



HAL
open science

Stable lattice Boltzmann schemes with a dual entropy approach for monodimensional nonlinear waves

François Dubois

► **To cite this version:**

François Dubois. Stable lattice Boltzmann schemes with a dual entropy approach for monodimensional nonlinear waves. *Computers & Mathematics with Applications*, 2013, 65, pp.142-159. 10.1016/j.camwa.2012.09.005 . hal-00545244v2

HAL Id: hal-00545244

<https://hal.science/hal-00545244v2>

Submitted on 8 Mar 2013

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Stable lattice Boltzmann schemes with a dual entropy approach for monodimensional nonlinear waves

François Dubois ^{ab}

^a *Conservatoire National des Arts et Métiers,
Department of Mathematics and LMSSC, Paris, France.*

^b *Department of Mathematics, University Paris-Sud,
Bât. 425, F-91405 Orsay Cedex, France.
francois.dubois@math.u-psud.fr*

20 September 2012 *

Abstract. We follow the mathematical framework proposed by Bouchut [6] 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.

Keywords: Hyperbolic conservation laws, entropy, convex hull, shock wave, nonlinear acoustics.

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

* Contribution published in *Computers And Mathematics With Applications*, volume 65, pages 142-159, 2013, doi: 10.1016/j.camwa.2012.09.005. Edition 04 March 2013.

1) Introduction

An hyperbolic partial differential equation like the Burgers equation

$$(1) \quad \partial_t u + \partial_x(F(u)) = 0, \quad F(u) \equiv \frac{u^2}{2}$$

exhibits shock waves (see *e.g.* [24]), *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

$$(2) \quad \partial_t(\eta(u)) + \partial_x(\zeta(u)) \leq 0$$

as suggested by Godunov [25] and Friedrichs and Lax [22]. In the relation (2), $\eta(\bullet)$ is a strictly convex function and $\zeta(\bullet)$ the associated entropy flux (see *e.g.* [24], [16] or [34]). For the Burgers equation, the quadratic entropy is usually considered

$$(3) \quad \eta(u) \equiv \frac{u^2}{2}, \quad \zeta(u) \equiv \frac{u^3}{3}.$$

Remark that the entropy condition (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.* [24] or [34]).

- 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 [3], Elton [19], Elton *et al.* [20]). With the lattice Boltzmann methods described *e.g.* by Lallemand and Luo [33], first tentatives were proposed by d’Humières [28], Alexander *et al.* [1], Qian and Zhou [40]. The study of nonlinear scalar equation with the help of the lattice Boltzmann scheme has been emphasized by Buick *at al.* [11] for nonlinear acoustics. The approximation of the Burgers equation with a quantum variant of the method has been presented by Yenez [43]. A D1Q2 entropic scheme for the one-dimensional viscous Burgers equation has been developed by Boghosian *et al.* [4] and we refer to Duan and Liu [17] 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.*, [38], Brownlee *et al.* [10], Nie, Shan and Chen [35], Karlin and Asinari [30], Chikatamarla and Karlin [14].

- 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 [6] making the link between the finite volume method and kinetic models in the framework of the BGK [2] 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.

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,

$$(4) \quad \eta^*(\varphi) = \sup_W \left(\varphi \bullet W - \eta(W) \right).$$

The upper bound in the right hand side of relation (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 :

$$(5) \quad \eta'(W) = \varphi.$$

A first example is simply $\eta(w) \equiv e^w$ at one space dimension. Then $e^w = \varphi$, $\eta^*(\varphi) = \varphi \log \varphi - \varphi$ and we recover in this way the fundamental tool to define the so-called ‘‘Shannon entropy’’ [42].

- We can derive the dual function : if $d\eta(W) \equiv \varphi \bullet dW$ then

$$(6) \quad d\eta^*(\varphi) = d\varphi \bullet W$$

and the ‘‘physical state’’ W is the Jacobian of the dual entropy. In an analogous way, we can introduce (see *e.g.* [24], [16] or [34]) in the context of hyperbolic conservation laws

$$(7) \quad \partial_t W + \partial_x(F(W)) = 0$$

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 (5) as previously. Then $d\zeta^*(\varphi) = d\varphi \bullet F(W)$ 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 (7) can be expressed in terms of the dual entropy η^* and of the dual entropy flux ζ^* . The example of Burgers equation (1) with the quadratic entropy and associated flux gives without difficulty

$$(8) \quad \eta^*(\varphi) = \frac{\varphi^2}{2}, \quad \zeta^*(\varphi) = \frac{\varphi^3}{6}.$$

- Independently of the framework relative to hyperbolic conservation laws, the Boltzmann equation with discrete velocities has been studied by Broadwell [9] (see also Gatignol [23] and Cabannes [12]). In this contribution, we write this model for $(J+1)$ velocities in one space dimension :

$$(9) \quad \partial_t f_j + v_j \partial_x f_j = Q_j(f), \quad 0 \leq j \leq J.$$

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 (9) admits N microscopic collision invariants M_{kj} :

$$\sum_j M_{kj} Q_j(f) = 0, \quad 1 \leq k \leq N$$

and $N = 1$ for a scalar (*e.g.* Burgers) equation. The N first conserved moments :

$$(10) \quad W_k \equiv \sum_j M_{kj} f_j, \quad 1 \leq k \leq N$$

satisfy a system of conservation laws :

$$(11) \quad \partial_t W_k + \partial_x \left(\sum_j M_{kj} v_j f_j \right) = 0, \quad 1 \leq k \leq N.$$

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* $d\eta = \varphi \bullet dW$) 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 :

$$(12) \quad \varphi \bullet M_j \equiv \sum_{k=1}^N \varphi_k M_{kj}, \quad 0 \leq j \leq J,$$

is well defined. In some sense, the vector $\varphi \in \mathbb{R}^N$ can be split into $J+1$ (with $J \geq N$) **scalar** contributions $\varphi \bullet M_j$ associated with the particle distribution of the Boltzmann method. In the following, we denote this contribution as the “ j° particle component of the entropy variables”.

- The link between the Boltzmann models and the entropy variables has been first proposed by Perthame [37]. We follow here the approach developed by Bouchut [6]. We say that the “dual entropy approach” is satisfied if we suppose that there exists J **convex** scalar functions h_j^* such that

$$(13) \quad \sum_j h_j^*(\varphi \bullet M_j) \equiv \eta^*(\varphi), \quad \sum_j v_j h_j^*(\varphi \bullet M_j) \equiv \zeta^*(\varphi), \quad \forall \varphi.$$

We introduce $h_j(f_j) \equiv \sup_y (y f_j - h_j^*(y))$ 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 (5) making for each j the link between f_j and $\varphi \bullet M_j$ under the scalar form

$$(14) \quad h_j'(f_j) = \varphi \bullet M_j, \quad 0 \leq j \leq J.$$

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 (13) is satisfied, we can prove a discrete version of the Boltzmann H-theorem. If

$$(15) \quad \sum_j h_j'(f_j) Q_j(f) \leq 0,$$

we have dissipation of the microscopic entropy :

$$(16) \quad \partial_t H(f) + \partial_x \left(\sum_j v_j h_j(f_j) \right) \leq 0$$

and this function is a natural Lyapunov function. The equilibrium distribution $f_j^{\text{eq}}(W)$ is then defined by

$$(17) \quad f_j^{\text{eq}}(W) \equiv (h_j^*)'(\varphi \bullet M_j), \quad 0 \leq j \leq J$$

because the relation (6) holds. Then we recover the Karlin *et al* [31] minimization property : $H(f) \geq H(f^{\text{eq}})$ for each f such that $\sum_j M_{kj} f_j = \sum_j M_{kj} f_j^{\text{eq}} \equiv W_k$ with $1 \leq k \leq N$.

• By differentiation of the relations (13) relative to the entropy variable φ and taking into account the previous relations (17), we have the necessary equilibrium conditions $\sum_j M_j f_j^{\text{eq}} = W$ and $\sum_j v_j M_j f_j^{\text{eq}} = F(W)$. In other terms, the conserved variables are given by the relations (17)(10) and the macroscopic fluxes by

$$F_k(W) \equiv \sum_j M_{kj} v_j f_j^{\text{eq}}, \quad 1 \leq k \leq N.$$

The macroscopic entropy and associated entropy fluxes satisfy

$$\eta(W) = \sum_j h_j(f_j^{\text{eq}}), \quad \zeta(W) = \sum_j v_j h_j(f_j^{\text{eq}}).$$

When the Boltzmann equation with discrete velocities satisfies the so-called BGK hypothesis [2], *id est*

$$(18) \quad Q_j(f) = \frac{1}{\tau} (f_j^{\text{eq}} - f_j), \quad 0 \leq j \leq J$$

for some constant $\tau > 0$, the Boltzmann H-theorem is satisfied. We give the proof for completeness : we first have the following convexity inequality

$$\left(h_j'(f_j^{\text{eq}}) - h_j'(f_j) \right) \left(f_j^{\text{eq}} - f_j \right) \geq 0, \quad 0 \leq j \leq J.$$

If the BGK hypothesis (18) occurs, we have by summation over j ,

$$\begin{aligned} \tau \sum_j h_j'(f_j) Q_j(f) &= \sum_j h_j'(f_j) \left(f_j^{\text{eq}} - f_j \right) \leq \sum_j h_j'(f_j^{\text{eq}}) \left(f_j^{\text{eq}} - f_j \right) = \\ &= \sum_j (\varphi \bullet M_j) \left(f_j^{\text{eq}} - f_j \right) = \varphi \bullet \sum_j M_j \left(f_j^{\text{eq}} - f_j \right) = 0 \end{aligned}$$

and due to (14), the hypothesis (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 (1) equipped with a quadratic entropy. If there exists **convex** functions $h_j^*(\varphi)$ of the entropy variable φ such that

$$(19) \quad \sum_j h_j^*(\varphi) \equiv \eta^*(\varphi) = \frac{\varphi^2}{2}, \quad \sum_j v_j h_j^*(\varphi) \equiv \zeta^*(\varphi) = \frac{\varphi^3}{6}$$

then the equilibrium $f_j^{\text{eq}}(u) \equiv \frac{dh_j^*}{d\varphi}$ defines a **stable** approximation in a sense detailed in Chen *et al* [13] and extended by Bouchut [5, 7].

