one $\xi \in [0, M]$ yields

$$
\begin{aligned}
f_0^\star &= \Big(1 - \frac{s}{2}\Big(1 + \frac{\varphi'(\xi)}{\lambda}\Big)\Big) f_0 + \frac{s}{2}\Big(1 - \frac{\varphi'(\xi)}{\lambda}\Big) f_1,\\
f_1^\star &= \frac{s}{2}\Big(1 + \frac{\varphi'(\xi)}{\lambda}\Big) f_0 + \Big(1 - \frac{s}{2}\Big(1 - \frac{\varphi'(\xi)}{\lambda}\Big)\Big) f_1.
\end{aligned}
$$

The assumptions $s \in [0, 1]$ and $\lambda \geqslant K$ then immediately imply that $f_0^\star$ and $f_1^\star$ are nonnegative linear combinations of f_0 and f_1, so that are nonnegative. The superior bound is then a consequence of the conservation of the global first moment $\mathrm{u}^{\mathrm{tot}}$. □

Remark 9.2.7. The assumption $\mathrm{u}^{\mathrm{tot}} \leqslant M$ can be removed in the case where the flux φ is K-lipschitzienne over $\mathbb{R}$.

9.2.5 NUMERICAL ILLUSTRATIONS

In this section, we perform two numerical simulations, one for the transport equation with a constant velocity, and one for Burger's equation. The lattice $\mathscr{L}$ is reduced to $[0, 1]$ and a homogeneous Neumann condition is added to treat the boundaries. In order to visualize the properties of the $\mathsf{D}_1\mathsf{Q}_2$ scheme, the initial condition is chosen of two types: first a smooth function and second a Riemann problem type function.

9.2.5.1 THE TRANSPORT EQUATION

Let c be a real constant, we consider in this section $\varphi(u) = cu$.

In Fig. 9.1, the left (*r*esp. right) plot shows the initial and the final (at time $T = 0.4$) moment u for several relaxation parameters s for smooth initial condition (*r*esp. Riemann problem). The number of points in space $N = 200$ had been chosen in order to visualize that the maximum principle is fulfilled when $s \in [0, 1]$ and is not when $s \in]1, 2]$ (the condition $\lambda \geqslant |c|$ is true). Tbl. 9.1 (*r*esp. Tbl. 9.2) shows the convergence of the L^2-norm for several relaxation parameters s when Δx goes to zero for smooth initial condition (*r*esp. Riemann problem). Each line corresponds to the integer $k \in \{3, \dots, 16\}$ with $\Delta x = 2^{-k}$. We then verify numerically that the scheme is consistent at order 1 with the transport equation in the general case and at order 2 if $s = 2$, for smooth solutions. The convergence is lowered when the solution is less regular.

Remark 9.2.8. The decrease of the convergence rate for discontinuous solution is in conformity with previous results for the hyperbolic systems: Kuznetsov established the 1/2 order for the non linear Lax's scheme on a multi-dimensional Cartesian mesh [94]; Delarue and Lagoutière prove that the upwind scheme is of order 1/2 in $L^\infty([0, T], L^1(\mathbb{R}^d))$ for an integrable initial datum of bounded variation for the transport equation on a polygonal mesh [35]; finally, concerning the mono-dimensional non linear equation investigated in this section, Sabac established that the 1/2 order is optimal for

k s	2.000	1.900	1.750	1.000	0.750	0.500
3	1.536e-01	1.416e-01	1.256e-01	8.104e-02	7.881e-02	8.113e-02
4	1.733e-01	1.714e-01	1.712e-01	2.062e-01	2.288e-01	2.550e-01
5	1.319e-01	1.153e-01	1.073e-01	1.495e-01	1.757e-01	2.100e-01
6	4.897e-02	4.697e-02	5.138e-02	1.145e-01	1.405e-01	1.719e-01
7	1.254e-02	1.429e-02	2.162e-02	7.983e-02	1.049e-01	1.357e-01
8	3.113e-03	4.850e-03	9.913e-03	4.990e-02	7.081e-02	9.927e-02
9	7.761e-04	1.991e-03	4.836e-03	2.863e-02	4.329e-02	6.599e-02
10	1.943e-04	9.263e-04	2.412e-03	1.551e-02	2.448e-02	3.990e-02
11	4.863e-05	4.522e-04	1.208e-03	8.096e-03	1.311e-02	2.233e-02
12	1.216e-05	2.241e-04	6.041e-04	4.138e-03	6.794e-03	1.188e-02
13	3.039e-06	1.117e-04	3.022e-04	2.092e-03	3.461e-03	6.136e-03
14	7.598e-07	5.577e-05	1.512e-04	1.052e-03	1.747e-03	3.121e-03
15	1.900e-07	2.787e-05	7.559e-05	5.277e-04	8.778e-04	1.574e-03
16	4.749e-08	1.393e-05	3.780e-05	2.642e-04	4.400e-04	7.904e-04
slope	2.000e+00	1.000e+00	9.999e-01	9.979e-01	9.965e-01	9.937e-01

Table 9.1 – *Transport equation with* $c = 0.75$ *at final time* $T = 0.4$ *(smooth solution: error in* L^2 *norm)*

k s	2.000	1.900	1.750	1.000	0.750	0.500
3	2.722e-01	2.657e-01	2.590e-01	2.649e-01	2.758e-01	2.893e-01
4	8.353e-02	8.611e-02	9.415e-02	1.696e-01	2.027e-01	2.389e-01
5	1.488e-01	1.372e-01	1.304e-01	1.434e-01	1.587e-01	1.832e-01
6	1.055e-01	9.036e-02	8.323e-02	1.066e-01	1.225e-01	1.444e-01
7	8.651e-02	7.416e-02	7.188e-02	9.591e-02	1.082e-01	1.251e-01
8	6.158e-02	4.995e-02	5.070e-02	7.838e-02	8.932e-02	1.038e-01
9	5.568e-02	4.470e-02	4.497e-02	6.609e-02	7.494e-02	8.675e-02
10	4.421e-02	3.434e-02	3.570e-02	5.515e-02	6.270e-02	7.268e-02
11	3.460e-02	2.684e-02	2.954e-02	4.657e-02	5.289e-02	6.125e-02
12	2.710e-02	2.089e-02	2.424e-02	3.909e-02	4.442e-02	5.146e-02
13	2.230e-02	1.732e-02	2.043e-02	3.288e-02	3.735e-02	4.326e-02
14	1.783e-02	1.406e-02	1.707e-02	2.763e-02	3.140e-02	3.637e-02
15	1.403e-02	1.151e-02	1.432e-02	2.324e-02	2.641e-02	3.059e-02
16	1.111e-02	9.517e-03	1.202e-02	1.954e-02	2.220e-02	2.572e-02
slope	3.374e-01	2.746e-01	2.527e-01	2.502e-01	2.501e-01	2.501e-01

Table 9.2 – *Transport equation with* $c = 0.75$ *at final time* $T = 0.4$ *(Riemann problem: error in* L^2 *norm)*

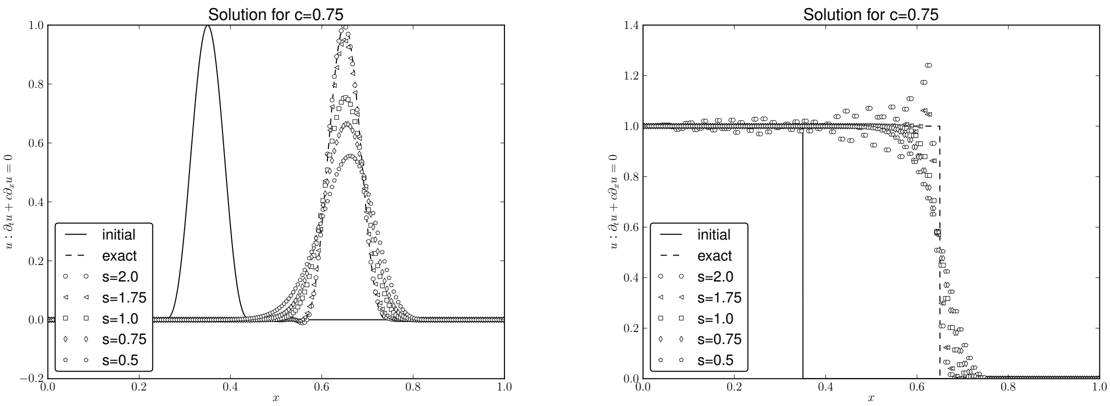

Figure 9.1 – *Transport equation with* $c = 0.75$ *at final time* $T = 0.4$ *(left: smooth solution, right: Riemann problem)*

the monotone finite differences schemes [118]. High order accurate methods like the streamline upwind Petrov-Galerkin (SUPG) method introduced by Hughes and Brooks [19] or like the essentially non-oscillatory (ENO) and the weighted essentially non-oscillatory (WENO) methods initiated by Harten, Engquist, Osher, and Chakravarthy [74] have also a decrease of their convergence rates [86, 126].

9.2.5.2 BURGER'S EQUATION

In this section, the flux φ is taken to simulate Burger's equation $\varphi(\mathrm{u}) = \mathrm{u}^2/2$.

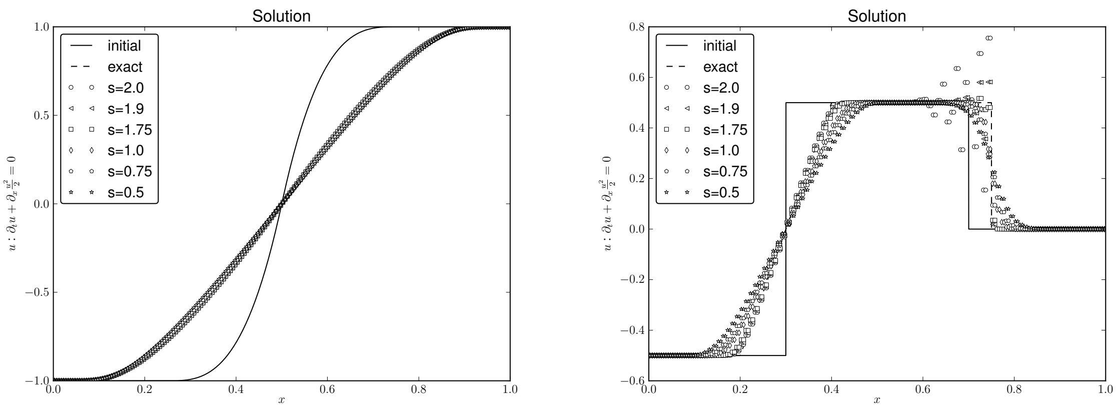

Figure 9.2 – *Burger's equation at final time* $T = 0.2$ *(left: smooth solution, right: discontinuous solution)*

In Fig. 9.2, the left (*r*esp. right) plot shows the initial and the final (at time $T = 0.2$) moment u for several relaxation parameters s for smooth (*r*esp. discontinuous) initial condition. Concerning the maximum principle, the conditions of Prop. 9.2.6 are more complicated. The initial data are chosen in order to have $|\varphi'(\mathrm{u})| \leqslant \lambda$ and we can observe that the principle is fulfilled for $s \in [0, 1]$ and is not for $s > 1$ with the discontinuous solution.

