arXiv:1012.2094v1 [math.NA] 9 Dec 2010

Stable lattice Boltzmann scheme for a moving Burgers shock wave

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9 december 2010 *

Abstract. – We follow the mathematical framework proposed by Bouchut [3] in order to derive equilibrium functions for D1Q3 lattice Boltzmann simulations of the Burgers equation. When a particular convexity property is satisfied, we observe for strong nonlinear shocks and rarefactions that the resulting scheme is numerically stable.

Keywords: Hyperbolic conservation laws, entropy, convex hull.

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

* Invited Presentation, Seventh International Conference for Mesoscopic Methods in Engineering and Science (ICMMES-2010), Edmonton, Alberta, Canada, July 12-16, 2009. Submitted to *Computers And Mathematics With Applications*.

1) Introduction

• An hyperbolic partial differential equation like the Burgers equation

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

exhibits shock waves (see *e.g.* [17]), *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

$$\partial_t\big(\eta(u)\big) \,+\, \partial_x\big(\zeta(u)\big) \,\leq\, 0 \tag{2}$$

as suggested by Godunov [18] and Friedrichs and Lax [15]. In the relation (2), $\eta(\bullet)$ is a strictly convex function and $\zeta(\bullet)$ the associated entropy flux (see *e.g.* [17], [10] or [25]). For the Burgers equation, the quadratic entropy is usually considered

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

• The computation of weak solutions of hyperbolic problems with the lattice Boltzmann scheme as described *e.g.* by Lallemand and Luo [24] is a difficult task. A first tentative has been proposed in the pioneering work of d'Humières [11]. The study of nonlinear scalar equation with the help of the lattice Boltzmann scheme has been emphasized by Buick *at al* [6] for nonlinear acoustics. The approximation of the Burgers equation with a quantum variant of the method has been presented by Yepez [31] and we refer to Duan and Liu [12] for the approximation of two-dimensional Burgers equation with the lattice Boltzmann scheme. The extension for gas dynamics equations is under study with *e.g.* the works of Philippi *et al*, [29], Nie, Shan and Chen [26] and Karlin and Asinari [21].

• In this contribution, we start from the mathematical framework developed by Bouchut [3] making the link between the finite volume method and kinetic models in the framework of the BGK [1] approximation. The key notion is the representation of the dual entropy with the help of the discrete velocities of the lattice. In section 2, we recal this framework with emphasis to the one-dimensional scalar case and in section 3 we derive three equilibria for a kinetic distribution associated with the lattice Boltzmann method. In section 4, we recall the numerical D1Q3 scheme and in section 5 the link between this scheme and the finite volume approach. We present our numerical experiments with the Burgers equation in section 6 and propose natural extensions to other systems 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 any convex function $\eta(\bullet)$ is parametrized by the slopes of the tangent planes. In other terms,

$$\eta^*(\varphi) \,=\, \sup_W \Big(\varphi \bullet W \,-\, \eta(W)\Big)\,. \tag{4}$$

The maximum 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) $$\eta'(W) = \varphi \, .$$

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" [30].

• We can derive the dual function : if $\mathrm{d}\eta(W) \equiv \varphi \bullet \mathrm{d}W$ then $\mathrm{d}\eta^*(\varphi) = \mathrm{d}\varphi \bullet W$ and the "physical state" W is the jacobian of the dual entropy. In an analogous way, we can introduce (see *e.g.* [17], [10] or [25]) in the context of hyperbolic conservation laws

(6) $$\partial_t W \,+\, \partial_x \big(F(W) \big) \,=\, 0$$

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

(7) $$\mathrm{d}\zeta^*(\varphi) = \mathrm{d}\varphi \bullet F(W)$$

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

• Independently of the framework relative to hyperbolic conservation laws, the Boltzmann equation with discrete velocities has been studied by Gatignol [16] (see also [7]). In this contribution, we write this model for J velocities in one space dimension :

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

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 $J = 2$ for the D1Q3 lattice Boltzmann scheme (presented in section 4). The equation (9) admits N microscopic collision invariants M_{kj} :

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

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

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

satisfy a system of conservation laws :

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

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* $\mathrm{d}\eta = \varphi \bullet \mathrm{d}W$). Then the following scalar expression :

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

is well defined. We call it the $j^{\rm o}$ "particle component of the entropy variables".