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.* [33]). For the Burgers equation (1) a possible mathematical entropy is the quadratic one (3). The dual entropy $\eta^*(\varphi)$ and the associated dual entropy flux $\zeta^*(\varphi)$ are given according to the relations (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 (19) holds, *id est* for D1Q3 :

$$(20) \quad h_+(\varphi) + h_0^*(\varphi) + h_-(\varphi) \equiv \frac{\varphi^2}{2}, \quad \lambda (h_+(\varphi) - h_-(\varphi)) \equiv \frac{\varphi^3}{6}.$$

- 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

$$(21) \quad h_0^*(\varphi) = (1 - \alpha) \frac{\varphi^2}{2}.$$

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 (20), the two other dual functions $h_+(\varphi)$ and $h_-(\varphi)$ are determined :

$$(22) \quad h_+ = \alpha \frac{\varphi^2}{4} + \frac{\varphi^3}{12\lambda}, \quad h_- = \alpha \frac{\varphi^2}{4} - \frac{\varphi^3}{12\lambda}.$$

The associated dual functions can be written explicitly without particular difficulty :

$$(23) \quad \begin{cases} h_+(f_+) &= \frac{\lambda^2}{6} \left[\left(\alpha^2 + 4 \frac{f_+}{\lambda} \right)^{3/2} - 6\alpha \frac{f_+}{\lambda} - \alpha^3 \right] \\ h_0(f_0) &= \frac{1}{2(1-\alpha)} f_0^2 \\ h_-(f_-) &= \frac{\lambda^2}{6} \left[\left(\alpha^2 - 4 \frac{f_-}{\lambda} \right)^{3/2} + 6\alpha \frac{f_-}{\lambda} - \alpha^3 \right]. \end{cases}$$

The three functions h_j^* introduced in (21) and (22) are convex when

$$(24) \quad |\varphi| \leq \alpha \lambda$$

and the relation (24) can be interpreted as a Courant-Friedrichs-Lewy stability condition :

$$\Delta t \leq \frac{\alpha}{|u|} \Delta x.$$

The dual entropy approach contains in particular the numerical stability condition (24). The stability is in fact defined as the domain of convexity of the dual functions h_j^* presented algebraically by relations (21) (22) and illustrated in Figure 1. The explicit determination of the equilibrium distribution is then a consequence of the relation (17) taking also into account that $\varphi \equiv u$ for the quadratic entropy. We have

$$(25) \quad f_+^{\text{eq}}(u) = \frac{\alpha}{2} u + \frac{u^2}{4\lambda}, \quad f_0^{\text{eq}} = (1 - \alpha) u, \quad f_-^{\text{eq}} = \frac{\alpha}{2} u - \frac{u^2}{4\lambda}.$$

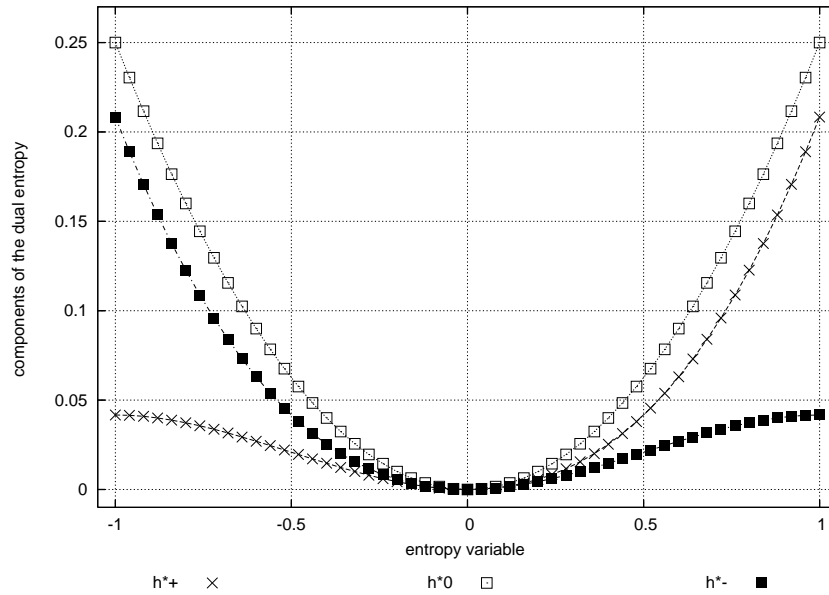


Figure 1. Kinetic decomposition (21) (22) of the dual entropy for the Burgers equation with a “centered” D1Q3 scheme ($\alpha = \frac{1}{2}$).

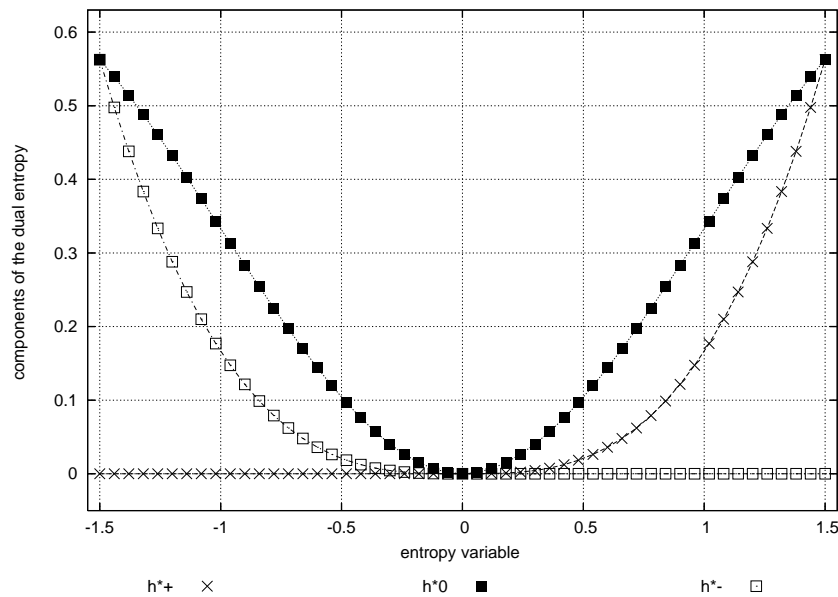


Figure 2. Kinetic decomposition for Burgers equation, equilibria (26) for the lattice Boltzmann upwind scheme D1Q3.

- Another solution of the previous system (20) can be obtained as follows. Derive the two relations in (20) two times. Then

$$(h_+^*)''(\varphi) = (h_-^*)''(\varphi) + \frac{\varphi}{\lambda}, \quad (h_0^*)''(\varphi) + 2(h_-^*)''(\varphi) = 1 - \frac{\varphi}{\lambda}.$$

In order to have a better stability property than the condition (24) obtained previously, we try to enforce the convexity condition $(h_j^*)''(\varphi) \geq 0$ if $|\varphi| \leq \lambda$ instead of (24). For

$\varphi \leq 0$, we propose to replace the inequality $(h_+^*)''(\varphi) \equiv (h_-^*)''(\varphi) + \frac{\varphi}{\lambda} \geq 0$ by an equality. Then $(h_-^*)''(\varphi) = -\frac{\varphi}{\lambda}$ if $\varphi \leq 0$. We deduce $(h_+^*)''(\varphi) = 0$ and $(h_0^*)''(\varphi) = 1 + \frac{\varphi}{\lambda}$ if $\varphi \leq 0$. With analogous arguments, we obtain $(h_+^*)''(\varphi) = \frac{\varphi}{\lambda}$, $(h_0^*)''(\varphi) = 1 - \frac{\varphi}{\lambda}$ and $(h_-^*)''(\varphi) = 0$ when $\varphi \geq \lambda$. We construct in this way an ‘‘upwind’’ distribution for the decomposition of the dual entropy:

$$(26) \quad h_+^*(\varphi) = \begin{cases} \frac{\varphi^3}{6\lambda} \\ 0 \end{cases}, \quad h_0^*(\varphi) = \begin{cases} \frac{\varphi^2}{2} - \frac{\varphi^3}{6\lambda} \\ \frac{\varphi^2}{2} + \frac{\varphi^3}{6\lambda} \end{cases}, \quad h_-^*(\varphi) = \begin{cases} 0, & \varphi \geq 0 \\ -\frac{\varphi^3}{6\lambda}, & \varphi \leq 0. \end{cases}$$