k s	2.000	1.900	1.750	1.000	0.750	0.500
3	1.378e-01	1.378e-01	1.378e-01	1.378e-01	1.378e-01	1.378e-01
4	4.301e-02	4.019e-02	3.878e-02	7.735e-02	1.029e-01	1.344e-01
5	1.416e-02	1.036e-02	1.047e-02	4.100e-02	6.042e-02	8.991e-02
6	4.256e-03	2.441e-03	4.038e-03	2.142e-02	3.334e-02	5.389e-02
7	1.200e-03	8.378e-04	1.836e-03	1.114e-02	1.789e-02	3.033e-02
8	3.172e-04	3.565e-04	8.763e-04	5.698e-03	9.306e-03	1.620e-02
9	8.073e-05	1.655e-04	4.274e-04	2.878e-03	4.743e-03	8.381e-03
10	2.036e-05	7.977e-05	2.111e-04	1.448e-03	2.398e-03	4.271e-03
11	5.142e-06	3.919e-05	1.050e-04	7.270e-04	1.207e-03	2.161e-03
12	1.289e-06	1.942e-05	5.238e-05	3.644e-04	6.061e-04	1.087e-03
13	3.206e-07	9.669e-06	2.616e-05	1.825e-04	3.037e-04	5.456e-04
14	8.019e-08	4.824e-06	1.307e-05	9.131e-05	1.521e-04	2.734e-04
15	2.017e-08	2.410e-06	6.534e-06	4.568e-05	7.610e-05	1.369e-04
16	5.043e-09	1.204e-06	3.267e-06	2.285e-05	3.807e-05	6.850e-05
slope	2.000e+00	1.001e+00	1.000e+00	9.994e-01	9.992e-01	9.988e-01

Table 9.3 – *Burger's equation at final time $T = 0.2$ (smooth solution: error in L^2 norm)*

k s	2.000	1.900	1.750	1.000	0.750	0.500
3	2.216e-01	2.216e-01	2.216e-01	2.216e-01	2.216e-01	2.216e-01
4	6.980e-02	7.162e-02	7.667e-02	1.323e-01	1.616e-01	1.971e-01
5	6.115e-02	6.021e-02	6.318e-02	1.031e-01	1.246e-01	1.555e-01
6	6.144e-02	5.565e-02	5.328e-02	7.651e-02	9.299e-02	1.173e-01
7	5.498e-02	3.606e-02	3.560e-02	5.471e-02	6.796e-02	8.742e-02
8	5.584e-02	1.553e-02	1.163e-02	3.619e-02	4.732e-02	6.312e-02
9	8.526e-02	1.030e-02	1.119e-02	2.506e-02	3.308e-02	4.498e-02
10	6.426e-02	1.220e-02	1.202e-02	1.755e-02	2.283e-02	3.132e-02
11	7.534e-02	8.772e-03	8.165e-03	1.192e-02	1.545e-02	2.130e-02
12	6.869e-02	3.545e-03	2.193e-03	7.612e-03	1.022e-02	1.429e-02
13	7.320e-02	2.403e-03	2.532e-03	5.269e-03	6.969e-03	9.674e-03
14	7.377e-02	3.012e-03	2.930e-03	3.808e-03	4.852e-03	6.611e-03
15	7.302e-02	2.175e-03	2.001e-03	2.645e-03	3.346e-03	4.526e-03
16	7.229e-02	8.734e-04	4.971e-04	1.706e-03	2.254e-03	3.091e-03
slope	⋆⋆⋆	⋆⋆⋆	⋆⋆⋆	6.324e-01	5.700e-01	5.500e-01

Table 9.4 – *Burger's equation at final time $T = 0.2$ (discontinuous solution: error in L^2 norm)*

The smooth initial data has been chosen as a piecewise polynomial function of order three so that an expression of the exact solution can be given. Moreover, this function is increasing so that no shock appears. Its expression reads

$$\mathrm{u}(x+1/2, t=0) = \begin{cases} \operatorname{sign}(x) & \text{for } |x| \geqslant 1/4, \\ \operatorname{sign}(x)\big(1+(4|x|-1)^3\big) & \text{for } |x| \leqslant 1/4. \end{cases}$$

The discontinuous initial data is a piecewise constant function with two discontinuities: the first one at $x = 0.3$ and the second one at $x = 0.7$. The left discontinuity leads to a rarefaction wave whereas the right one leads to a shock wave.

Tbl. 9.3 (*r*esp. Tbl. 9.4) shows the convergence of the L^2-norm for several relaxation parameters when Δx goes to zero for smooth initial condition (*r*esp. discontinuous initial condition). We then verify numerically that the scheme is consistent at order 1 with Burger's equation in the general case and at order 2 if $s = 2$, for smooth solutions. In the case of the discontinuous initial condition, we observe a lower convergence if $s \in [0, 1]$ but no convergence rate if $s > 1$ even if the error seems to be small.

9.3 THE $\mathsf{D}_1\mathsf{Q}_2^n$ SCHEME FOR THE $1-D$ SYSTEM

In this section, we consider the following mono-dimensional hyperbolic system

$$\partial_t \mathrm{u}(t,x) + \partial_x \varphi(\mathrm{u})(t,x) = 0, \qquad t>0,\ x \in \mathbb{R}, \tag{9.19}$$

where the unknown u is a vector of $\mathbb{R}^n$ and the flux φ is a smooth function over $\mathbb{R}^n$, for which the jacobian matrix $\mathrm{d}\varphi(\mathrm{u})$ is diagonalizable for each u, with eigenvalues $\lambda_k(\mathrm{u}) \in \mathbb{R}$, $1 \leqslant k \leqslant n$. For the numerical illustrations, we consider the p-system and the full compressible Euler system ($n = 2$ or 3 in these cases). We propose an extension of the $\mathsf{D}_1\mathsf{Q}_2$ scheme compatible with the framework of the Multiple Relaxation Times lattice Boltzmann Schemes proposed by d'Humière [80].

9.3.1 DESCRIPTION OF THE SCHEME

We use the same notations for the regular lattice $\mathscr{L}$ with mesh size Δx. The time step Δt is linked with the scheme velocity by the relation $\lambda = \Delta x/\Delta t$. Finally, the set of velocities $\mathcal{V}$ is also defined by $\mathcal{V} = (-\lambda, \lambda)$. The $\mathsf{D}_1\mathsf{Q}_2^n$ scheme is then defined by concatenate n $\mathsf{D}_1\mathsf{Q}_2$ schemes coupled through the equilibrium.

Let us introduce the particles distributions vector $\boldsymbol{f} = (f_{1,0}, f_{1,1}, \dots, f_{n,0}, f_{n,1})^{\mathrm{T}}$ and the moments vector $\mathbf{m} = (\mathrm{u}_1, \dots, \mathrm{u}_n, \mathrm{v}_1, \dots, \mathrm{v}_n)^{\mathrm{T}}$. For the sake of readibility, we also define $\mathrm{u} = (\mathrm{u}_1, \dots, \mathrm{u}_n)^{\mathrm{T}}$ and $\mathrm{v} = (\mathrm{v}_1, \dots, \mathrm{v}_n)^{\mathrm{T}}$. The matrix of the moments $\boldsymbol{M}$ then reads

$$\boldsymbol{M} = \begin{pmatrix} 1\ 1 & 0\ 0 & \dots & 0\ 0 \\ 0\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0\ 0 \\ 0\ 0 & \dots & 0\ 0 & 1\ 1 \\ -\lambda\ \lambda & 0\ 0 & \dots & 0\ 0 \\ 0\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0\ 0 \\ 0\ 0 & \dots & 0\ 0 & -\lambda\ \lambda \end{pmatrix}. \tag{9.20}$$

The inverse matrix $\boldsymbol{M}^{-1}$ is not given but can easily be obtained by the concatenatation of n matrices corresponding to the scalar case. The starting point is the density vector $\boldsymbol{f}(x,t)$ in $x \in \mathscr{L}$ at time t, the moments are then computed by

$$\mathbf{m}(x,t) = \boldsymbol{M}\boldsymbol{f}(x,t). \tag{9.21}$$

The relaxation phase in the space of the moments reads

$$\mathrm{u}_k^\star(x,t) = \mathrm{u}_k(x,t), \quad \mathrm{v}_k^\star(x,t) = \mathrm{v}_k(x,t) + s_k(\mathrm{v}_k^{\mathrm{eq}}(x,t) - \mathrm{v}_k(x,t)), \quad 1 \leqslant k \leqslant n, \tag{9.22}$$

where s_k, $1 \leqslant k \leqslant n$, is the k-th relaxation parameter and $\mathrm{v}_k^{\mathrm{eq}}$ the moment at equilibrium that is a function of the vector u. As a consequence, the first moment u is conserved during the relaxation phase. The densities are then computed by

$$\boldsymbol{f}^\star(x,t) = \boldsymbol{M}^{-1}\mathbf{m}^\star(x,t). \tag{9.23}$$

The transport finally reads

$$f_{k,j}(x,t+\Delta t) = f_{k,j}^\star(x - v_j\Delta t, t), \qquad 0 \leqslant j \leqslant 1,\ 1 \leqslant k \leqslant n. \tag{9.24}$$

Concerning the treatment of the boundaries, as the densities of each moment are decoupled, the standard Bouzidi conditions [17] can be applied independently on each moment: for instance, anti-bounce back conditions in order to impose first-order Dirichlet conditions. These simplicity is remarkable in particular for the full compressible Euler system for which the first and the third moments (corresponding to the mass and the energy) are usually coupled with a standard lattice Boltzmann scheme like D_1Q_5 or more elaborated schemes with seven velocities for instance [37, 38].

9.3.2 ASYMPTOTIC ANALYSIS: THE TAYLOR EXPANSION METHOD

In this section, we use the Taylor expansion method to write the system of the equivalent equations as in section 9.2.2. No additional difficulties are involved by the dimension n.

Proposition 9.3.1 (zeroth order)**.** *Defining* $\mathbf{m}^{\mathrm{eq}} = (\mathrm{u}_1,\dots,\mathrm{u}_n,\mathrm{v}_1^{\mathrm{eq}},\dots,\mathrm{v}_n^{\mathrm{eq}})$ *and* $\boldsymbol{f}^{\mathrm{eq}} = \boldsymbol{M}^{-1}\mathbf{m}^{\mathrm{eq}}$*, we have*

$$f_{k,j} = f_{k,j}^{\mathrm{eq}} + \mathcal{O}(\Delta t), \qquad f_{k,j}^\star = f_{k,j}^{\mathrm{eq}} + \mathcal{O}(\Delta t), \qquad 0 \leqslant j \leqslant 1, \quad 1 \leqslant k \leqslant n. \tag{9.25}$$

Proposition 9.3.2 (First order macroscopic equation)**.** *The first moment* $\mathrm{u} = (\mathrm{u}_1,\dots,\mathrm{u}_n)$ *satisfies the partial differential equation*

$$\partial_t \mathrm{u} + \partial_x \mathrm{v}^{\mathrm{eq}} = \mathcal{O}(\Delta t), \tag{9.26}$$

with $\mathrm{v}^{\mathrm{eq}} = (\mathrm{v}_1^{\mathrm{eq}},\dots,\mathrm{v}_n^{\mathrm{eq}})$*. The choice* $\mathrm{v}^{\mathrm{eq}} = \varphi(\mathrm{u})$ *is then done so that* u *satisfies* (9.19) *at order 1.*