• The link between the Boltzmann models and the entropy variables has been first proposed by Perthame [28]. We follow here the approach developed by Bouchut [3]. We suppose that there exists J **convex** scalar functions h_j^* such that

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

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 (5) making for each j the link between f_j and $\varphi \bullet M_j$ under the scalar form

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

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

$$\sum_j h_j'(f_j) \, Q_j(f) \leq 0, \tag{15}$$

we have dissipation of the microscopic entropy :

$$\partial_t H(f) + \partial_x \Big(\sum_j v_j \, h_j(f_j) \Big) \leq 0 \tag{16}$$

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

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

because the relation (7) holds. Then we recover the Karlin *et al* [22] minimization property : $H(f) \geq H(f^{\rm eq})$ for each f such that $\sum_j M_{kj} \, f_j = \sum_j M_{kj} \, f_j^{\rm eq} \equiv W_k$ with $1 \leq k \leq N$.

• We recall that the equilibrium distribution of particles, the conserved variables and the macroscopic fluxes are given respectively by the relations (17), (10) and

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

The macroscopic entropy and associated entropy fluxes satisfy

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

When the Boltzmann equation with discrete velocities satisfies the so-called BGK hypothesis [1], *id est*

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

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 (18) occurs, we have by summation over j,

$$\tau \sum_j h'_j(f_j)\, Q_j(f) \,=\, \sum_j h'_j(f_j)\,\Big(f_j^{\rm eq} - f_j\Big) \,\leq\, \sum_j h'_j(f_j^{\rm eq})\,\Big(f_j^{\rm eq} - f_j\Big) \,=$$

$$= \sum_j \big(\varphi \bullet M_j\big)\,\Big(f_j^{\rm eq} - f_j\Big) \,=\, \varphi \bullet \sum_j M_j\,\Big(f_j^{\rm eq} - f_j\Big) \,=\, 0$$

and due to (14), the hypothesis (15) is satisfied and the H-theorem is established in this case.

- As a summary of this mathematical section in the case of the Burgers equation (1) and following the work of Bouchut [2], if there exists **convex** functions $h_j^*(\varphi)$ of the entropy variable φ such that

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

then the equilibrium $f_j^{\rm eq}(u) \equiv \frac{{\rm d}h_j^*}{{\rm d}\varphi}$ defines a **stable** approximation in a sense detailed in Chen *et al* [8] and extended by Bouchut [4].

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.* [24]). 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 method proposed in the previous section, we search three convex functions $h_+^*(\varphi)$, $h_0^*(\varphi)$ and $h_-^*(\varphi)$ such that

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

- 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

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

Due to (20), the two other dual fuctions $h^*_+(\varphi)$ and $h^*_-(\varphi)$ are determined :

$$h^*_+ \,=\, \alpha \, \frac{\varphi^2}{4} \,+\, \frac{\varphi^3}{12\,\lambda} \,, \qquad h^*_- \,=\, \alpha \, \frac{\varphi^2}{4} \,-\, \frac{\varphi^3}{12\,\lambda} \,. \tag{22}$$

The associated dual functions can be explicited without particular difficulty :

$$\left\{ \begin{array}{rcl} h_+(f_+) & = & \dfrac{\lambda^2}{6} \Big[\Big(\alpha^2 + 4 \, \dfrac{f_+}{\lambda} \Big)^{3/2} \,-\, \Big(\alpha^3 + 6\,\alpha\,\dfrac{f_+}{\lambda} \Big) \Big] \\ h_0\big(f_0\big) & = & \dfrac{1}{2\,(1-\alpha)} \, f_0^2 \\ h_-\big(f_-\big) & = & \dfrac{\lambda^2}{6} \Big[\Big(\alpha^2 - 4 \, \dfrac{f_-}{\lambda} \Big)^{3/2} + 6\,\alpha\,\dfrac{f_-}{\lambda} - \alpha^3 \Big] \,. \end{array} \right. \tag{23}$$