It is presented in Figure 2. The associated equilibrium distribution (17) takes the form

$$(27) \quad f_+^{\text{eq}}(u) = \begin{cases} \frac{u^2}{2\lambda} \\ 0 \end{cases}, \quad f_0^{\text{eq}}(u) = \begin{cases} u - \frac{u^2}{2\lambda} \\ u + \frac{u^2}{2\lambda} \end{cases}, \quad f_-^{\text{eq}}(u) = \begin{cases} 0, & u \geq 0 \\ -\frac{u^2}{2\lambda}, & u \leq 0. \end{cases}$$

By considering the Legendre duals of the relations (26), we have

$$(28) \quad \begin{cases} h_+(f_+) = \frac{2}{3} f_+ \sqrt{2\lambda f_+} & \text{with } f_+ \geq 0 \\ h_0(f_0) = \frac{\lambda^2}{3} \left[\left(1 - 2 \frac{|f_0|}{\lambda}\right)^{3/2} + 3 \frac{|f_0|}{\lambda} - 1 \right] & \text{with } f_0 \in \mathbb{R} \\ h_-(f_-) = -\frac{2}{3} f_- \sqrt{-2\lambda f_-} & \text{with } f_- \leq 0. \end{cases}$$

• 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

$$(29) \quad h_+^*(\varphi) = \frac{\varphi^2}{4} + \frac{\varphi^3}{12\lambda}, \quad h_-^* = \frac{\varphi^2}{4} - \frac{\varphi^3}{12\lambda}.$$

These two functions represented in Figure 3 are convex if

$$(30) \quad |\varphi| \leq \lambda$$

and the associated Courant-Friedrichs-Lewy stability condition states as follows

$$\Delta t \leq \frac{1}{|u|} \Delta x.$$

The dual equilibrium entropy function defined at relations (29) are represented on Figure 3. The associated components $h_+(f_+)$ and $h_-(f_-)$ of the microscopic entropy follow from (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

$$(31) \quad f_+^{\text{eq}}(u) = \frac{1}{2} u + \frac{u^2}{4\lambda}, \quad f_-^{\text{eq}} = \frac{1}{2} u - \frac{u^2}{4\lambda}.$$

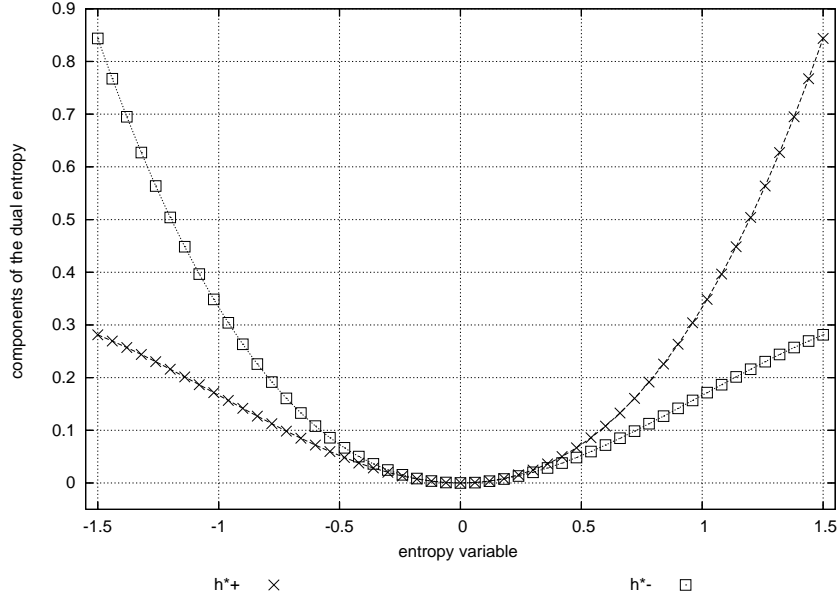


Figure 3. Kinetic decomposition for Burgers ; D1Q2 centered scheme.

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 [28], we discretize in space and time the Boltzmann equation with discrete velocities (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

$$(32) \quad m \equiv M \bullet f, \quad M = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \lambda^2 & 0 & \lambda^2 \end{pmatrix}, \quad u \equiv f_{-1} + f_0 + f_1 = m_1.$$

- The first equilibrium (25) can be translated in terms of moments under the form

$$m^{\text{eq},1} \equiv \left(u, \frac{u^2}{2}, \alpha \lambda^2 u \right)^t.$$

When using the “upwind” equilibrium (27), we obtain an other possible value for moments at equilibrium :

$$m^{\text{eq},2} \equiv \left(u, \frac{u^2}{2}, \lambda \operatorname{sgn}(u) \frac{u^2}{2} \right)^t.$$

The simpler scheme D1Q2 corresponds to the first equilibrium (25) with the particular value $\alpha = 1$ as proposed in relations (31). We have only two components in this case :

$$m^{\text{eq},3} \equiv \left(u, \frac{u^2}{2} \right)^t.$$

- The relaxation step is nonlinear and local in space :

$$(33) \quad m_1^* = m_1^{\text{eq}} = u, \quad m_k^* = m_k + s_k (m_k^{\text{eq}} - m_k) \text{ for } k \geq 2,$$

with $s_2 = s_3 = 1.7$ in our simulations unless otherwise stated. For nonlinear hyperbolic systems (7) of two conservation laws in one space dimension, the moments m_1 and m_2 are at equilibrium and the relation (33) is written in this case

$$(34) \quad m_1^* = m_1^{\text{eq}} = W_1, \quad m_2^* = m_2^{\text{eq}} = W_2, \quad m_3^* = m_3 + s_3 (m_3^{\text{eq}} - m_3).$$

The particle distribution f_j^* after relaxation is obtained by inversion of relation (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 [18] 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

$$\frac{1}{\Delta t} \left(u(x, t + \Delta t) - u(x, t) \right) + \frac{1}{\Delta x} \left[\psi \left(x + \frac{\Delta x}{2}, t \right) - \psi \left(x - \frac{\Delta x}{2}, t \right) \right] = 0$$

with a numerical flux $\psi \left(x + \frac{\Delta x}{2}, t \right)$ at the interface between the vertices x and $x + \Delta x$ defined according to

$$(35) \quad \psi \left(x + \frac{\Delta x}{2}, t \right) = \lambda \left(f_+^*(x, t) - f_-^*(x + \Delta x, t) \right).$$

We observe that the resulting lattice Boltzmann scheme is **not** a traditional finite volume scheme (in the sense proposed *e.g.* in [16]) 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 (33). On the contrary, the lattice Boltzmann method is mainly a particle method with given velocities, as analyzed *e.g.* in Junk *al.* [29] with an asymptotic expansion technique. Nevertheless, if $s_2 = s_3 = 1$, we can give an interpretation of the associated flux (35) because in this case, $f_j^* \equiv f_j^{\text{eq}}$ for all j .

- We observe that we can also decompose the “physical” flux $F(\bullet)$ (see the relation (1) or (7) in all generality) under the form $F(u) \equiv F_+(u) + F_-(u)$ with

$$(36) \quad F_+(u) = \lambda f_+^{\text{eq}}(u), \quad F_-(u) = -\lambda f_-^{\text{eq}}(u).$$

We have $F_+(u(x, t)) + F_-(u(x + \Delta x, t)) = \lambda (f_+^{\text{eq}}(u(x, t)) - f_+^{\text{eq}}(u(x + \Delta x, t)))$ and when $s_2 = s_3 = 1$ the numerical flux ψ introduced in (35) admits the classical so-called flux splitting form :

$$(37) \quad \psi \left(x + \frac{\Delta x}{2}, t \right) = F_+(u(x, t)) + F_-(u(x + \Delta x, t)).$$

With this above link between fluxes and particle distributions (37) it is natural to re-interpret, with classical flux decompositions as (36), those proposed in this contribution at relations (25), (27) and (31). As remarked by Bouchut [8], the relations (25) and (31) are associated with two variants of the Lax-Friedrichs scheme (see *e.g.* Lax [34]) whereas the upwind scheme (27) corresponds exactly to the Engquist-Osher [21] scheme !