We then define the equilibrium default θ_k, $1 \leqslant k \leqslant n$, by using the particular derivatives $\mathrm{d}_t^j = \partial_t + v_j\partial_x$, $0 \leqslant j \leqslant 1$,

$$\theta_k = \sum_{j=0}^{1} v_j\, \mathrm{d}_t^j f_{k,j}^{\mathrm{eq}}, \qquad 1 \leqslant k \leqslant n.$$

The equilibrium default θ_k can then be rewritten into the form

$$\theta_k = \partial_t \mathrm{v}_k^{\mathrm{eq}} + \lambda^2 \partial_x \mathrm{u}_k, \qquad 1 \leqslant k \leqslant n. \tag{9.27}$$

Lemma 9.3.3 (Transition lemma)**.** *The second moment* v *satisfies*

$$\mathrm{v}_k = \mathrm{v}_k^{\mathrm{eq}} - \frac{\Delta t}{s_k}\theta_k + \mathcal{O}(\Delta t^2), \quad \mathrm{v}_k^{\star} = \mathrm{v}_k^{\mathrm{eq}} + \Delta t\Big(1 - \frac{1}{s_k}\Big)\theta_k + \mathcal{O}(\Delta t^2), \quad 1 \leqslant k \leqslant n. \tag{9.28}$$

Moreover, we have

$$f_{k,j}^{\star} - f_{k,j} = \Delta t \, \mathrm{d}_t^j f_{k,j}^{\mathrm{eq}} + \mathcal{O}(\Delta t^2), \quad 0 \leqslant j \leqslant 1, \quad 1 \leqslant k \leqslant n.$$

Proposition 9.3.4 (Second order macroscopic equation)**.** *The first moment* u *satisfies the following system of second-order partial differential equations:*

$$\partial_t \mathrm{u} + \partial_x \varphi(\mathrm{u}) = \Delta t \, \mathfrak{S} \, \partial_x \Big(\big(\lambda^2 \boldsymbol{I}_n - (\mathrm{d}\varphi(\mathrm{u}))^2\big) \partial_x \mathrm{u} \Big) + \mathcal{O}(\Delta t^2), \tag{9.29}$$

with $\mathfrak{S} = \mathrm{diag}(\sigma_1, \dots, \sigma_n)$*,* $\sigma_k = 1/s_k - 1/2$*,* $1 \leqslant k \leqslant n$*, and* $\boldsymbol{I}_n$ *the identity matrix of size* $n \times n$*.*

Let us remark that this system of second-order macroscopic equations (9.29) then contains a diffusion term with a regularization effect if $\sigma_k > 0$ (that is $s_k < 2$), $1 \leqslant k \leqslant n$, and $|\lambda_k(\mathrm{u})| < \lambda$, for $\lambda_k(\mathrm{u})$ eigenvalue of $\mathrm{d}\varphi(\mathrm{u})$.

9.3.3 LINK WITH THE RELAXATION METHOD

Jin and Xin [85] extended the relaxation method to solve hyperbolic systems of conservation laws by forming the linear system with a stiff source term :

$$\begin{cases} \partial_t \mathrm{u}^{\epsilon} + \partial_x \mathrm{v}^{\epsilon} = 0, \\ \partial_t \mathrm{v}^{\epsilon} + A \partial_x \mathrm{u}^{\epsilon} = \dfrac{1}{\epsilon}(\varphi(\mathrm{u}^{\epsilon}) - \mathrm{v}^{\epsilon}), \end{cases} \tag{9.30}$$

where A is a $n \times n$-dimensional matrix.

If all the relaxation parameters s_k, $1 \leqslant k \leqslant n$, are equal to s (BGK type lattice Boltzmann scheme), the $\mathsf{D}_1\mathsf{Q}_2^n$ scheme is then rewritten as a discretization of the relaxation system (9.30). Indeed, denoting $\mathrm{u}_i^n = \mathrm{u}(x_i, t^n)$, $\mathrm{v}_i^n = \mathrm{v}(x_i, t^n)$, $x_i \in \mathscr{L}$ and $t^n = n\Delta t$, relations (9.15, 9.16, 9.17) are satisfied in a vectorial sens. We then reinterpret the scheme $\mathsf{D}_1\mathsf{Q}_2^n$ as a splitting between the relaxation part (9.15) and the hyperbolic part (9.16,9.17). The relaxation part is treated by the explicit Euler method with $\epsilon = \Delta t / s$, and the hyperbolic part by the Lax-Friedrichs method with $A = \lambda^2 \boldsymbol{I}_n$. Moreover, as for the scalar case, the transport phase of the $\mathsf{D}_1\mathsf{Q}_2^n$ treats the hyperbolic part of the relaxation system (9.30) by an upwind scheme in the base of the eigenvectors.

The relaxation proposed by Jin and Xin does not require that A is proportional to $\boldsymbol{I}_n$ (even if this particular case is specifically investigated). On the other hand, the stiff source term corresponding to the relaxation is proportional to $\boldsymbol{I}_n$ when the $\mathsf{D}_1\mathsf{Q}_2^n$ allows different values for the relaxation parameters.

9.3.4 NUMERICAL ILLUSTRATIONS

In this section, we perform numerical illustrations for the p-system and the full Euler compressible equation. The lattice $\mathscr{L}$ is reduced to $[0,1]$ and homogeneous Neumann conditions are added to treat the boundaries. The initial condition is constant over $[0,0.5]$ and $]0.5,1]$ in order to numerically solve the corresponding Riemann problem. We then denote u_{kL} and u_{kR} the left and the right value of the k^{th} moment, so that we have at initial time

$$u_k(0,x) = \begin{cases} u_{kL} & \text{if } x \leqslant 0.5, \\ u_{kR} & \text{if } x > 0.5. \end{cases}$$

The presented numerical results try to cover all the typical cases: the plots and the numerical convergence rates can be extended to all Riemann problems.

9.3.4.1 p-SYSTEM

In this section, we consider the following p-system:

$$\begin{cases} \partial_t u_1 - \partial_x u_2 = 0, \\ \partial_t u_2 - \partial_x p(u_1) = 0, \end{cases} \tag{9.31}$$

where $p(u) = -u^{-\gamma}$, with $\gamma = 2/3$. This system of equations is hyperbolic as $\gamma > 0$ and the eigenvalues of the jacobian matrix are $\pm\sqrt{\gamma}u^{-\frac{\gamma+1}{2}}$.

In Fig. 9.3 (*resp.* Fig. 9.4), the two plots show the initial and the final (at time $T = 0.3$) moments u_1 and u_2 for several relaxation parameters s_1, s_2, where the initial conditions are chosen in order to obtain 1-shock, 2-rarefaction waves (*resp.* 1-rarefaction, 2-shock waves). For the numerical values, we have the velocity of the scheme $\lambda = 1$, the number of points $N = 200$, and the initial condition given by

- for the 1-shock, 2-rarefaction: $u_{1L} = 1.5$, $u_{2L} = 1.25$, $u_{1R} = 1.0$, $u_{2R} = 1.0$,
- for the 1-rarefaction, 2-shock: $u_{1L} = 1.0$, $u_{2L} = 1.0$, $u_{1R} = 1.5$, $u_{2R} = 1.25$.

The Tbl. 9.5 (*resp.* Tbl. 9.6) shows the convergence of the L^2-norm for several relaxation parameters s_1, s_2 when Δx goes to zero for the 1-shock, 2-rarefaction waves (*resp.* 1-rarefaction, 2-shock waves). Each line corresponds to the integer $k \in \{3,\dots,16\}$ with $\Delta x = 2^{-k}$. Essentially, we observe a convergence at order 0.5 due to the discontinuity of the solution. In the case of 1-rarefaction, 2-rarefaction waves (the solution is then continuous for $t > 0$), the same investigation yields to a higher order, between 0.64 and 0.8 depending on the relaxation parameters.

9.3.4.2 FULL COMPRESSIBLE EULER SYSTEM

In this section, the $D_1Q_2^n$ scheme is tested to simulate the mono-dimensional Euler equations

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0, \\ \partial_t E + \partial_x(Eu + pu) = 0, \end{cases} \tag{9.32}$$

where ρ is the mass, u the velocity, $E = \rho u^2 + p/(\gamma-1)$ the energy, and p the pressure. The Euler equations can then be viewed as a conservative hyperbolic system in the variable $u_1 = \rho$, $u_2 = \rho u$, and $u_3 = E$. For the numerical simulations, the test case is the Sod shock tube ($\rho_L = 1.0$, $p_L = 1.0$, $u_L = 0.0$, $\rho_R = 0.125$, $p_R = 0.1$, $u_R = 0.0$), γ is taken to 1.4, the number of points $N = 800$, and the scheme velocity is $\lambda = 3.0$.

s_1	0.500	1.000	1.500	1.900	0.500	1.000	1.500
k s_2	0.500	1.000	1.500	1.900	1.000	0.500	1.000
3	1.527e-01	1.428e-01	1.379e-01	1.378e-01	1.497e-01	1.459e-01	1.396e-01
4	1.057e-01	9.754e-02	1.007e-01	1.154e-01	1.030e-01	1.012e-01	9.777e-02
5	9.398e-02	7.297e-02	6.757e-02	7.972e-02	8.562e-02	8.371e-02	6.930e-02
6	7.163e-02	4.956e-02	3.718e-02	5.121e-02	6.313e-02	6.259e-02	4.366e-02
7	5.801e-02	4.057e-02	3.138e-02	4.426e-02	5.111e-02	5.102e-02	3.605e-02
8	4.754e-02	3.313e-02	2.520e-02	3.552e-02	4.177e-02	4.158e-02	2.925e-02
9	3.697e-02	2.376e-02	1.496e-02	1.721e-02	3.177e-02	3.171e-02	1.986e-02
10	2.859e-02	1.803e-02	1.274e-02	1.776e-02	2.425e-02	2.418e-02	1.534e-02
11	2.118e-02	1.287e-02	9.210e-03	1.192e-02	1.764e-02	1.763e-02	1.098e-02
12	1.520e-02	8.813e-03	5.519e-03	6.085e-03	1.246e-02	1.246e-02	7.262e-03
13	1.083e-02	6.426e-03	4.486e-03	6.092e-03	8.899e-03	8.889e-03	5.436e-03
14	7.638e-03	4.376e-03	2.539e-03	2.883e-03	6.237e-03	6.233e-03	3.553e-03
15	5.402e-03	3.088e-03	1.769e-03	2.052e-03	4.408e-03	4.404e-03	2.502e-03
16	3.816e-03	2.178e-03	1.226e-03	1.500e-03	3.112e-03	3.108e-03	1.760e-03
slope	5.014e-01	5.035e-01	5.288e-01	4.519e-01	5.021e-01	5.027e-01	5.073e-01

s_1	1.000	1.900	1.000	0.500	1.500	1.500	1.900
k s_2	1.500	1.000	1.900	1.500	0.500	1.900	1.500
3	1.412e-01	1.397e-01	1.409e-01	1.481e-01	1.427e-01	1.376e-01	1.380e-01
4	9.755e-02	9.936e-02	9.863e-02	1.025e-01	1.014e-01	1.052e-01	1.056e-01
5	6.961e-02	6.835e-02	6.861e-02	8.253e-02	8.053e-02	6.968e-02	6.974e-02
6	4.346e-02	4.156e-02	4.100e-02	5.978e-02	5.937e-02	3.790e-02	3.841e-02
7	3.581e-02	3.443e-02	3.392e-02	4.836e-02	4.841e-02	3.210e-02	3.245e-02
8	2.928e-02	2.756e-02	2.757e-02	3.939e-02	3.918e-02	2.468e-02	2.471e-02
9	1.982e-02	1.805e-02	1.795e-02	2.960e-02	2.956e-02	1.372e-02	1.385e-02
10	1.539e-02	1.417e-02	1.424e-02	2.248e-02	2.239e-02	1.244e-02	1.241e-02
11	1.096e-02	1.023e-02	1.019e-02	1.625e-02	1.624e-02	8.956e-03	8.980e-03
12	7.241e-03	6.595e-03	6.543e-03	1.141e-02	1.142e-02	5.173e-03	5.222e-03
13	5.441e-03	5.023e-03	5.027e-03	8.164e-03	8.153e-03	4.348e-03	4.346e-03
14	3.552e-03	3.173e-03	3.163e-03	5.698e-03	5.695e-03	2.207e-03	2.224e-03
15	2.502e-03	2.227e-03	2.223e-03	4.025e-03	4.022e-03	1.511e-03	1.521e-03
16	1.762e-03	1.560e-03	1.561e-03	2.841e-03	2.836e-03	1.014e-03	1.017e-03
slope	5.055e-01	5.137e-01	5.098e-01	5.027e-01	5.037e-01	5.757e-01	5.798e-01