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

$$|\,\varphi\,| \leq \, \alpha \, \lambda \tag{24}$$

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

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

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

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

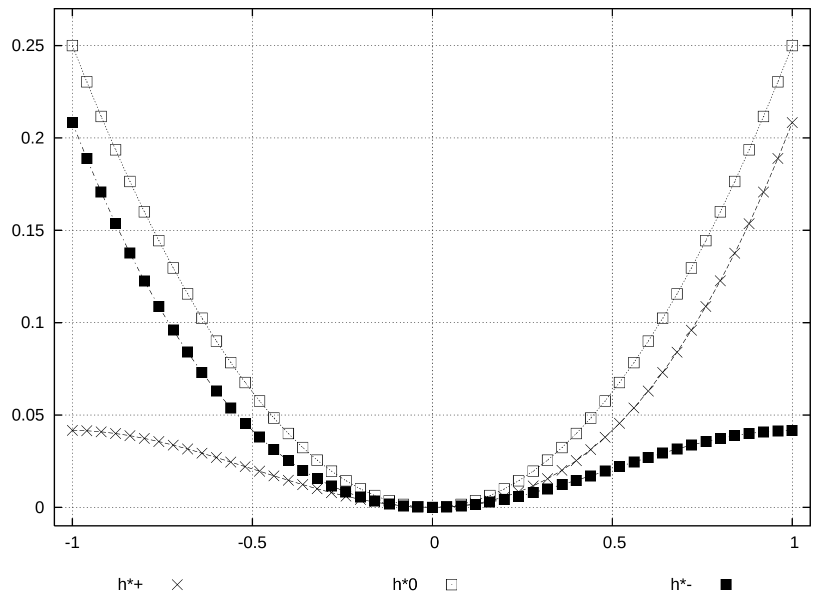

Figure 1. Kinetic decomposition (21) (22) for the Burgers equation with a "centered" D1Q3 scheme ($\alpha = \frac{1}{2}$).

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

$$\big(h^*_+\big)''(\varphi) \,=\, \big(h^*_-\big)''(\varphi) \,+\, \frac{\varphi}{\lambda} \,, \quad \big(h^*_0\big)''(\varphi) \,+\, 2\,\big(h^*_-\big)''(\varphi) \,=\, 1 - \frac{\varphi}{\lambda} \,.$$

In order to have a better stability property than the condition (24) obtained previously, we try to enforce the convexity condition $\big(h_j^*\big)''(\varphi) \geq 0$ if $|\,\varphi\,| \leq \lambda$ instead of (24). For $\varphi \leq 0,$ we propose to replace the inequality $\big(h_+^*\big)''(\varphi) \equiv \big(h_-^*\big)''(\varphi) + \frac{\varphi}{\lambda} \geq 0$ by an equality. Then $\big(h_-^*\big)''(\varphi) = -\frac{\varphi}{\lambda}$ if $\varphi \leq 0$. We deduce $\big(h_+^*\big)''(\varphi) = 0$ and $\big(h_0^*\big)''(\varphi) = 1 + \frac{\varphi}{\lambda}$ if $\varphi \leq 0$. With analogous arguments, we obtain $\big(h_+^*\big)''(\varphi) = \frac{\varphi}{\lambda}$, $\big(h_0^*\big)''(\varphi) = 1 - \frac{\varphi}{\lambda}$ and $\big(h_-^*\big)''(\varphi) = 0$ when $\varphi \geq \lambda$.

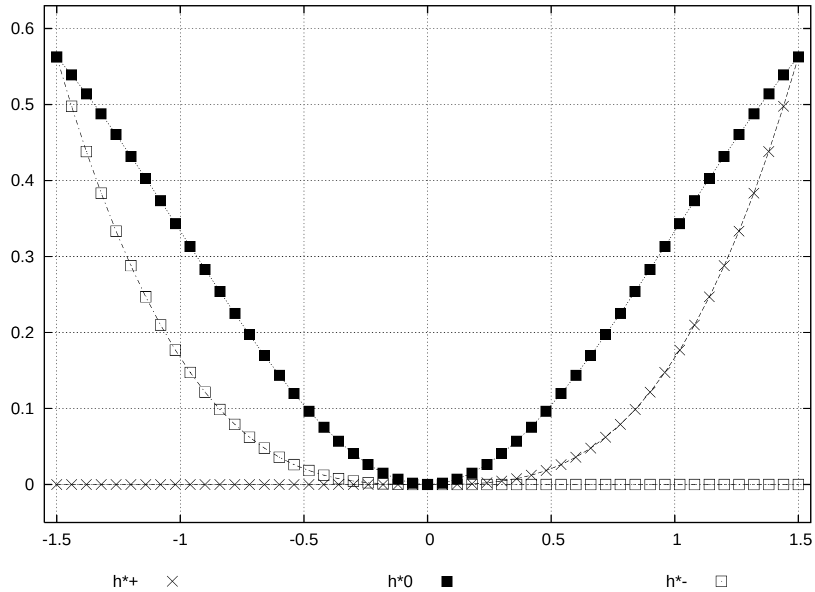

Figure 2. Kinetic decomposition for Burgers equation, equilibria (26) for the lattice Boltzmann upwind scheme D1Q3.