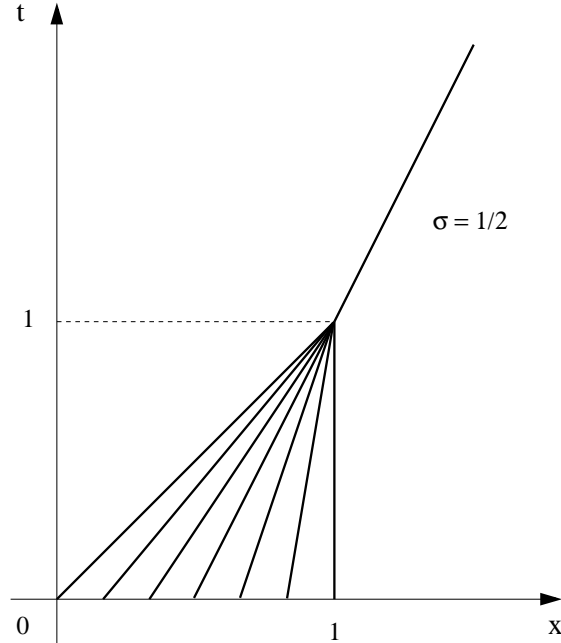


Figure 4. A converging shock wave for the Burgers equation. The decreasing profile (38) at $t = 0$ leads to an admissible discontinuity at $t = 1$. Then a shock wave with velocity $\sigma = \frac{1}{2}$ develops.

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 (25), (27) and (31) of the lattice Boltzmann scheme for each problem.

- 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

$$(38) \quad u_0(x) = \begin{cases} 1 & \text{if } x \leq 0 \\ 1 - x & \text{if } 0 \leq x \leq 1 \\ 0 & \text{if } x \geq 1. \end{cases}$$

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.* [24], [16] or [34]). 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 (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 $u(x, t) \geq 1$ have to be considered. But the convexity-stability condition (24) reads as $|u| \leq \frac{\lambda}{2}$ 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 (24), the lattice Boltzmann scheme is unstable in this strongly nonlinear situation, even if we respect the linear stability condition

$$(39) \quad 0 < s_j < 2$$

proposed initially by Hénon [27].

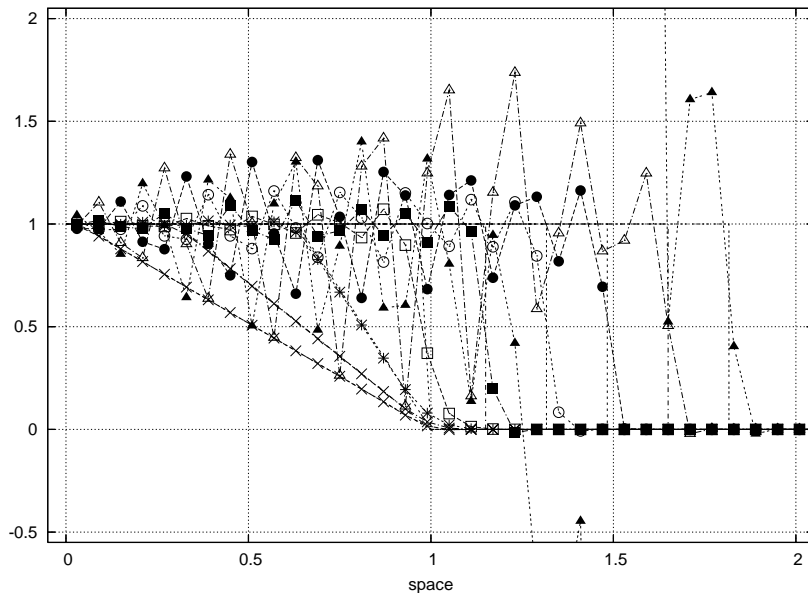


Figure 5. Burgers equation. Unstable D1Q3 lattice Boltzmann simulation for a converging shock with equilibrium (25) associated to the parameters $\alpha = \frac{1}{2}$, $s_2 = s_3 = 1.7$ and $\lambda = 1.8$. Computed values are displayed every 10 time steps.

- We repeat the same numerical experiment with a smaller time step. We take $\lambda = 3$ in a second experiment. The condition (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 (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 (39).

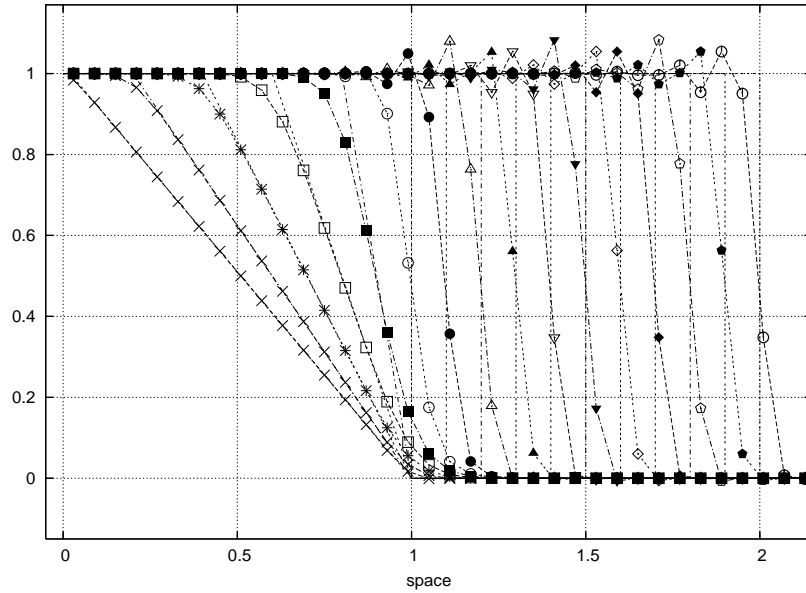


Figure 6. Burgers equation. Stable D1Q3 lattice Boltzmann simulation for a converging shock with equilibrium (25) associated to the parameters $\alpha = \frac{1}{2}$, $\lambda = 3$ and $s_2 = s_3 = 1.7$. Computed values are displayed every 10 time steps.

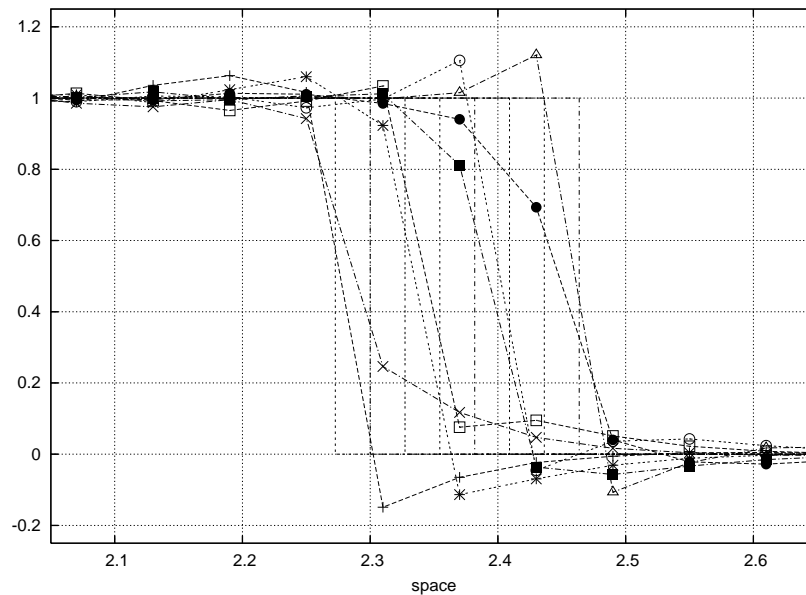


Figure 7. Burgers equation. Stable D1Q3 lattice Boltzmann simulation for a converging shock with upwind equilibrium (27) with $\lambda = 1.1$ and $s_2 = s_3 = 1.7$. Eight consecutive discrete time steps.

- With the same initial condition (38), we use the D1Q3 upwind version (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 (38), using the D1Q2 version (31) leads to results presented on Figure 8. We observe only an over-shooting at the discrete shock profile without any under-overshooting.

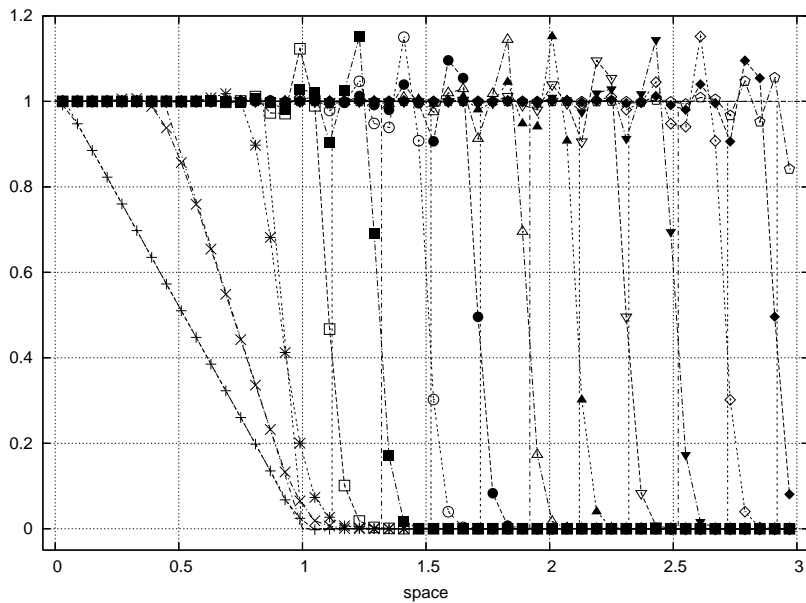


Figure 8. Burgers equation. Stable D1Q2 lattice Boltzmann simulation for a converging shock with equilibrium (31), $\lambda = 1.5$ and $s_2 = 1.7$. Computed values are displayed every 10 time steps.