Table 9.5 – *p-system at final time $T = 0.3$ (1-shock, 2-rarefaction: error in L^2 norm)*

s_1	0.500	1.000	1.500	1.900	0.500	1.000	1.500
k s_2	0.500	1.000	1.500	1.900	1.000	0.500	1.000
3	1.105e-01	1.016e-01	9.836e-02	1.003e-01	1.092e-01	1.030e-01	9.895e-02
4	1.005e-01	8.795e-02	8.294e-02	8.454e-02	9.734e-02	9.316e-02	8.549e-02
5	8.301e-02	6.054e-02	4.975e-02	5.020e-02	7.503e-02	7.365e-02	5.544e-02
6	6.483e-02	4.451e-02	3.236e-02	2.993e-02	5.678e-02	5.661e-02	3.924e-02
7	4.948e-02	3.265e-02	2.172e-02	1.831e-02	4.262e-02	4.283e-02	2.807e-02
8	3.807e-02	2.425e-02	1.513e-02	1.113e-02	3.244e-02	3.253e-02	2.040e-02
9	2.870e-02	1.753e-02	1.034e-02	6.624e-03	2.408e-02	2.416e-02	1.448e-02
10	2.114e-02	1.243e-02	7.105e-03	4.193e-03	1.747e-02	1.753e-02	1.015e-02
11	1.519e-02	8.681e-03	4.883e-03	2.745e-03	1.240e-02	1.244e-02	7.032e-03
12	1.071e-02	6.009e-03	3.363e-03	1.755e-03	8.662e-03	8.684e-03	4.852e-03
13	7.445e-03	4.150e-03	2.312e-03	1.158e-03	5.997e-03	6.011e-03	3.349e-03
14	5.149e-03	2.869e-03	1.586e-03	7.763e-04	4.146e-03	4.153e-03	2.312e-03
15	3.560e-03	1.978e-03	1.081e-03	5.688e-04	2.867e-03	2.872e-03	1.587e-03
16	2.460e-03	1.350e-03	7.328e-04	3.875e-04	1.976e-03	1.979e-03	1.078e-03
slope	5.332e-01	5.505e-01	5.607e-01	5.540e-01	5.373e-01	5.373e-01	5.575e-01

s_1	1.000	1.900	1.000	0.500	1.500	1.500	1.900
k s_2	1.500	1.000	1.900	1.500	0.500	1.900	1.500
3	1.010e-01	1.007e-01	1.011e-01	1.087e-01	1.004e-01	9.851e-02	1.002e-01
4	8.547e-02	8.633e-02	8.467e-02	9.583e-02	9.263e-02	8.289e-02	8.331e-02
5	5.515e-02	5.375e-02	5.306e-02	7.179e-02	7.116e-02	4.854e-02	4.900e-02
6	3.906e-02	3.697e-02	3.654e-02	5.364e-02	5.374e-02	2.979e-02	3.013e-02
7	2.783e-02	2.593e-02	2.547e-02	3.988e-02	4.031e-02	1.885e-02	1.916e-02
8	2.032e-02	1.851e-02	1.836e-02	3.016e-02	3.035e-02	1.249e-02	1.259e-02
9	1.443e-02	1.297e-02	1.287e-02	2.222e-02	2.235e-02	8.136e-03	8.207e-03
10	1.011e-02	9.021e-03	8.952e-03	1.600e-02	1.610e-02	5.461e-03	5.512e-03
11	7.007e-03	6.227e-03	6.183e-03	1.130e-02	1.136e-02	3.712e-03	3.746e-03
12	4.842e-03	4.287e-03	4.271e-03	7.869e-03	7.900e-03	2.540e-03	2.553e-03
13	3.342e-03	2.958e-03	2.945e-03	5.441e-03	5.461e-03	1.727e-03	1.738e-03
14	2.308e-03	2.037e-03	2.032e-03	3.762e-03	3.772e-03	1.178e-03	1.182e-03
15	1.583e-03	1.395e-03	1.389e-03	2.600e-03	2.608e-03	8.064e-04	8.126e-04
16	1.075e-03	9.464e-04	9.415e-04	1.788e-03	1.793e-03	5.473e-04	5.525e-04
slope	5.581e-01	5.595e-01	5.609e-01	5.403e-01	5.401e-01	5.591e-01	5.565e-01

Table 9.6 – *p-system at final time $T = 0.3$ (1-rarefaction, 2-shock: error in L^2 norm)*

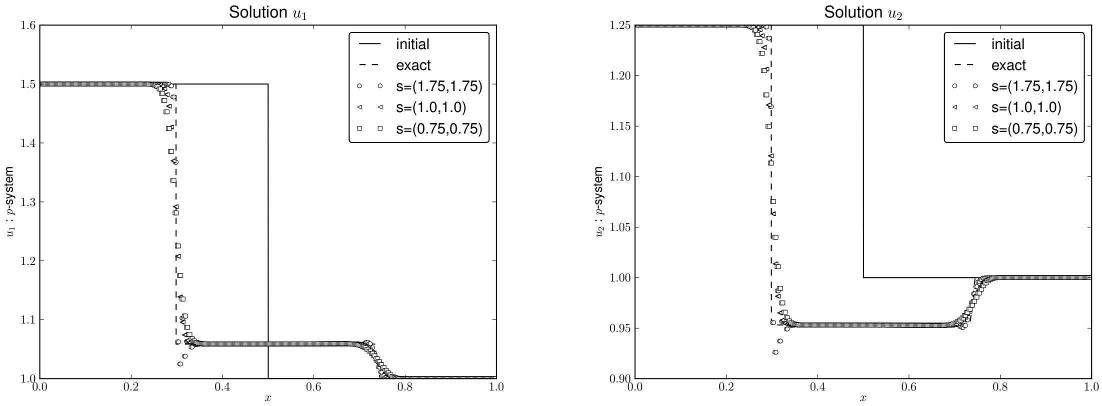

Figure 9.3 – *p-system at final time $T = 0.3$ (left:* u_1*, right:* u_2*) Riemann problem corresponding to* 1*-shock,* 2*-rarefaction*

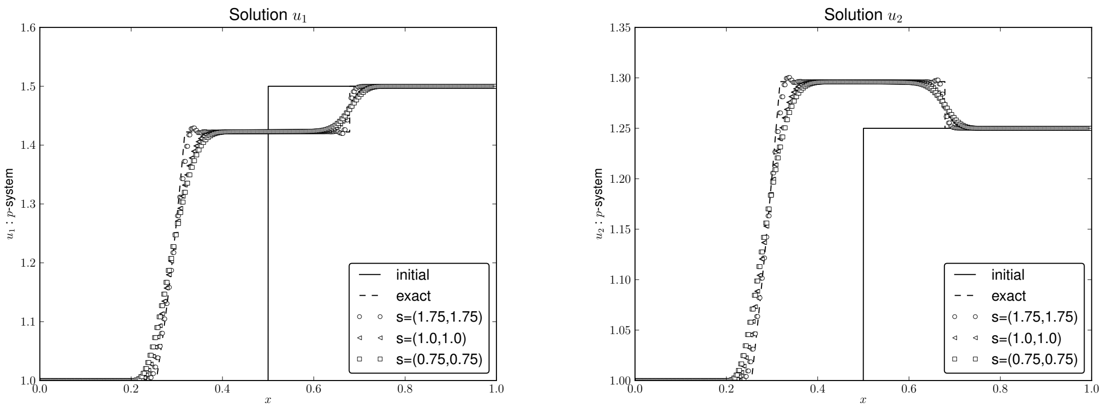

Figure 9.4 – *p-system at final time $T = 0.3$ (left:* u_1*, right:* u_2*) Riemann problem corresponding to* 1*-rarefaction,* 2*-shock*

In Fig. 9.5, the mass ρ is plotted at time $T = 0.2$ for several relaxation parameters: $s_1 = s_2 = s_3 = s$, with $s \in \{0.5, 0.75, 1.0, 1.5, 1.75, 1.9\}$. The numerical diffusion is as expected higher for small relaxation parameters, whereas numerical oscillations are observed for large relaxation parameters (after the shock wave and also after the contact discontinuity).

Numerical convergence results in L^2 norm are given in Tbl. 9.7 for several relaxation parameters s_1, s_2, and s_3 when Δx goes to zero, each line corresponding to the integer $k \in \{3, \dots, 16\}$ with $\Delta x = 2^{-k}$. The error in L^2 norm goes to zero with an order that depends on the relaxation parameters. The convergence seems to be quicker when the three relaxation parameters move nearer to 2, the order approaching 0.5.

In Fig. 9.6, the mass, the velocity, and the pressure are plotted, the exact solution with a solid line and the approximate one with a dashed line. The parameters of this simulation are $N = 1000$, $T = 0.14$, $s_1 = 1.9$, $s_2 = 1.5$, and $s_3 = 1.4$. It appears as a good compromise between numerical diffusion and oscillations in the area of discontinuities.