We construct in this way an "upwind" distribution for the decomposition of the dual entropy:

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

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

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

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

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

• 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

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

These two functions represented in Figure 3 are convex if

$$
(30) \qquad |\,\varphi\,| \leq \lambda
$$

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

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

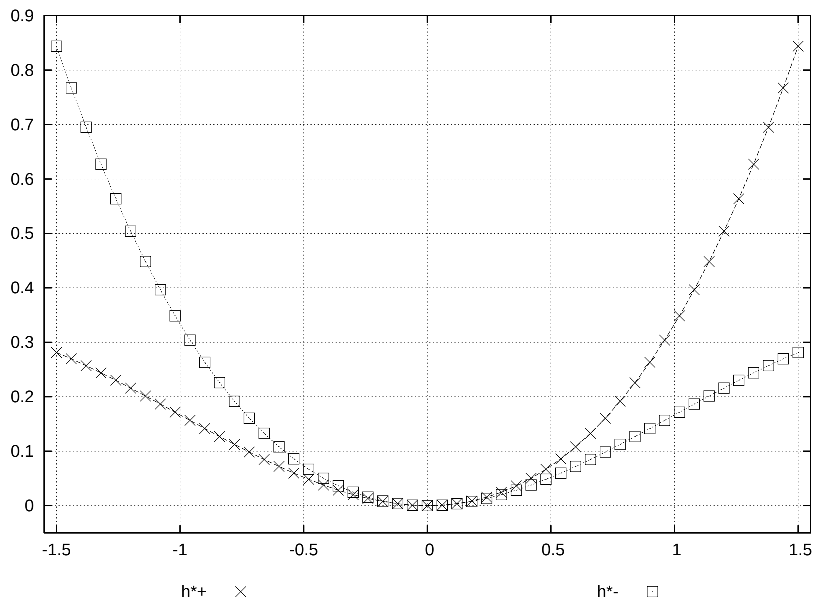

Figure 3. Kinetic decomposition for Burgers ; D1Q2 centered scheme.

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 [11], 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

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

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

$$m^{\mathrm{eq},1} \equiv \Big(u \,,\, \frac{u^2}{2} \,,\, \alpha\, \lambda^2\, u \Big)^{\mathrm{t}} .$$

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

$$m^{\mathrm{eq},2} \equiv \Big(u \,,\, \frac{u^2}{2} \,,\, \lambda \, \mathrm{sgn}(u)\, \frac{u^2}{2} \Big)^{\mathrm{t}} .$$

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 :

$$m^{\mathrm{eq},3} \equiv \Big(u \,,\, \frac{u^2}{2} \Big)^{\mathrm{t}} .$$

• The relaxation step is nonlinear and local in space :

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

with $s_2 = s_3 = 1.7$ in our simulations unless otherwise stated. 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 neighbours.

5) Comparison with finite volumes

• In [13] 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

$$\psi\Big(x + \frac{\Delta x}{2},\, t\Big) = \lambda\, \Big(f_+^*(x,\, t) - f_-^*(x + \Delta x,\, t) \Big) \,. \tag{34}$$

We observe that the resulting lattice Boltzmann scheme is **not** a traditional finite volume scheme (in the sense proposed *e.g.* in [10]) 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). Nevertheless, if $s_2 = s_3 = 1,$ we can give an interpretation of the associated flux (34) because in this case, $f_j^* \equiv f_j^{\rm eq}$ for all j.

• We observe that we can also decompose the "physical" flux $F(\bullet)$ (see the relation (1) or (6) in all generality) under the form $F(u) \equiv F_+(u) + F_-(u)$ with

$$F_+(u) = \lambda\, f_+^{\rm eq}(u)\,, \quad F_-(u) = -\lambda\, f_-^{\rm eq}(u)\,. \qquad (35)$$

We have $F_+\big(u(x,\, t)\big) + F_-\big(u(x+\Delta x,\, t)\big) \,=\, \lambda\, \big(f_+^{\rm eq}\big(u(x,\, t)\big) - f_+^{\rm eq}\big(u(x+\Delta x,\, t)\big)\big)$ and when $s_2 = s_3 = 1$ the numerical flux ψ introduced in (34) admits the classical so-called flux splitting form :

$$\psi\Big(x + \frac{\Delta x}{2},\, t\Big) = F_+\big(u(x,\, t)\big) + F_-\big(u(x+\Delta x,\, t)\big)\,. \qquad (36)$$

With this above link between fluxes and particle distributions (36) it is natural to re-interpret with classical flux decompositions as (35) those proposed in this contribution at relations (25), (27) and (31). As remarked by Bouchut [5], the relations (25) and (31) are associated with two variants of the Lax-Friedrichs scheme (see *e.g.* Lax [25]) whereas the upwind scheme (27) corresponds exactly to the Engquist-Osher [14] scheme !