- In a second set of experiments, we use the very simple “two steps” or “Riemann” initial condition. The first one is simply

$$(40) \quad u_0(x) = \begin{cases} 1 & \text{if } x < 0.2 \\ 0 & \text{if } x > 0.2. \end{cases}$$

The entropic solution of this Riemann problem composed by the Burgers equation (1) associated with the initial condition (40) is a discontinuity propagating at the velocity $\sigma = \frac{1}{2}$ (see *e.g.* [24], [16] or [34]). 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 (25), (27) and (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.

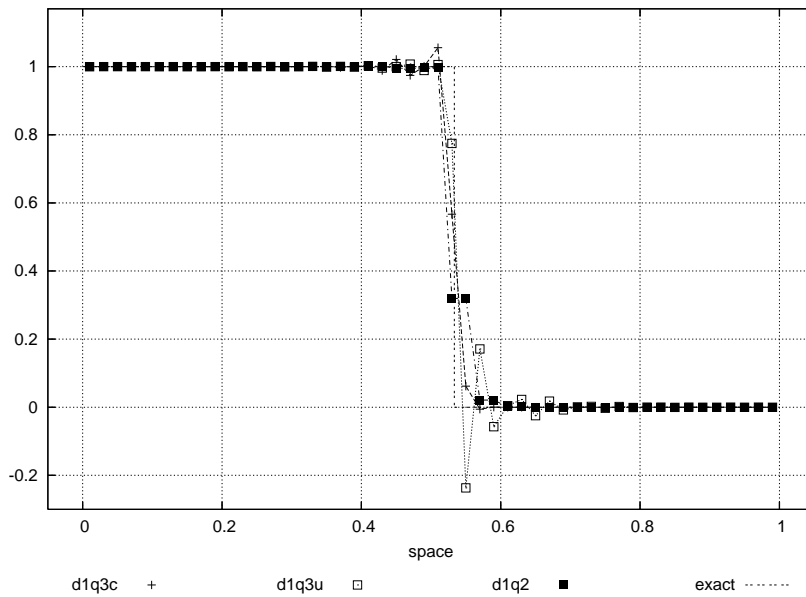


Figure 9. The Riemann problem for the Burgers equation associated with the initial condition (40) develops a shock wave. The figures shows the numerical solutions with the three variants of the scheme after 100 discrete time steps and parameters $\lambda = 3$ and $s_2 = s_3 = 1.7$.

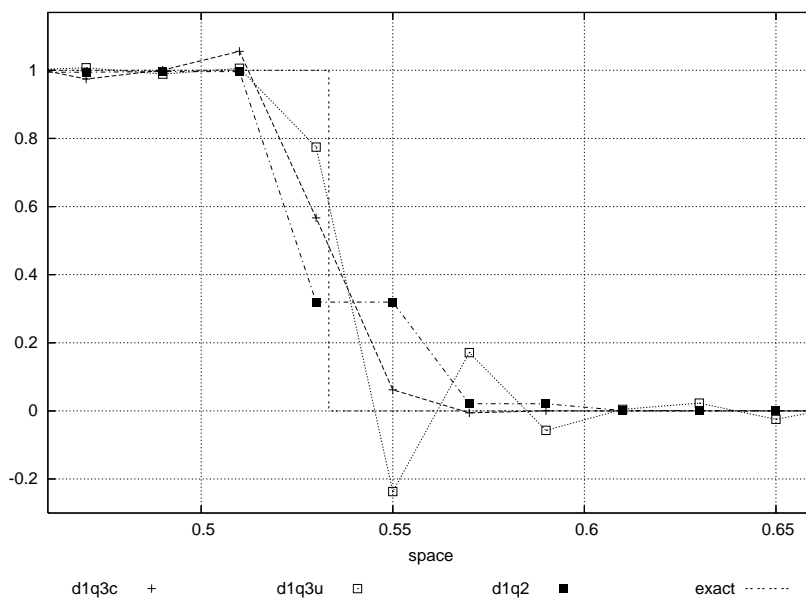


Figure 10. Zoom of Figure 10 around the location of the shock wave.

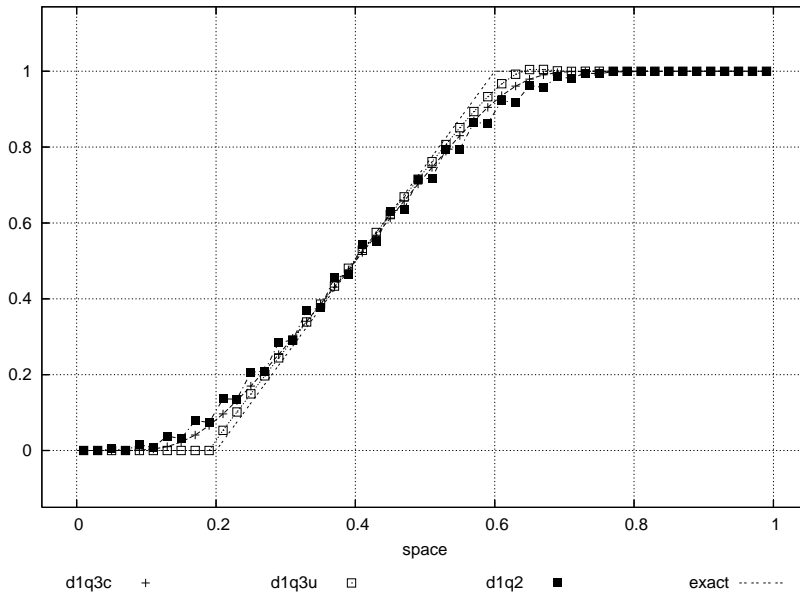


Figure 11. The Riemann problem for the Burgers equation associated with the initial condition (41) develops a rarefaction wave. Numerical solutions with the three variants of the lattice Boltzmann scheme after 100 discrete time steps and parameters $\lambda = 3$, $s_2 = s_3 = 1.7$.

- We reverse the values 0 and 1 in the initial condition (40) and obtain in this way a new initial condition :

$$(41) \quad u_0(x) = \begin{cases} 0 & \text{if } x < 0.2 \\ 1 & \text{if } x > 0.2. \end{cases}$$

The entropic solution of (1)(41) is a rarefaction wave : a continuous solution with two constant states and a self-similar component as detailed *e.g.* [24], [16] or [34]. 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 discontinuous and the solution of the problem (1)(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 (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 (33) can be found the work of Brownlee *et al.* [10] with a totally different point of view. Second, under the convexity condition of the h_j^* functions of the particle decomposition (20), we observe that the entropy condition is automatically enforced. No so-called rarefaction shock has never been observed with the initial condition (41).

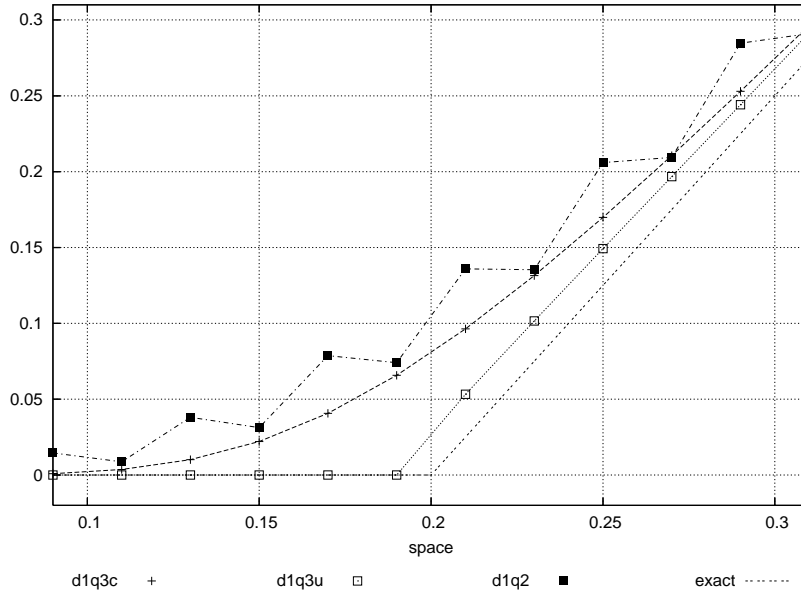


Figure 12. Zoom of Figure 12 at the foot of the rarefaction.