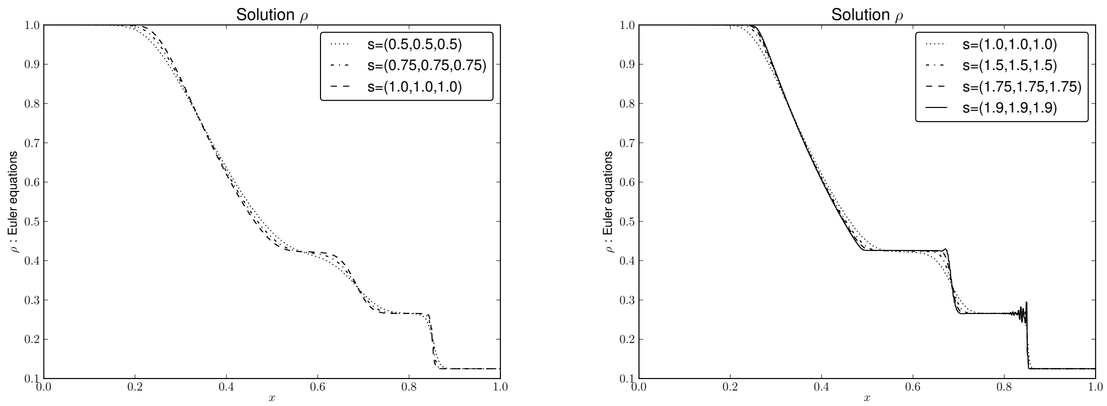

Figure 9.5 – *Euler system at final time $T = 0.2$ (left: $s \leqslant 1$, right: $s \geqslant 1$) Sod Shock Tube*

	s_1	1.900	0.500	1.000	1.500	1.900	1.990
	s_2	1.500	0.500	1.000	1.500	1.900	1.990
k	s_3	1.400	0.500	1.000	1.500	1.900	1.990
3		1.297e-01	1.709e-01	1.278e-01	1.133e-01	1.297e-01	1.361e-01
4		9.789e-02	1.242e-01	8.141e-02	7.408e-02	8.542e-02	9.103e-02
5		6.229e-02	8.670e-02	5.454e-02	4.380e-02	4.041e-02	4.230e-02
6		4.795e-02	6.764e-02	4.643e-02	3.445e-02	2.644e-02	3.112e-02
7		3.136e-02	5.136e-02	3.691e-02	2.528e-02	1.639e-02	2.358e-02
8		2.205e-02	4.132e-02	2.951e-02	1.957e-02	1.377e-02	2.085e-02
9		1.421e-02	3.369e-02	2.229e-02	1.416e-02	9.334e-03	1.944e-02
10		1.008e-02	2.645e-02	1.651e-02	1.023e-02	6.232e-03	1.591e-02
11		7.191e-03	1.974e-02	1.220e-02	7.995e-03	5.324e-03	1.173e-02
12		5.129e-03	1.452e-02	9.122e-03	6.169e-03	4.011e-03	8.173e-03
13		3.903e-03	1.080e-02	7.035e-03	4.876e-03	3.069e-03	6.121e-03
14		3.011e-03	8.179e-03	5.547e-03	3.980e-03	2.531e-03	4.304e-03
15		2.443e-03	6.363e-03	4.484e-03	3.301e-03	2.163e-03	3.177e-03
16		1.968e-03	5.064e-03	3.665e-03	2.738e-03	1.769e-03	2.259e-03
slope		3.119e-01	3.296e-01	2.908e-01	2.699e-01	2.901e-01	4.924e-01

Table 9.7 – *Sod shock tube at final time $T = 0.1$ (error in L^2 norm)*

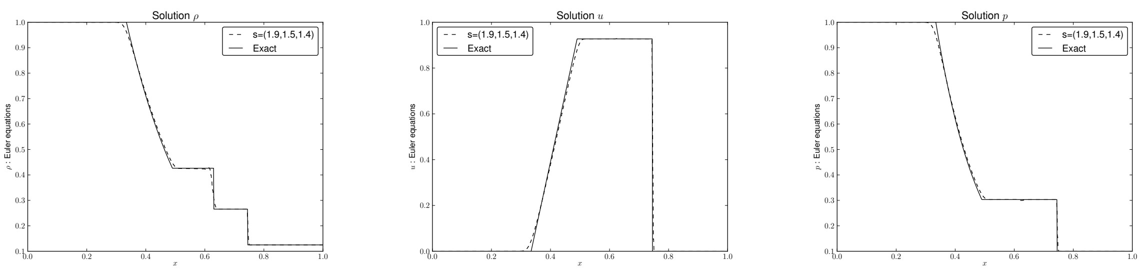

Figure 9.6 – *Euler system at final time $t = 0.14$ Sod Shock Tube*

9.4 CONCLUSION

In this paper, a new Lattice Boltzmann scheme is introduced in order to simulate mono-dimensional hyperbolic systems. This scheme is described in the framework of d'Humières and related to the relaxation method proposed by Jin and Xin. The equivalent conservation equations are given up to the second order and stability conditions are investigated in the scalar case. Numerical illustrations are produced for the scalar advection, Burger's equation, the p-system, and Euler's equations.

Let us finally remark that the method can be generalized to any other elementary schemes: the $\mathsf{D}_1\mathsf{Q}_2$ scheme can be replaced by the $\mathsf{D}_1\mathsf{Q}_3$ for instance. However, using more velocities increases the size of the systems and does not necessarily improve the accuracy.

9.A TAYLOR EXPANSION METHOD FOR THE SCALAR CASE

The Taylor expansion method consists in expanding the distribution functions with respect to the small parameter Δt. Considering Eq. (9.8), we have

$$f_j + \Delta t \partial_t f_j + \tfrac{1}{2}\Delta t^2 \partial_{tt} f_j = f_j^\star - v_j \Delta t \partial_x f_j^\star + \tfrac{1}{2} {v_j}^2 \Delta t^2 \partial_{xx} f_j^\star + \mathcal{O}(\Delta t^3), \qquad 0 \leqslant j \leqslant 1, \tag{9.33}$$

where the variables $x \in \mathscr{L}$ and t have been removed for readability. As the relaxation phase is written in the space of moments, we immediately take the moments of order 0 and 1 of Eq. (9.33) by summing over j after multiplication by ${v_j}^0$ or ${v_j}^1$:

$$\mathrm{u} + \Delta t \partial_t \mathrm{u} + \tfrac{1}{2}\Delta t^2 \partial_{tt}\mathrm{u} = \mathrm{u}^\star - \Delta t \partial_x \mathrm{v}^\star + \tfrac{\lambda^2}{2}\Delta t^2 \partial_{xx}\mathrm{u}^\star + \mathcal{O}(\Delta t^3), \qquad 0 \leqslant j \leqslant 1, \tag{9.34}$$

$$\mathrm{v} + \Delta t \partial_t \mathrm{v} + \tfrac{1}{2}\Delta t^2 \partial_{tt}\mathrm{v} = \mathrm{v}^\star - \lambda^2 \Delta t \partial_x \mathrm{u}^\star + \tfrac{\lambda^2}{2}\Delta t^2 \partial_{xx}\mathrm{v}^\star + \mathcal{O}(\Delta t^3), \qquad 0 \leqslant j \leqslant 1. \tag{9.35}$$

We then consider Eqs. (9.34) and (9.35) at order k for $0 \leqslant k \leqslant 2$.

• Eq. (9.34) at zeroth-order does not give information: as the first moment u is conserved during the relaxation phase, $\mathrm{u} = \mathrm{u}^\star$.

• Eq. (9.35) at zeroth-order reads $\mathrm{v} = \mathrm{v}^\star + \mathcal{O}(\Delta t)$. Using Eq. (9.6) $\mathrm{v}^\star = \mathrm{v} + s(\mathrm{v}^{\mathrm{eq}} - \mathrm{v})$, it yields to Eq. (9.9)

$$\mathrm{v} = \mathrm{v}^{\mathrm{eq}} + \mathcal{O}(\Delta t), \qquad \mathrm{v}^\star = \mathrm{v}^{\mathrm{eq}} + \mathcal{O}(\Delta t), \tag{9.9}$$

as the relaxation parameter s is considered as a constant.

• Eq. (9.34) at first-order (after division by Δt) can be rewritten in the form

$$\partial_t \mathrm{u} + \partial_x \mathrm{v}^{\mathrm{eq}} = \mathcal{O}(\Delta t), \tag{9.10}$$

by using (9.9).

• Eq. (9.35) at first-order reads

$$\mathrm{v}^\star - \mathrm{v} = \Delta t (\partial_t \mathrm{v}^{\mathrm{eq}} + \lambda^2 \partial_x \mathrm{u}) + \mathcal{O}(\Delta t^2) = \Delta t\, \theta + \mathcal{O}(\Delta t^2),$$

by using the definition of the equilibrium default (9.11). Combining this equation with Eq. (9.6) then yields

$$\mathrm{v} = \mathrm{v}^{\mathrm{eq}} - \frac{\Delta t}{s}\theta + \mathcal{O}(\Delta t^2), \qquad \mathrm{v}^\star = \mathrm{v}^{\mathrm{eq}} + \Delta t\Big(1 - \frac{1}{s}\Big)\theta + \mathcal{O}(\Delta t^2). \tag{9.12}$$

• Eq. (9.34) at second-order reads

$$\partial_t \mathrm{u} + \partial_x \mathrm{v}^{\mathrm{eq}} = -\partial_x(\mathrm{v}^\star - \mathrm{v}^{\mathrm{eq}}) + \tfrac{1}{2}\Delta t \left[-\partial_{tt}\mathrm{u} + \lambda^2 \partial_{xx}\mathrm{u}\right] + \mathcal{O}(\Delta t^2).$$

The derivation of Eq. (9.10) over t gives

$$-\partial_{tt}\mathrm{u} + \lambda^2 \partial_{xx}\mathrm{u} = \partial_x \theta + \mathcal{O}(\Delta t),$$

so replacing $\mathrm{v}^\star - \mathrm{v}^{\mathrm{eq}}$ by its expression (9.12) yields

$$\partial_t \mathrm{u} + \partial_x \mathrm{v}^{\mathrm{eq}} = \Delta t\, \sigma\, \partial_x \theta + \mathcal{O}(\Delta t^2).$$

As v^{eq} is a function of u, $\mathrm{v}^{\mathrm{eq}} = \varphi(\mathrm{u})$, we have

$$\theta = \left[\lambda^2 - \left(\varphi'(\mathrm{u})\right)^2\right]\partial_x \mathrm{u} + \mathcal{O}(\Delta t),$$

and we obtain the second-order macroscopic equation

$$\partial_t \mathrm{u} + \partial_x \varphi(\mathrm{u}) = \Delta t\, \sigma\, \partial_x \left(\left(\lambda^2 - \left(\varphi'(\mathrm{u})\right)^2\right)\partial_x \mathrm{u}\right) + \mathcal{O}(\Delta t^2). \tag{9.13}$$

CHAPTER 10

STRONG NONLINEAR WAVES WITH VECTORIAL LATTICE BOLTZMANN SCHEMES

In this chapter [1], we show that a hyperbolic system with a mathematical entropy can be discretized with vectorial lattice Boltzmann schemes using the methodology of kinetic representation of the dual entropy. We test this approach for the shallow water equations in one and two spatial dimensions. We obtain interesting results for a shock tube, reflection of a shock wave and non-stationary two-dimensional propagation. This contribution shows the ability of vectorial lattice Boltzmann schemes to simulate strong nonlinear waves in non-stationary situations.

10.1 INTRODUCTION

The computation of discrete shock waves with lattice Boltzmann approaches began with viscous Burgers approximations in the framework of lattice-gas automata (see Boghosian and Levermore[10] and Elton *et al.* [54]). With the lattice Boltzmann methods described *e.g.* by Lallemand and Luo[95], the first tentative results were proposed by d'Humières[80] and Alexander *et al.* [3] among others. A D1Q2 entropic scheme for the one-dimensional viscous Burgers equation has been developed by Boghosian *et al.* [11]. The extension to gas-dynamic equations, and in particular to shock tube problems, is studied in the works of Philippi *et al.* [111], Nie, Shan and Chen [106], Karlin and Asinari [90], and Chikatamarla and Karlin [33].

In this contribution, we test the ability of lattice Boltzmann schemes to approach weak entropy solutions of hyperbolic equations. It is well known that a first-order hyperbolic equation exhibits shock waves. In order to enforce uniqueness, the notion of mathematical entropy has been proposed by Godunov[70] and Friedrichs and Lax[58]. A mathematical entropy is a strictly convex function of the conserved variables satisfying *ad hoc* differential constraints to ensure a complementary conservation law for regular solutions (see, *e.g.*, our book with Després[39]). The gradient of the entropy defines the so-called "entropy variables." The Legendre-Fenchel-Moreau duality for convex functions allows us to define the dual of the entropy, which is a convex function of the entropy variables.