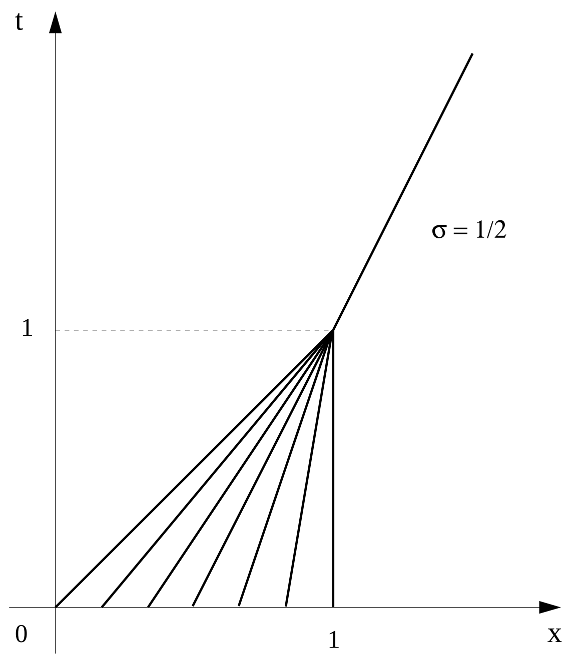

Figure 4. A converging schock wave for the Burgers equation. The decreasing profile (37) at $t = 0$ leads to an admissible discontinuity at $t = 1$. Then a shock wave with velocity $\sigma = \frac{1}{2}$ develops.

6) Test cases

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 physical 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

$$u_0(x) = \begin{cases} 1 & \text{if} \quad x \leq 0 \\ 1 - x & \text{if} \quad 0 \leq x \leq 1 \\ 0 & \text{if} \quad x \geq 1\,. \end{cases} \tag{37}$$

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.* [17], [10] or [25]). It is a challenge if a lattice Boltzmann scheme is able to capture in a systematic way such a discontinuous solution.

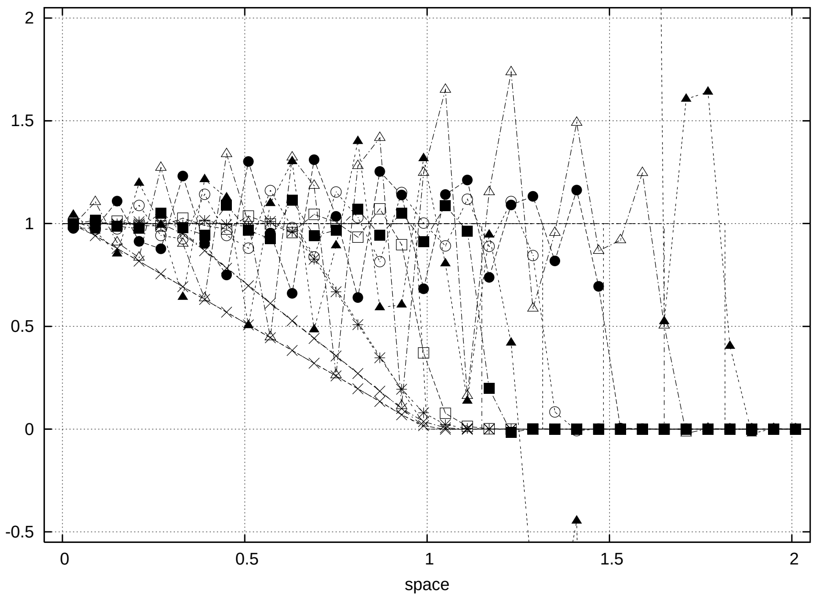

Figure 5. Burgers equation. Instable D1Q3 lattice Boltzmann simulation for a converging shock with equilibrium (25) associated to the parameters $\alpha = \frac{1}{2}$, $s_2 = s_3 = 1.7$ and $\lambda = 1.8$. Computed values are displayed every 10 time steps.

- 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

(38) $$0 < s_j < 2$$

proposed initially by Hénon [20].