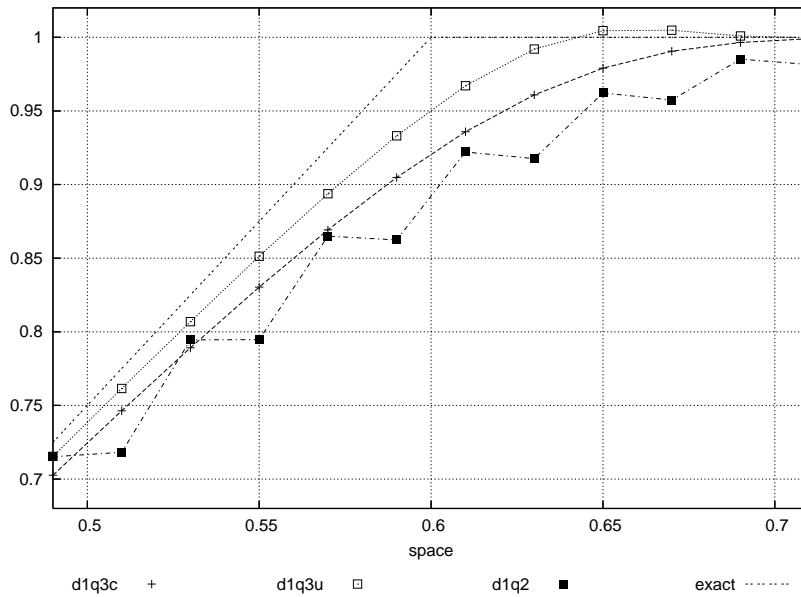


Figure 13. Zoom of Figure 12 at the top of the rarefaction.

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 :

$$(42) \quad \partial_t \begin{pmatrix} \rho \\ q \end{pmatrix} + \partial_x \begin{pmatrix} q \\ c_0^2 \rho \end{pmatrix} = 0.$$

Then a mathematical entropy is simply a quadratic form that corresponds to the physical energy :

$$(43) \quad \eta(W) \equiv \frac{\rho^2}{2} + \frac{q^2}{2c_0^2}.$$

The entropy variables are the gradients of the entropy (43) relative to the conserved variables (ρ, q) and we have

$$(44) \quad \varphi = \left(\rho, \frac{q}{c_0^2} \right).$$

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

$$(45) \quad \eta^*(\varphi) = \eta(W), \quad \zeta^*(\varphi) = \zeta(W);$$

all is quadratic in this system !

- We approach the system (42) with a D1Q3 lattice Boltzmann scheme. We use the moments m associated with the same matrix M used for the Burgers equation (see (32)). The associated particle components of the entropy variables $\varphi \bullet M_j$ introduced in (12) are given according to

$$(46) \quad \varphi \bullet M_+ \equiv \rho + \frac{\lambda q}{c_0^2}, \quad \varphi \bullet M_0 \equiv \rho, \quad \varphi \bullet M_- \equiv \rho - \frac{\lambda q}{c_0^2}.$$

The identities (13) take now the form

$$(47) \quad \begin{cases} h_+^*(\varphi \bullet M_+) + h_0^*(\varphi \bullet M_0) + h_-^*(\varphi \bullet M_-) & \equiv \eta^*(\varphi) \\ \lambda h_+^*(\varphi \bullet M_+) - \lambda h_-^*(\varphi \bullet M_-) & \equiv \zeta^*(\varphi). \end{cases}$$

We search a possible solution of system (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 (47) leads to

$$(48) \quad \begin{cases} h_+^*\left(\rho + \frac{\lambda q}{c_0^2}\right) & = \frac{c_0^2}{4\lambda^2} \left(\rho + \frac{\lambda q}{c_0^2}\right)^2 \\ h_0^*(\rho) & = \frac{1}{2} \left(1 - \frac{c_0^2}{\lambda^2}\right) \rho^2 \\ h_-^*\left(\rho - \frac{\lambda q}{c_0^2}\right) & = \frac{c_0^2}{4\lambda^2} \left(\rho - \frac{\lambda q}{c_0^2}\right)^2. \end{cases}$$

The functions proposed in (48) are convex under the stability condition :

$$(49) \quad |c_0| \leq \lambda.$$

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.* [34]). A microscopic

entropy $H(f) = h_+(f_+) + h_0(f_0) + h_-(f_-)$ can be easily derived from (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 (17) and (48) and we have

$$(50) \quad f_+^{\text{eq}} = \frac{c_0^2}{2\lambda^2} \left(\rho + \frac{\lambda q}{c_0^2}\right), \quad f_0^{\text{eq}} = \frac{1}{2} \left(1 - \frac{c_0^2}{\lambda^2}\right) \rho, \quad f_-^{\text{eq}} = \frac{c_0^2}{2\lambda^2} \left(\rho - \frac{\lambda q}{c_0^2}\right).$$

In terms of moments, the relations (50) reduce to $m_3^{\text{eq}} = c_0^2 \rho$ as proposed in Qian *et al.* [39]. Observe that the equilibrium (50) for acoustics satisfies the dual entropy approach if the CFL condition (49) is satisfied.

- We propose now to introduce a system of nonlinear acoustics obtained by replacing the linear pressure law in (42) by a nonlinear one. We consider to fix the ideas the particular example of barotropic pressure law $p(\rho)$ given according to

$$(51) \quad p(\rho) = \frac{1}{\gamma} \rho_0 c_0^2 \left(\frac{\rho}{\rho_0}\right)^\gamma,$$

with $\gamma > 1$. The corresponding nonlinear system of equations is quite similar to the so-called *p-system*. It can be written as

$$(52) \quad \partial_t \rho + \partial_x q = 0, \quad \partial_t q + \partial_x (p(\rho)) = 0.$$

It admits a mathematical entropy η and an associated entropy flux ζ satisfying

$$(53) \quad \eta(W) = \Phi(\rho) + \frac{q^2}{2}, \quad \zeta(W) = p(\rho) q,$$

where $\Phi(\bullet)$ is a primitive of the function $p(\bullet)$ introduced at the relation (51). In consequence of (53), the entropy variables $\varphi \equiv (\alpha, \beta)$ take the form

$$(54) \quad \alpha = p(\rho), \quad \beta = q.$$

The dual entropy $\eta^*(\bullet)$ and dual entropy flux $\zeta^*(\bullet)$ admit the expressions

$$(55) \quad \begin{cases} \eta^*(\alpha, \beta) &= \frac{\rho_0^2 c_0^2}{\gamma + 1} \left(\frac{\gamma \alpha}{\rho_0 c_0^2}\right)^{\frac{\gamma+1}{\gamma}} + \frac{\beta^2}{2} \equiv \frac{\rho_0^2 c_0^2}{\gamma + 1} \left(\frac{\rho}{\rho_0}\right)^{\gamma+1} + \frac{\beta^2}{2} \\ \zeta^*(\alpha, \beta) &= \alpha \beta \equiv \zeta(\rho, q). \end{cases}$$

- With the matrix M introduced at relation (32), we denote by φ_+ , φ_0 and φ_- the particle components of the entropy variables $\varphi \bullet M_j$ and we have

$$(56) \quad \varphi_+ = \alpha + \lambda \beta, \quad \varphi_0 = \alpha, \quad \varphi_- = \alpha - \lambda \beta.$$

It is possible to find nonlinear convex functions satisfying (47) with the new entropy data (55). By differentiating the relations (55) relative to the two entropy variables (54), the equilibrium functions f_+^{eq} , f_0^{eq} and f_-^{eq} must satisfy the relations

$$(57) \quad \begin{cases} f_+^{\text{eq}}(\alpha + \lambda \beta) + f_0^{\text{eq}}(\alpha) + f_-^{\text{eq}}(\alpha - \lambda \beta) &= \rho \\ \lambda f_+^{\text{eq}}(\alpha + \lambda \beta) - \lambda f_-^{\text{eq}}(\alpha - \lambda \beta) &= q \equiv \beta \\ \lambda^2 f_+^{\text{eq}}(\alpha + \lambda \beta) + \lambda^2 f_-^{\text{eq}}(\alpha - \lambda \beta) &= p(\rho) \equiv \alpha. \end{cases}$$

Then

$$(58) \quad f_+^{\text{eq}}(\alpha + \lambda\beta) = \frac{1}{2\lambda^2}(\alpha + \lambda\beta), \quad f_0^{\text{eq}}(\alpha) = \rho - \frac{\alpha}{\lambda^2}, \quad f_-^{\text{eq}}(\alpha - \lambda\beta) = \frac{1}{2\lambda^2}(\alpha - \lambda\beta)$$

and by integration of (17) and (58), we deduce that the relations (48) have to be replaced by

$$(59) \quad h_+^*(\alpha) = h_-^*(\alpha) = \frac{1}{4\lambda^2}\alpha^2, \quad h_0^*(\alpha) = \frac{\rho_0^2 c_0^2}{\gamma + 1} \left(\frac{\gamma\alpha}{\rho_0 c_0^2} \right)^{\frac{\gamma+1}{\gamma}} - \frac{\alpha^2}{2\lambda^2}.$$

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:

$$(60) \quad \left(\frac{\rho}{\rho_0} \right)^{\gamma-1} \left(\frac{c_0}{\lambda} \right)^2 \leq 1.$$