We start from the mathematical framework developed by Bouchut[14], making the link between the finite-volume method and kinetic models in the framework of the BGK approximation. The key notion is the representation of the dual entropy with the help of convex functions associated with the discrete velocities of the lattice. If we suppose that a single distribution of particles is present, our previous contribution[47] shows that Burgers equation can be simulated in this way. We have also shown that the approach can be extended to the nonlinear wave equation but is not compatible with the system of shallow water equations.

[1] This contribution has been originally published in [48].

In Section 1, we develop vectorial lattice Boltzmann schemes with a kinetic representation of the dual entropy. This framework is applied in Section 2 for the approximation of one-dimensional shallow water equations, and in Section 3 for the two-dimensional case. Stationary and non-stationary two-dimensional simulations are presented in Section 4.

10.2 DUAL ENTROPY VECTORIAL LATTICE BOLTZMANN SCHEMES

In order to treat complex physics with particle-like methods, a classical idea is to multiply the number of particle distributions, as proposed by Khobalatte and Perthame[92], Shan and Chen[122], Bouchut[13], Dellar[36], and Wang *et al.* [132]. We follow here the idea of a dual entropy decomposition with vectorial particle distributions, as proposed by Bouchut[14]. We consider a hyperbolic system composed of N conservation laws with space described by points in $x \in \mathbb{R}^d$. The unknowns are the conserved variables $W \in \mathbb{R}^N$ (*i.e.* $W^k \in \mathbb{R}$). The nonlinear physical fluxes : $F_\alpha(W) \in \mathbb{R}^N$ (with $1 \leqslant \alpha \leqslant d$) are given regular functions. The system is of first-order:

$$\partial_t W^k + \sum_{\alpha=1}^{d} \partial_\alpha F_\alpha^k(W) = 0\,, \quad 1 \leqslant k \leqslant N. \tag{10.1}$$

We suppose that a mathematical entropy $\eta(W)$ is given, with associated entropy fluxes $\zeta_\alpha(W)$ for $0 \leqslant \alpha \leqslant d$:

$$\mathrm{d}\zeta_\alpha(W) \equiv \mathrm{d}\eta(W) \bullet \mathrm{d}F_\alpha(W)\,.$$

The entropy variables $\varphi_k \equiv \dfrac{\partial \eta(W)}{\partial W^k}$ are defined as the jacobian of the entropy:

$$\mathrm{d}\eta(W) \equiv \sum_{k=1}^{N} \varphi_k \,\mathrm{d}W^k.$$

The dual entropy $\eta^*(\varphi)$ and the so-called "dual entropy fluxes" $\zeta^*_\alpha(\varphi)$ satisfy

$$\eta^*(\varphi) = \varphi \bullet W - \eta(W)\,, \quad \zeta^*_\alpha(\varphi) \equiv \varphi \bullet F_\alpha(W) - \zeta_\alpha(W)\,. \tag{10.2}$$

They can be differentiated without difficulty (see *e.g.* [39]):

$$\mathrm{d}\eta^*(\varphi) \equiv \sum_k \mathrm{d}\varphi_k \, W^k\,, \qquad \mathrm{d}\zeta^*_\alpha(\varphi) \equiv \sum_k \mathrm{d}\varphi_k \, F^k_\alpha(W)\,.$$

- With Bouchut[14], we introduce N particle distributions f_j^k (for $1 \leqslant k \leqslant N$) and q velocities ($0 \leqslant j \leqslant q-1$). The conserved moments W^k are simply the first discrete integrals of these distributions:

$$W^k = \sum_{j=0}^{q-1} f_j^k\,, \quad 1 \leqslant k \leqslant N. \tag{10.3}$$

We suppose that the particle distributions f_j^k are solutions of the Boltzmann equations with discrete velocities:

$$\partial_t f_j^k + v_j^\alpha \partial_\alpha f_j^k = Q_j^k\,, \quad 0 \leqslant j \leqslant q-1\,, \qquad 1 \leqslant k \leqslant N$$

We suppose $\sum_j Q_j^k = 0$ in order to enforce the conservation laws (10.1). The non-equilibrium fluxes take the natural form $\Phi_\alpha^k \equiv \sum_j v_j^\alpha f_j^k$ and we have a system of N conservation laws:

$$\partial_t W^k + \sum_\alpha \partial_\alpha \Phi_\alpha^k = 0\,, \quad 1 \leqslant k \leqslant N\,.$$

In the following, we use the term "Perthame-Bouchut hypothesis" to refer to the fact that the dual mathematical entropy $\eta^*(\varphi)$ can be is decomposed into q scalar potentials, h_j^*. The potentials h_j^* are supposed to be regular convex functions of the entropy variables φ, and satisfy the two identities

$$\sum_{j=0}^{q-1} h_j^*(\varphi) \equiv \eta^*(\varphi)\,, \quad \sum_{j=0}^{q-1} v_j^\alpha\, h_j^*(\varphi) \equiv \zeta_\alpha^*(\varphi)\,, \quad \forall \varphi\,. \tag{10.4}$$

The equilibrium fluxes $(f^{\mathrm{e}q})_j^k$ are easy to derive from the potentials h_j^*:

$$\left(f^{\mathrm{e}q}\right)_j^k = \frac{\partial h_j^*}{\partial \varphi_k}\,, \quad \sum_{j=0}^{q-1} \left(f^{\mathrm{e}q}\right)_j^k = W^k\,, \quad 1 \leqslant k \leqslant N\,.$$

- We introduce the Legendre dual of the convex potentials h_j^*:

$$h_j(f_j\hat{\mathrm{A}}^1, f_j^2, \ldots, f_j^N) \equiv \sup_\varphi \Big(\big[\sum_{k=1}^N \varphi_k f_j^k \big] - h_j^*(\varphi) \Big)\,, \quad 0 \leqslant j \leqslant q-1\,.$$

We observe that each function $h_j(\bullet)$ is a convex function of N variables. The so-called "microscopic entropy" $H(f)$ can now be defined according to

$$H(f) \equiv \sum_{j=0}^{q-1} h_j(f_j^1, f_j^2, \ldots, f_j^N)\,.$$

This is a convex function in the domain where the h_j's are convex.

- We can establish a "H-theorem" for the continuous dynamics relative to time and space in a way similar to the maximal entropy approach developed by Karlin and his co-workers[91]. Under a BGK-type hypothesis

$$Q_j^k \equiv \frac{1}{\tau} \big((f^{\mathrm{e}q})_j^k - f_j^k \big)$$

we have

$$\partial_t H(f) + \sum_\alpha \partial_\alpha \Big(\sum_j v_j^\alpha\, h_j(f_j^1, f_j^2, \ldots, f_j^N) \Big) \leqslant 0\,.$$

To establish this result, we derive the microscopic entropy relative to time:

$$\frac{\partial H}{\partial t} = \sum_{jk} \frac{\partial h_j}{\partial f_j^k} \frac{\partial f_j^k}{\partial t} = \sum_{jk} \frac{\partial h_j}{\partial f_j^k} Q_j^k - \sum_{jk} \frac{\partial h_j}{\partial f_j^k} v_j^\alpha \partial_\alpha f_j^k = \sum_{jk} \frac{\partial h_j}{\partial f_j^k} Q_j^k - \partial_\alpha \Big(\sum_{j=0}^{q-1} v_j^\alpha h_j \Big).$$

Then

$$\frac{\partial H}{\partial t} + \partial_\alpha \big(\sum_j v_j^\alpha \, h_j \big) = \frac{1}{\tau} \sum_{jk} \frac{\partial h_j}{\partial f^k} (f_j^k) \, [\, (f^{\rm eq})_j^k - f_j^k \,]$$
$$\leq \frac{1}{\tau} \sum_{jk} \frac{\partial h_j}{\partial f_j^k} (f_j^{\rm eq}) \, [(f^{\rm eq})_j^k - f_j^k] \text{ by convexity of the potentials } h_j .$$

This last expression is equal to $\frac{1}{\tau} \sum_{jk} \varphi_k [(f^{\rm eq})_j^k - f_j^k]$ due to Legendre duality:

$$\frac{\partial h_j}{\partial f_j^k} (f^{\rm eq}) = \varphi_k \,.$$

In consequence,

$$\frac{\partial H}{\partial t} + \partial_\alpha \big(\sum_j v_j^\alpha \, h_j \big) \leq \sum_k \varphi_k \sum_j \, [(f^{\rm eq})_j^k - f_j^k] = 0$$

by construction of the values $f^{\rm eq}$ in equilibrium. The H-theorem is thereby proven. □

10.3 “D1Q3Q2” LATTICE BOLTZMANN SCHEME FOR SHALLOW WATER

We apply the previous ideas to the shallow-water equations in one spatial dimension

$$\partial_t \rho + \partial_x q = 0 , \qquad \partial_t q + \partial_x \Big(\frac{q^2}{\rho} + \frac{p_0}{\rho_0^\gamma} \, \rho^\gamma \Big) = 0 ,$$

Velocity u, pressure p and sound velocity $c > 0$ are given by the expressions:

$$u \equiv \frac{q}{\rho} , \quad p \equiv \frac{p_0}{\rho_0^\gamma} \rho^\gamma , \quad c^2 \equiv \frac{\gamma \, p}{\rho} = \gamma \, \frac{p_0}{\rho_0^\gamma} \, \rho^{\gamma - 1} .$$

The entropy η and the entropy flux ζ can be determined explicitly without difficulty (see *e.g.* [47]):

$$\eta = \frac{1}{2} \rho \, u^2 + \frac{p}{\gamma - 1} , \quad \zeta = \eta \, u + p \, u$$

Then the entropy variables $\varphi = (\theta \equiv \partial_\rho \eta, \, \beta \equiv \partial_q \eta)$ can be related to the usual ones:

$$\theta = \frac{c^2}{\gamma - 1} - \frac{u^2}{2} , \quad \beta = u .$$

Thanks to (10.2), the dual entropy η^* and the dual entropy flux ζ^* can be worked out explicitly: $\eta^* = p$ and $\zeta^* = p \, u$. We observe that

$$\eta^* = K \Big(\theta + \frac{\beta^2}{2} \Big)^2 = p , \, \zeta^* = K \beta \Big(\theta + \frac{\beta^2}{2} \Big)^2 = p \, u , \, with \, K = k \Big(\frac{\gamma - 1}{\gamma \, k} \Big)^{\frac{\gamma}{\gamma - 1}} .$$

- We model this system with a kinetic approach and a D1Q3 stencil. We have to find the particle components of the entropy variables, *id est* the (still unknown) convex functions h_j^* satisfing the Perthame-Bouchut hypothesis (10.4), that now can be written in the form:

$$h_+^* (\theta, \beta) + h_0^* (\theta, \beta) + h_-^* (\theta, \beta) = p , \quad \lambda \, h_+^* (\theta, \beta) - \lambda \, h_-^* (\theta, \beta) = p \, u , \tag{10.5}$$

where $\lambda \equiv \frac{\Delta x}{\Delta t}$ is the numerical velocity of the mesh. We use a simple quadratic function as in our previous contribution[47]. We suggest that when $\gamma = 2$:

$$h_0^* = h_0^*(\theta) = \frac{a}{2} K \theta^2 , \tag{10.6}$$

with the introduction of a parameter a that has to be made precise for real numerical computations. With this choice (10.6), the resolution of the system (10.5) with unknowns $h_\pm^*$ is straightforward, resulting in

$$h_\pm^*(\theta, \beta) = \frac{K}{2} \Big(\theta + \frac{\beta^2}{2}\Big)^2 \Big(1 \pm \frac{\beta}{\lambda}\Big) - \frac{a K}{4} \theta^2 . \tag{10.7}$$