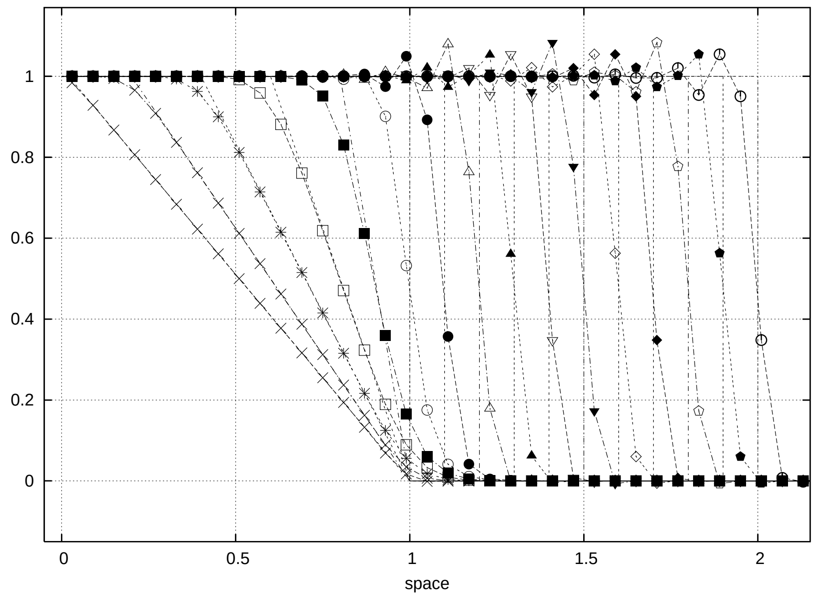

Figure 6. Burgers equation. Stable D1Q3 lattice Boltzmann simulation for a converging shock with equilibrium (25) associated to the parameters $\alpha = \frac{1}{2}$, $\lambda = 3$ and $s_2 = s_3 = 1.7$. Computed values are displayed every 10 time steps.

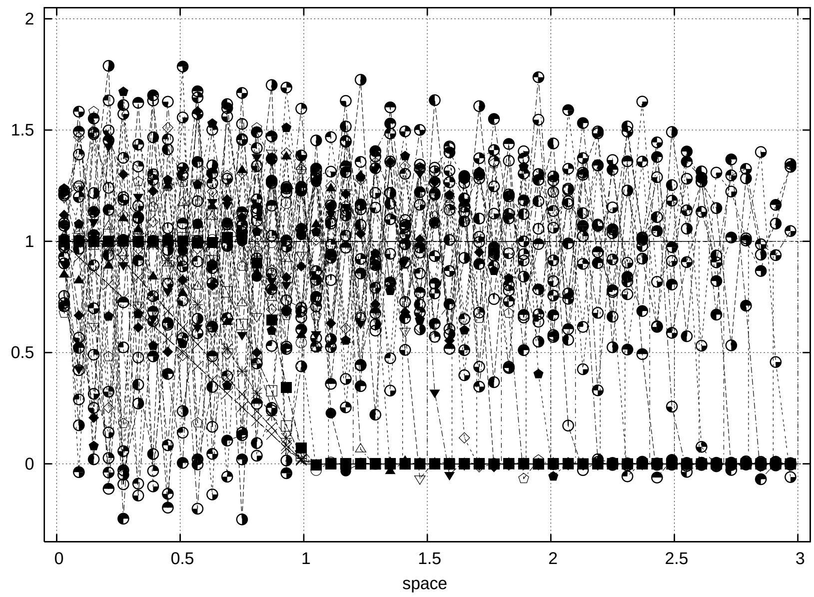

Figure 7. Burgers equation. Same experiment as in Figure 6 except that $s_2 = s_3 = 2$. The numerical algorithm remains stable but is no longer convergent. Computed values are displayed every 10 time steps.

• 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 (38)), the numerical experiment does not give correct results because no entropy is dissipated. But the scheme remains stable as presented on Figure 7 : 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 (38).

• With the same initial condition (37), we use the D1Q3 upwind version (27) of the lattice Boltzmann scheme. Now the stability condition is not so severe as in the previous case and we take $\lambda = 1.1$. The results, presented in Figure 8, are qualitatively analogous to the previous one (see Figure 6). We observe on Figure 8 an alternance of monotonic and over or undershooting discrete shock profiles.

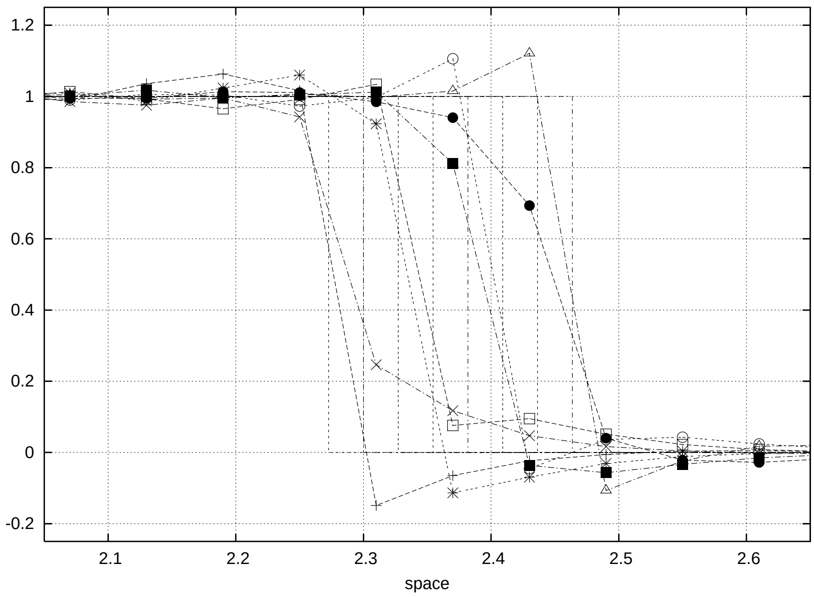

Figure 8. Burgers equation. Stable D1Q3 lattice Boltzmann simulation for a converging shock with upwind equilibrium (27) with $\lambda = 1.1$ and $s_2 = s_3 = 1.7$. Eight consecutive discrete time steps.