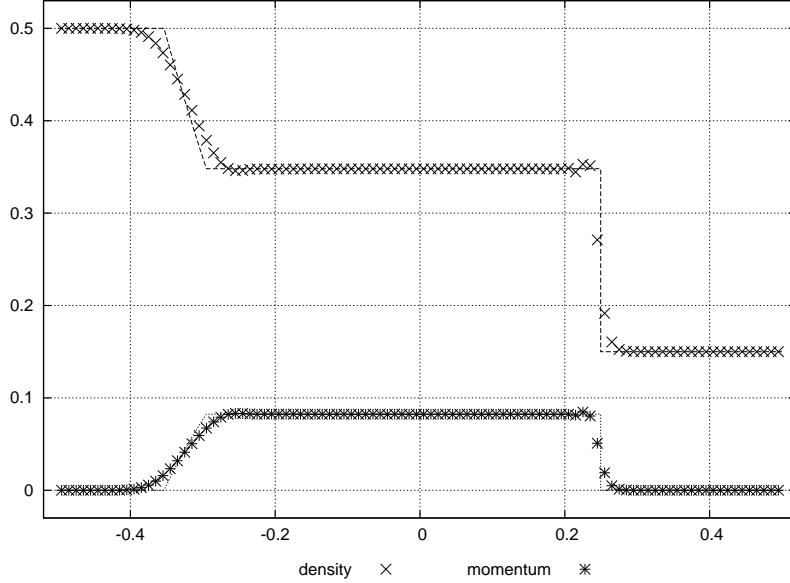


Figure 14. Riemann problem (52) (61) for the system of nonlinear acoustics. The numerical data are precised at the relations (62). A rarefaction wave is propagating from right to left and a shock wave from left to right. Exact (dotted lines) and approximated (discrete symbols) profiles of density (top) and momentum (bottom) for 100 mesh points and 60 time steps.

- We have tested the system of nonlinear acoustics (51) (52) with a D1Q3 lattice Boltzmann scheme for a Riemann problem. The initial condition is a discontinuity at $x = 0$:

$$(61) \quad (\rho(x, 0), q(x, 0)) = \begin{cases} (\rho_\ell, q_\ell) & \text{if } x < 0 \\ (\rho_r, q_r) & \text{if } x > 0. \end{cases}$$

We have chosen the physical and numerical parameters as follows:

$$(62) \quad \gamma = 2, \quad \frac{\rho_\ell}{\rho_0} = 0.5, \quad \frac{\rho_r}{\rho_0} = 0.15, \quad q_\ell = q_r = 0, \quad \frac{\lambda}{c_0} = 1.2, \quad s_3 = 1.7.$$

The exact solution of the nonlinear hyperbolic system (52) (61) can be obtained without difficulty with the general methods presented in [16] or [24]. In the case of initial data (61) (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 (62), the condition (60) is realized: $\left(\frac{\rho}{\rho_0}\right)^{\gamma-1} \left(\frac{cq}{\lambda}\right)^2 \leq 0.347$. 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 (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 (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.

7) The case of shallow water equations

The case of shallow water equations has been considered with the lattice Boltzmann scheme by Salmon [41] 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 :

$$(63) \quad \partial_t \rho + \partial_x q = 0, \quad \partial_t q + \partial_x \left(\frac{q^2}{\rho} + k \rho^\gamma \right) = 0,$$

where $k > 0$ and $\gamma \geq 1$ 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

$$(64) \quad u \equiv \frac{q}{\rho}, \quad p \equiv k \rho^\gamma, \quad c^2 \equiv \frac{\gamma p}{\rho} = \gamma k \rho^{\gamma-1}.$$

Then the entropy η and the entropy flux ζ satisfy

$$(65) \quad \eta = \frac{1}{2} \rho u^2 + \frac{p}{\gamma-1}, \quad \zeta = \eta u + p u;$$

the entropy variables $\varphi = (\partial_\rho \eta, \partial_q \eta) \equiv (\alpha, \beta)$ 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 :

$$(66) \quad \eta^* = K \left(\alpha + \frac{\beta^2}{2} \right)^{\frac{\gamma}{\gamma-1}}, \quad \zeta^* = K \left(\alpha + \frac{\beta^2}{2} \right)^{\frac{\gamma}{\gamma-1}} \beta, \quad K = k \left(\frac{\gamma-1}{\gamma k} \right)^{\frac{\gamma}{\gamma-1}}.$$

We remark that this dual entropy η^* explicited in (66) is no longer the sum of two functions of only one entropy variable as in (45) and (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 (56). The unknown **convex** functions h_j^* satisfy the identities (47) and take now the form

$$(67) \quad \begin{cases} h_+^*(\varphi_+) + h_0^*(\varphi_0) + h_-^*(\varphi_-) &= K \left(\alpha + \frac{\beta^2}{2} \right)^{\frac{\gamma}{\gamma-1}} \\ \lambda h_+^*(\varphi_+) - \lambda h_-^*(\varphi_-) &= K \left(\alpha + \frac{\beta^2}{2} \right)^{\frac{\gamma}{\gamma-1}} \beta. \end{cases}$$

• We prove in the following that the system of equations (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 (17). We differentiate the relations (67) relatively to α and β . We obtain relations very similar to (57):

$$(68) \quad \begin{cases} f_+^{\text{eq}}(\alpha + \lambda \beta) + f_0^{\text{eq}}(\alpha) + f_-^{\text{eq}}(\alpha - \lambda \beta) &= \rho \\ \lambda f_+^{\text{eq}}(\alpha + \lambda \beta) - \lambda f_-^{\text{eq}}(\alpha - \lambda \beta) &= \rho u \\ \lambda^2 f_+^{\text{eq}}(\alpha + \lambda \beta) + \lambda^2 f_-^{\text{eq}}(\alpha - \lambda \beta) &= \rho u^2 + p. \end{cases}$$

We are supposed to determine an increasing function f_0^{eq} of **only one** real variable α such that

$$(69) \quad f_0^{\text{eq}} \left(\frac{c^2}{\gamma-1} - \frac{u^2}{2} \right) \equiv \rho - \frac{1}{\lambda^2} (\rho u^2 + p).$$

Due to the elementary calculus $\frac{dc^2}{d\rho} = \gamma k (\gamma-1) \rho^{\gamma-2} = (\gamma-1) \frac{c^2}{\rho}$, we differentiate the relation (69) relative to ρ and independently relatively to u . We obtain

$$(70) \quad \frac{c^2}{\rho} (f_0^{\text{eq}})'(\alpha) + \frac{1}{\lambda^2} (u^2 + c^2) = 1, \quad -u (f_0^{\text{eq}})'(\alpha) + \frac{2\rho u}{\lambda^2} = 0.$$

We extract the derivative $(f_0^{\text{eq}})'(\alpha)$ from the second equation of (70) and report the result in the first equation. We deduce

$$(71) \quad u^2 + 3c^2 = \lambda^2$$

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 (69)) by a simple function of only one variable.

8) 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 [6]. If very interesting results are computed with

a very good lattice Boltzmann scheme in the framework proposed by d’Humières [28], 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

$$F_{\alpha k}(W) \equiv \sum_j M_{kj} v_j^\alpha f_j^{\text{eq}}.$$

First it is necessary to have a kinetic decomposition of the entropy and the associated entropy flux of the type

$$\eta(W) = \sum_j h_j(f_j^{\text{eq}}), \quad \zeta_\alpha(W) = \sum_j v_j^\alpha h_j(f_j^{\text{eq}}).$$

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

$$\varphi \mapsto h_j^*(\varphi \bullet M_j)$$

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 **vectorial** particle distribution as initially proposed by Khobalatte and Perthame in [32] and developed by Bouchut [5] 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 magnetohydrodynamics as suggested respectively by He, Chen and Doolen [26] and Dellar [15] and used by Peng, Shu and Chew [36] among others.

Acknowledgments

The author thanks François Bouchut, Benjamin Graille and Pierre Lallemand for helpful discussions during the elaboration of this work. Many thanks also to the Institute for Computer Based Modeling in Civil Engineering of Technische Universität Braunschweig (Germany) and to the “LaBS project” (Lattice Boltzmann Solver, www.labs-project.org), funded by the French FUI8 research program, for supporting this contribution. Last but not least, the author thanks the referees for very interesting remarks. Some of them have been directly incorporated into the present edition of the article.

Annex. On shallow water equations with $\gamma = 1$.

If $\gamma = 1$, we introduce a reference velocity c_* and replace the pressure law in (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

$$\alpha = \frac{\partial \eta}{\partial \rho} = c_*^2 \left(1 + \log \frac{\rho}{\rho_*} \right) - \frac{u^2}{2}, \quad \beta = \frac{\partial \eta}{\partial q} = u.$$

The entropy flux ζ is still obtained according to the relation (65): $\zeta = \eta u + p u$. After some lines of algebra, the dual entropy $\eta^* \equiv \alpha \rho + \beta q - \eta$ is equal to

$$\eta^* = c_*^2 \rho = p = \rho_* c_*^2 \exp \left(\frac{\alpha + \beta^2/2}{c_*^2} - 1 \right)$$

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 (67) are generalized without difficulty and the identity (69) can be now written

$$f_0^{\text{eq}} \left(c_*^2 \left(1 + \log \frac{\rho}{\rho_*} \right) - \frac{u^2}{2} \right) \equiv \rho - \frac{1}{\lambda^2} (\rho u^2 + p).$$

By derivation relative to density and velocity, we get respectively

$$\frac{c_*^2}{\rho} (f_0^{\text{eq}})'(\alpha) + \frac{1}{\lambda^2} (u^2 + c_*^2) = 1, \quad -u (f_0^{\text{eq}})'(\alpha) + \frac{2\rho u}{\lambda^2} = 0.$$

We deduce a necessary relation $u^2 + 3c_*^2 = \lambda^2$, very close to (71). This relation is satisfied only for exceptional values of velocity as in the case $\gamma > 1$.