• From the previous potentials, (10.6) and (10.7), it is possible to derive the entire distribution at equilibrium. Observe first that with a vectorial lattice Boltzmann scheme, it is necessary to use two families, f and g, of particle distributions, one for mass conservation and the other for momentum conservation. We have in this case

$$f_j^{\rm eq} = \frac{\partial h_j^*}{\partial \theta} , \quad g_j^{\rm eq} = \frac{\partial h_j^*}{\partial \beta} .$$

With (10.6), the function h_0^* is indepedent of β. Then $g_0 = \frac{\partial h_0^*}{\partial \beta}$ is unnecessary for the computation. With a very basic D1Q3 stencil, we define a "D1Q3Q2" lattice Boltzmann scheme. The equilibrium distribution is obtained by differentiation of the relations (10.6) and (10.7):

$$\left\{ \begin{array}{lll} f_0^{\rm eq} & = \dfrac{\partial h_0^*}{\partial \theta} & = a K \theta = a \dfrac{\rho_0}{2 c_0^2} \Big(c^2 - \dfrac{u^2}{2}\Big) = \dfrac{a}{2} \Big(\rho - \dfrac{\rho_0 u^2}{2 c_0^2}\Big) \\ f_\pm^{\rm eq} & = \dfrac{\partial h_\pm^*}{\partial \theta} & = \dfrac{\rho}{2} \Big(1 \pm \dfrac{u}{\lambda}\Big) - \dfrac{a}{4} \Big(\rho - \dfrac{\rho_0 u^2}{2 c_0^2}\Big) \\ g_\pm^{\rm eq} & = \dfrac{\partial h_\pm^*}{\partial \beta} & = \dfrac{\rho u}{2} \pm \dfrac{\rho}{2} \Big(\dfrac{u^2}{\lambda} + \dfrac{c^2}{2 \lambda}\Big) . \end{array} \right.$$

From these equilibria, we implement the lattice Boltzmann method within the multiple-relaxation-time (MRT) framework. The conserved moments follow the general paradigm introduced in (10.3):

$$\rho = f_0 + f_+ + f_- , \quad q = g_+ + g_- .$$

The non-conserved moments are chosen in the usual way:

$$J_\rho = \lambda(f_+ - f_-) , \quad \varepsilon_\rho = \lambda^2 (f_+ + f_- - 2 f_0) , \quad J_q = \lambda(g_+ - g_-) .$$

The relaxation step of the scheme is particularly simple when all the relaxation parameters are equal to a constant value τ as proposed in the BGK hypothesis. When a general MRT scheme is used, we follow the rule[95] of the moments m_ℓ^* after relaxation:

$$m_\ell^* = m_\ell + s_\ell (m_\ell^{\rm eq} - m_\ell) . \tag{10.8}$$

• We have tested the previous ideas for a Riemann problem for a shock tube. We have chosen the following numerical data and parameters:

$$\gamma = 2 , \ \frac{\rho_\ell}{\rho_0} = 2 , \ \frac{\rho_r}{\rho_0} = 0.5 , \ q_\ell = q_r = 0 , \ \frac{\lambda}{c_0} = 8 , \ a = 0.15 , \ s_j \equiv 1.8 .$$

The numerical results are displayed in Fig. 1. The rarefaction wave (on the left) and the shock wave (on the right) are correctly captured.

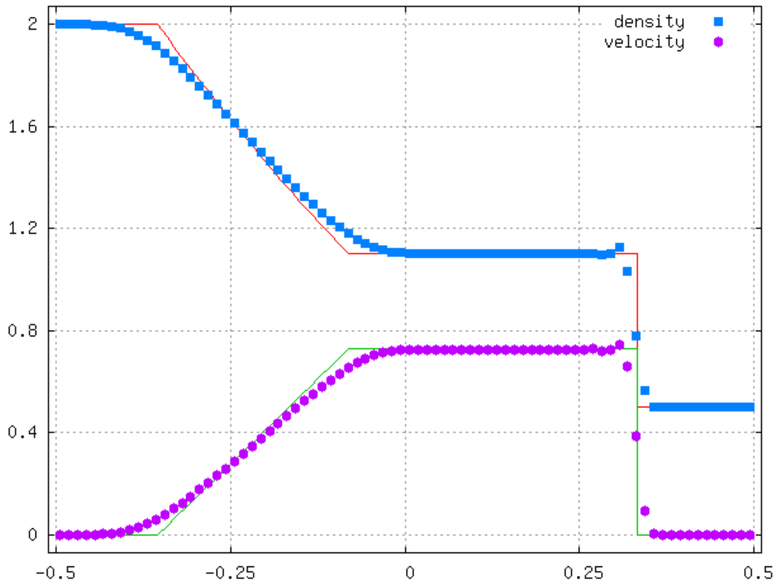

Figure 10.1 – *Riemann problem for shallow water equations. Density (blue, top) and velocity (pink, bottom) fields were computed with the D1Q3Q2 lattice Boltzmann scheme with 80 mesh points and compared to the exact solution.*

10.4 "D2Q5Q4Q4" VECTORIAL LATTICE BOLTZMANN SCHEME

We study now the two-dimensional shallow-water equations

$$\left\{\begin{array}{ll} \partial_t \rho + \partial_x(\rho\, u) + \partial_y(\rho\, v) & = 0 \\ \partial_t(\rho\, u) + \partial_x(\rho\, u^2 + \dfrac{p_0}{\rho_0^2}\,\rho^2) + \partial_y(\rho\, u\, v) & = 0 \\ \partial_t(\rho\, v) + \partial_x(\rho\, u\, v) + \partial_y(\rho\, v^2 + \dfrac{p_0}{\rho_0^2}\,\rho^2) & = 0\,. \end{array}\right. \tag{10.9}$$

We have three conservation laws in two spatial dimensions. We extend the previous D1Q3Q2 vectorial lattice Boltzmann scheme into a D2Q5Q4Q4 scheme. The D2Q5 stencil is associated with the following velocities:

$$v_0 = (0,0)\,,\quad v_1 = (\lambda, 0)\,,\quad v_2 = (0, \lambda)\,,\quad v_3 = (-\lambda, 0)\,,\quad v_4 = (0, -\lambda)\,. \tag{10.10}$$

We now have three particle distributions: $f \in$ D2Q5, $g_x \in$ D2Q4 and $g_y \in$ D2Q4. The natural question is to find an intrinsic method to determine the equilibrium values f_j^{eq} for $0 \leqslant j \leqslant 4$ and $\big(g_{xj}^{eq}, g_{yj}^{eq}\big)$ for $1 \leqslant j \leqslant 4$. As in the one-dimensional case, a key point is to be able to explicitly determine the dual entropy. In this two-dimensional case, the entropy variables $\varphi \in \mathbb{R}^3$ can be written as

$$\varphi = (\theta\,, u\,, v)\,,\; \theta = \frac{\partial \eta}{\partial \rho} = \frac{c^2}{\gamma - 1} - \frac{u^2 + v^2}{2}$$

$$\eta^*(\theta,\, u,\, v) \equiv p \equiv \frac{\rho_0}{2\, c_0^2}\Big(\theta + \frac{1}{2}(u^2 + v^2)\Big)^2\,.$$

In order to determine the equilibrium distributions, we search for convex functions $h_j^*(\theta, u, v)$ for $0 \leqslant j \leqslant 4$, such that the first set of Perthame-Bouchut conditions (10.4) are satisfied:

$$\sum_{j=0}^{4} h_j^*(\theta, u, v) \equiv \eta^*(\theta, u, v) \,. \tag{10.11}$$

Then

$$f_j^{eq} = \frac{\partial h_j^*}{\partial \theta}\,, \quad g_{xj}^{eq} = \frac{\partial h_j^*}{\partial u}\,, \quad g_{yj}^{eq} = \frac{\partial h_j^*}{\partial v}\,.$$

We also have to take into account the dual entropy fluxes ζ_α in order to correctly represent the first-order terms of the model, (10.1) or (10.9) in our case. With the second set of Perthame-Bouchut conditions (10.4), we have:

$$\sum_{j=0}^{4} v_j^1\, h_j^*(\theta, u, v) \equiv \eta^*\, u\,, \quad \sum_{j=0}^{4} v_j^2\, h_j^*(\theta, u, v) \equiv \eta^*\, v\,. \tag{10.12}$$

For the D2Q5 stencil, the conditions of (10.11) (10.12) take the form

$$h_0^* + h_1^* + h_2^* + h_3^* + h_3^* \equiv p\,, \quad \lambda\left(h_1^* - h_3^*\right) \equiv p\,u\,, \quad \lambda\left(h_2^* - h_4^*\right) \equiv p\,v\,. \tag{10.13}$$

We mimic for shallow water in two spatial dimensions what we have done for the one-dimensional case (10.6), and we suggest here to set as previously

$$h_0^*(\theta) \,=\, \frac{a}{2}\, K \theta^2 .$$

Because this function h_0^* does not depend explicitly on the variables u and v, we are not defining a D1Q5Q5Q5 scheme, but rather simply a D1Q5Q4Q4 vectorial lattice Boltzmann scheme. The positive parameter a still has to be fixed. Nevertheless, we still have many degrees of freedom. We suggest moreover to break into two parts the first relation of (10.13):

$$h_1^* + h_3^* \,=\, \frac{1}{2}\left(p - h_0^*\right), \quad h_2^* + h_4^* \,=\, \frac{1}{2}\left(p - h_0^*\right). \tag{10.14}$$

We have now a set of five independent equations (10.6), (10.13) and (10.14) with 5 unknowns h_j^*. The end of the algebraic determination of the system (10.6), (10.13) and (10.14) is then completely elementary.