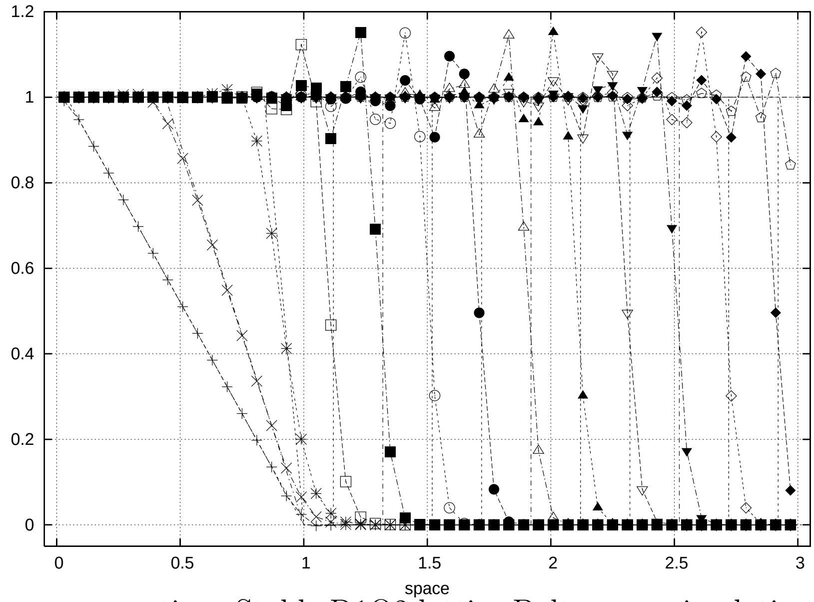

Figure 9. Burgers equation. Stable D1Q2 lattice Boltzmann simulation for a converging shock with quilibrium (31), $\lambda = 1.5$ and $s_2 = 1.7$. Computed values are displayed every 10 time steps.

- With the same decreasing initial condition (37), using the D1Q2 version (31) leads to results presented on Figure 9. We observe only an over-shooting at the discrete shock profile without any under-overshooting.
- In a second set of experiments, we use the very simple "two steps" or "Riemann" initial condition. The first one is simply

$$u_0(x) = \begin{cases} 1 & \text{if} \quad x < 0.2 \\ 0 & \text{if} \quad x > 0.2\,. \end{cases} \tag{39}$$

The entropic solution of this Riemann problem composed by the Burgers equation (1) associated with the initial condition (39) is a discontinuity propagating at the velocity $\sigma = \frac{1}{2}$ (see *e.g.* [17], [10] or [25]). With the numerical schemes introduced previously, this entropy satisfying solution is captured with a precision comparable to finite-volume type methods. The results are presented on Figure 10 for numerical schemes (25), (27) and (31). On Figure 11, a zoom of the previous data shows that this moving shock is captured by a stencil of four to five mesh points.

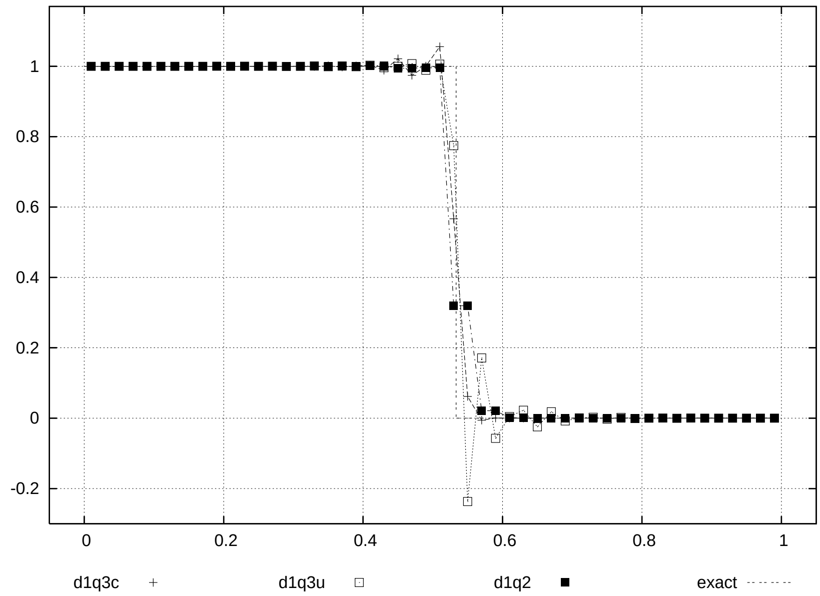

Figure 10. The Riemann problem for the Burgers equation associated with the initial condition (39) develops a shock wave. The figures shows the numerical solutions with the three variants of the scheme after 100 discrete time steps and parameters $\lambda = 3$ and $s_2 = s_3 = 1.7$.