References

- [1] F. Alexander, H. Chen, S. Chen, G. Doolen. “A lattice Boltzmann model for compressible fluids”, *Physical Review A*, vol. **46**, p 1967-1970, 1992.
- [2] P. Bhatnagar, E. Gross and M. Krook. “A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems”, *Physical Review*, vol. **94**, p. 511-525, 1954.

- [3] B. Boghosian, C. Levermore. “A Cellular Automaton for Burgers’s Equation”, *Complex Systems*, vol. **1**, p 17-30, 1987.
- [4] B. Boghosian, P. Love, J. Yezpez. “Entropic Lattice Boltzmann Model for Burgers’ Equation”, *Philosophical Transactions of the Royal Society A*, vol. **362**, p 1691-1702, 2004.
- [5] F. Bouchut. “Construction of BGK models with a family of kinetic entropies for a given system of conservation laws”, *Journal of Statistical Physics*, vol. **95**, p. 113-170, 1999.
- [6] F. Bouchut. “Entropy satisfying flux vector splittings and kinetic BGK models”, *Numerische Mathematik*, vol. **94**, p. 623-672, 2003.
- [7] F. Bouchut. “A reduced stability condition for nonlinear relaxation to conservation laws”, *Journal of Hyperbolic Differential Equations*, vol. **1**, p. 149-170, 2004.
- [8] F. Bouchut. Personal communication, Paris, June 2010.
- [9] J. Broadwell. “Study of a rarefied shear flow by the discrete velocity method”, *Journal of Fluid Mechanics*, vol. **19**, p. 401-14, 1964.
- [10] R. Brownlee, A. Gorban, J. Levesleye. “Stability and stabilization of the lattice Boltzmann method”, *Physical Review E*, vol. **75**, 036711, 2007.
- [11] J.M. Buick, C.L. Buckley, C.A. Greated, J. Gilbert. “Lattice Boltzmann BGK simulation of non-linear sound waves : the development of a shock front”, *Journal of Physics A: Mathematical and General*, vol. **33**, p. 3917-3928, 2000.
- [12] H. Cabannes. *The Discrete Boltzmann Equation (Theory and Applications)*, Lecture Notes, University of California at Berkeley, 1980. Revised edition by H. Cabannes, R. Gatignol and L.S. Luo, 2003 available at http://henri.cabannes.free.fr/Cours_de_Berkeley.pdf.
- [13] G.Q. Chen, C.D. Levermore, T.P. Liu. “Hyperbolic conservation laws with stiff relaxation and entropy”, *Communications on Pure and Applied Mathematics*, vol. **47**, p. 787-830, 1994.
- [14] S. Chikatamarla, I. Karlin, “Lattices for the lattice Boltzmann method”, *Physical Review E*, vol. **79**, 046701, 2009.
- [15] P. Dellar. “Lattice Kinetic Schemes for Magnetohydrodynamics”, *Journal of Computational Physics*, vol. **179**, p. 95-126, 2002.
- [16] B. Després, F. Dubois. *Systèmes hyperboliques de lois de conservation ; Application à la dynamique des gaz*, Editions de l’Ecole Polytechnique, Palaiseau, 2005.

- [17] Y. Duan, R.X. Liu. “Lattice Boltzmann model for two-dimensional unsteady Burgers’ equation”, *Journal of Computational and Applied Mathematics*, vol. **206**, p. 432-439, 2007.
- [18] F. Dubois. “On lattice Boltzmann scheme, finite volumes and boundary conditions”, *Progress in Computational Fluid Dynamics*, vol. **8**, p. 11-24, 2008.
- [19] B. Elton. “A lattice Boltzmann method for a two-dimensional viscous Burgers equation: computational results”. In *Supercomputing’91: Proceedings of the 1991 ACM/IEEE conference on Supercomputing*, p. 242-252. New York, NY, USA: ACM Press, 1991.
- [20] B. Elton, C. Levermore, G. Rodrigue. “Convergence of Convective-Diffusive Lattice Boltzmann Methods”, *SIAM Journal on Numerical Analysis*, vol. **32**, p. 1327-1354, 1995.
- [21] B. Engquist, S. Osher. “Stable and entropy satisfying approximations for transonic flow calculations”, *Mathematics of Computation*, vol. **34**, p. 45-75, 1980.
- [22] K.O. Friedrichs, P.D. Lax. “Systems of Conservation Equations with a Convex Extension”, *Proc. Nat. Sciences USA*, vol. **68**, p. 1686-1688, 1971.
- [23] R. Gatignol. “Théorie cinétique d’un gaz à répartition discrète de vitesses”, *Zeitschrift für Flugwissenschaften*, vol. **18**, p. 93-97, 1970.
- [24] E. Godlewski, P.A. Raviart. *Numerical Approximation of Hyperbolic Systems of Conservation Laws*, Springer-Verlag, New York Inc., 1996.
- [25] S. K. Godunov. “An interesting class of quasilinear systems”, *Dokl. Akad. Nauk SSSR*, vol. **139**, p. 521-523 , 1961; see also *Soviet. Math.*, vol. **2**, p. 947-949, 1961.
- [26] X. He, S. Chen, G.D. Doolen. “A Novel Thermal Model for the Lattice Boltzmann Method in Incompressible Limit”, *Journal of Computational Physics*, vol. **146**, p. 282-300, 1998.
- [27] M. Hénon. “Viscosity of a Lattice Gas”, *Complex Systems*, vol. **1**, p. 763-789, 1987.
- [28] D. d’Humières. “Generalized Lattice-Boltzmann Equations”, in *Rarefied Gas Dynamics: Theory and Simulations*, vol. **159** of *AIAA Progress in Astronautics and Astronautics*, p. 450-458, 1992.
- [29] M. Junk, A. Klar, L.S. Luo. “Asymptotic analysis of the lattice Boltzmann equation”, *Journal of Computational Physics*, vol. **210**, p. 676-704, 2005.
- [30] I.V. Karlin, P. Asinari. “Factorization symmetry in the lattice Boltzmann method”, *Physica A*, vol. **389**, p. 1530-1548, 2010.

- [31] I.V. Karlin, A.N. Gorban, S. Succi and V. Boffi. “Maximum Entropy Principle for Lattice Kinetic Equations”, *Physical Review Letters*, vol. **81**, p. 6-9, 1998.
- [32] B. Khobalatte, B. Perthame. “Maximum principle on the entropy and second-order kinetic schemes”, *Mathematics of Computation*, vol. **62**, p. 119-131, 1994.
- [33] P. Lallemand, L.-S. Luo. “Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability”, *Physical Review E*, vol. **61**, p. 6546-6562, June 2000.
- [34] P.D. Lax. *Hyperbolic Partial Differential Equations*, American Mathematical Society, Courant Lecture Notes, vol. **14**, 2006.
- [35] X. Nie, X. Shan, H. Chen. “Thermal lattice Boltzmann model for gases with internal degrees of freedom”, *Physical Review E*, vol. **77**, p. 035701(R), 2008.
- [36] Y. Peng, C. Shu, Y.T. Chew. “A 3D incompressible thermal lattice Boltzmann model and its application to simulate natural convection in a cubic cavity”, *Journal of Computational Physics*, vol. **193**, p. 260 - 274, 2004.
- [37] B. Perthame. “Boltzmann Type Schemes for Gas Dynamics and the Entropy Property”, *SIAM Journal on Numerical Analysis*, vol. **27**, p. 1405-1421, 1990.
- [38] P.C. Philippi, L.A. Hegele, R. Surmas, D.N. Siebert. “From the Boltzmann to the Lattice-Boltzmann equation: beyond BGK collision models”, *International Journal of Modern Physics C, Computational Physics and Physical Computation*, vol. **18**, p. 556-565, 2007.
- [39] Y. Qian, D. d’Humières, P. Lallemand, “Lattice BGK Models for Navier-Stokes Equation”, *Europhysics Letters*, vol. **17**, p. 479-484, 1992.
- [40] Y. Qian, Y. Zhou. “Complete Galilean-invariant lattice BGK models for the Navier-Stokes equation”, *Europhysics Letters*, vol. **42**, p. 359-364, 1998.
- [41] R. Salmon. “The lattice Boltzmann method as a basis for ocean circulation modeling”, *Journal of Marine Research*, vol. **57**, p. 503-535, 1999.
- [42] C. Shannon. “A mathematical theory of communication”, *The Bell Labs Systems Technical Journal*, vol. **27**, p. 379-423 and 623-656, 1948.
- [43] J. Yepez. “Quantum Lattice-Gas Model for the Burgers Equation”, *Journal of Statistical Physics*, vol. **107**, p. 203-224, 2002.