- When the potentials h_j^* are known, the computation of the equilibrium values is straightforward. With the $5+4+4=13$ particle distributions, we can construct 13 moments for the D2Q5Q4Q4 lattice Boltzmann scheme. We suggest the following five moments associated with the distribution f_j:

$$\left\{ \begin{array}{ll} \rho \,=\, f_0 + f_1 + f_2 + f_3 + f_4\,, & J_{x,\rho} \,=\, \lambda\left(f_1 - f_3\right), \quad J_{y,\rho} \,=\, \lambda\left(f_2 - f_4\right), \\ \varepsilon_\rho \,=\, f_1 + f_2 + f_3 + f_4 - 4\, f_0\,, & XX_\rho \,=\, f_1 - f_2 + f_3 - f_4\,. \end{array} \right.$$

For the eight moments relative to the distributions g_{xj} and g_{yj}, we have chosen

$$\left\{ \begin{array}{ll} q_x \,=\, g_{x1} + g_{x2} + g_{x3} + g_{x4}\,, & f_{xx} \,=\, \lambda\left(g_{x1} - g_{x3}\right), \\ f_{xy} \,=\, \lambda\left(g_{x2} - g_{x4}\right), & XX_u \,=\, g_{x1} - g_{x2} + g_{x3} - g_{x4} \end{array} \right.$$

and

$$\left\{ \begin{array}{ll} q_y = g_{y1} + g_{y2} + g_{y3} + g_{y4} \,, & f_{yx} = \lambda \big(g_{y1} - g_{y3} \big) \,, \\ f_{yy} = \lambda \big(g_{y2} - g_{y4} \big) \,, & XX_v = g_{y1} - g_{y2} + g_{y3} - g_{y4} \,. \end{array} \right.$$

• The value at equilibrium of the previous moments can be determined, taking into account that the three moments ρ, q_x and q_y are at equilibrium. We have:

$$\left\{ \begin{array}{ll} J_{x,\rho}^{\rm eq} = \rho\, u = q_x \,, & J_{y,\rho}^{\rm eq} = \rho\, v = q_y \,, \\ \varepsilon_{\rho}^{\rm eq} = \big(1 - \dfrac{5\,a}{2}\big)\, \rho + \dfrac{5}{4}\, \dfrac{\rho_0\, (u^2 + v^2)}{c_0^2} \,, & XX_{\rho}^{\rm eq} = 0 \end{array} \right.$$

We have also

$$\left\{ \begin{array}{lll} f_{xx}^{\rm eq} = \rho\, u^2 + p \,, & f_{xy}^{\rm eq} = \rho\, u\, v \,, & XX_u^{\rm eq} = 0 \\ f_{yx}^{\rm eq} = \rho\, u\, v \,, & f_{yy} = \lambda \big(g_{y2} - g_{y4} \big) \,, & XX_v^{\rm eq} = 0 \,. \end{array} \right.$$

The MRT algorithm can be implemented without difficulty. It is just necessary to write a relation of the type (10.8) for the 10 moments that are not at equilibrium. Our present choice is the BGK variant of the scheme, with all parameters s_ℓ set equal. The boundary conditions of wall constraint, supersonic inflow or supersonic outflow are treated with an easy adaptation of the usual methods of bounce-back and "anti-bounce-back".

10.5 FIRST TEST CASES

We propose two bi-dimensional test cases for the shallow-water equations: A stationary shock reflection and a classical non-stationary forward-facing step, first proposed by Emery [55] for gas dynamics. The first test case is a the reflection of an incident shock wave of angle $-\pi/4$ issued from a "left" state into a new shock of angle $a\,tan(4/3)$ due to the physical nature of the "top" state (in green on the left picture of Fig. 2) and the "right" state (in indigo). The exact solution is determined through the use of the Rankine-Hugoniot relations. We have chosen

$$\left\{ \begin{array}{lll} \rho_\ell = 1 \,, & u_\ell = 1.59497132403753 \,, & v_\ell = 0 \,, \\ \rho_t = 1.17150636388320 \,, & u_t = 1.47822089880855 \,, & v_t = -0.116750425228984 \,, \\ \rho_r = 1.38196199044604 \,, & u_r = 1.33228286727232 \,, & v_r = 0 \,. \end{array} \right.$$

The stationary result of the vectorial lattice Boltzmann scheme for this first test case can be compared with the pure finite-volume approach with the Godunov[70] scheme, solving a discontinuity at each interface at each time step. We have used three meshes of 35 × 20, 70 × 40 and 140 × 80 grid points. The contours of constant density are presented in Fig. 2. The numerical results are similar.

• The second test case (Emery[55]) is purely non-stationary. At time zero a small step is created inside a flow at Froude number equal to 3. A strong shock wave separates from the wall and various nonlinear waves are generated which mutually interact. Our present experiment (Figs. 3 and 4) shows the ability of a vectorial lattice Boltzmann scheme to approach such a flow. We have refined the mesh, using three families of meshes: 120 × 40, 240 × 80 and 480 × 120. We have used

$$\lambda = 80 \,, \quad a = 0.05 \,, \quad s_j = 1.8 \,\forall\, j$$

Figure 10.2 – *Shock reflection, mesh* 140 × 80. *Exact solution (left), Lattice Boltzmann scheme D2Q5Q4Q4 (middle) and Godunov scheme (right).*

to achieve experimental stability. The time step is very small (due to the high value of $\lambda = \frac{\Delta x}{\Delta t}$), and in consequence the computation is relatively slow.

- We present our results for the finer mesh, at a dimensionalized time equal to 1/2 (Fig. 3) and 4 (Fig. 4). The results show the ability of the vectorial scheme based on the decomposition of the dual entropy to capture such flows. Nevertheless, the Godunov scheme, well known to be only order one, gives better non-stationary results compared to the new approach.

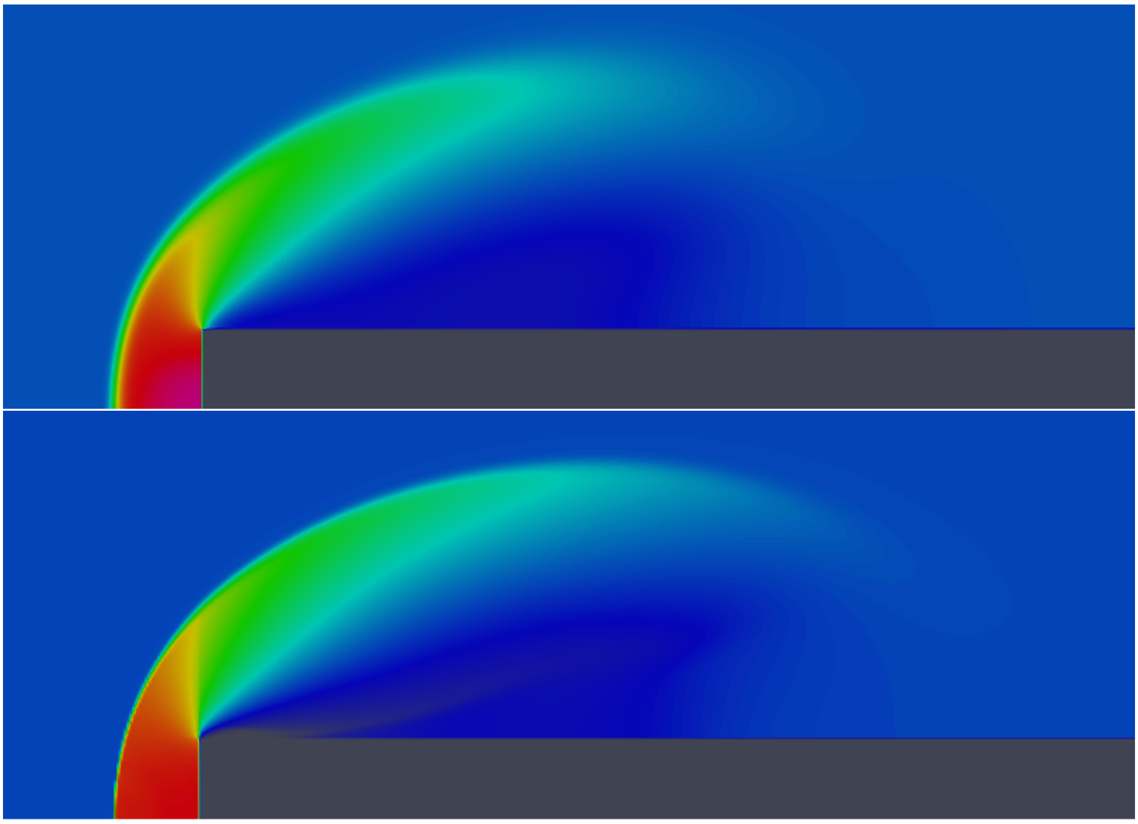

Figure 10.3 – *Emery test case for the shallow-water equations, mesh* 480 × 120, $t = 1/2$, *density profile, D2Q5Q4Q4 vectorial lattice Boltzmann scheme (top) and Godunov scheme (bottom).*

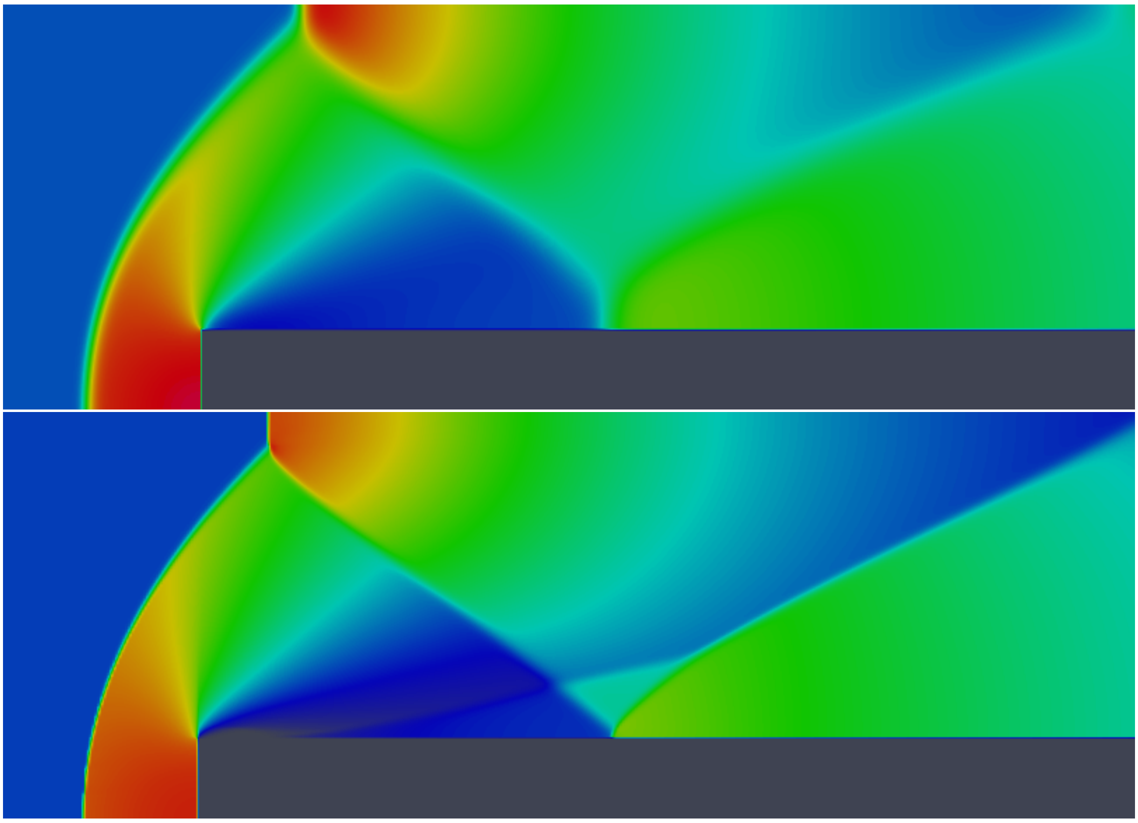

Figure 10.4 – *Emery test case for the shallow water equations, mesh* 480×120, $t = 4$, *density profile, D2Q5Q4Q4 vectorial lattice Boltzmann scheme (top) and Godunov scheme (bottom).*

CONCLUSION

We have extended the methodology of kinetic decomposition of the dual entropy previously studied for one-dimensional problems into a general framework of vectorial lattice Boltzmann schemes for systems of conservation laws in several spatial dimensions, in the spirit of Bouchut[14]. The key point is to decompose the dual entropy of the system into convex potentials satisfying the Perthame-Bouchut hypothesis. Our first choices show that the system of shallow-water equations can be solved numerically without major difficulty. Nevertheless, our first numerical experiments show that the resulting scheme contains high numerical viscosity. Future work is necessary to reduce this effect.

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