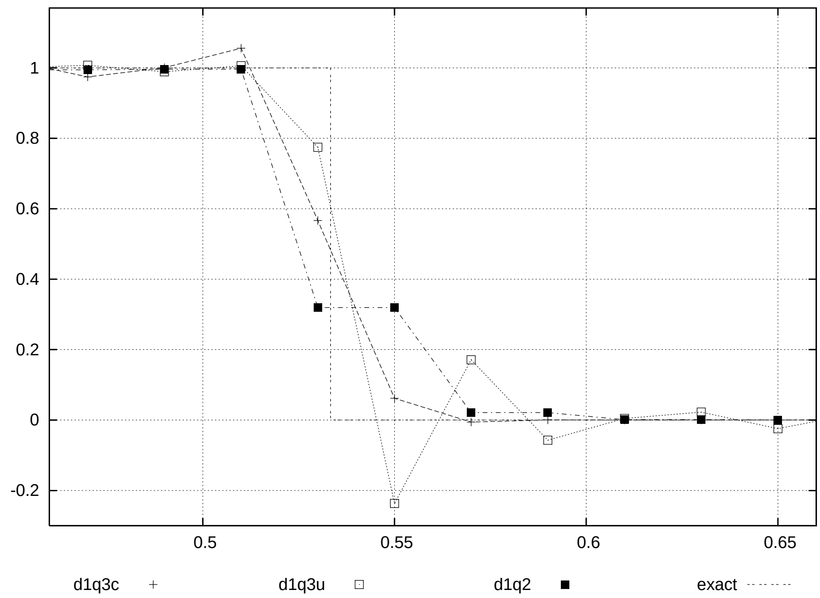

Figure 11. Zoom of Figure 10 around the location of the shock wave.

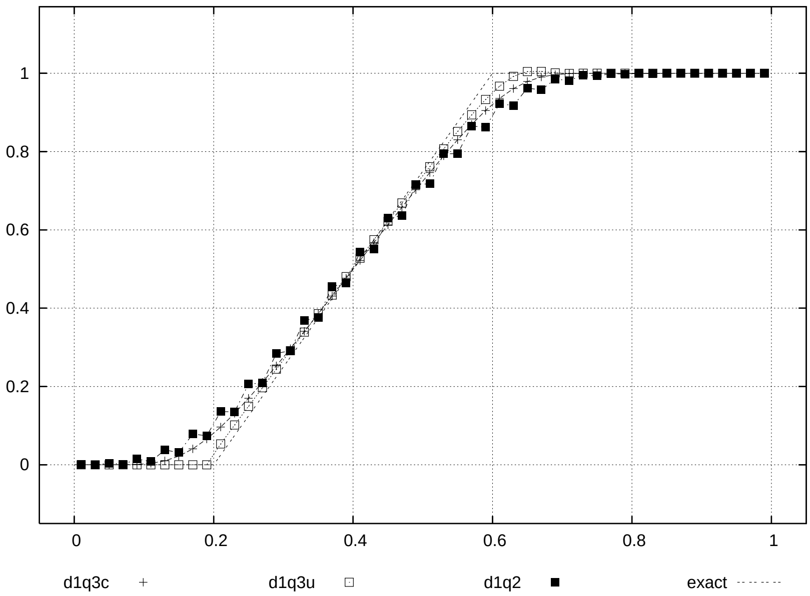

Figure 12. The Riemann problem for the Burgers equation associated with the initial condition (40) develops a rarefaction wave. Numerical solutions with the three variants of the lattice Boltzmann scheme after 100 discrete time steps and parameters $\lambda = 3$, $s_2 = s_3 = 1.7$.

• We reverse the values 0 and 1 in the initial condition (39) and obtain in this way a new initial condition :

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

The entropic solution of (1)(40) is a rarefaction wave : a continuous solution with two constant states and a self-similar component as detailed *e.g.* [17], [10] or [25]. Without any modification of the scheme, the numerical solution with the three previous variants are presented on Figure 12. At the tricky zones of the foot (Figure 13) and the top (Figure 14) of the rarefaction, the slope is discontinuous and the solution of the problem (1)(40) 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, a convex-satisfying lattice Boltzmann scheme associated with a particle decomposition (20) of the dual entropy 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) could be welcomed. 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 (40).

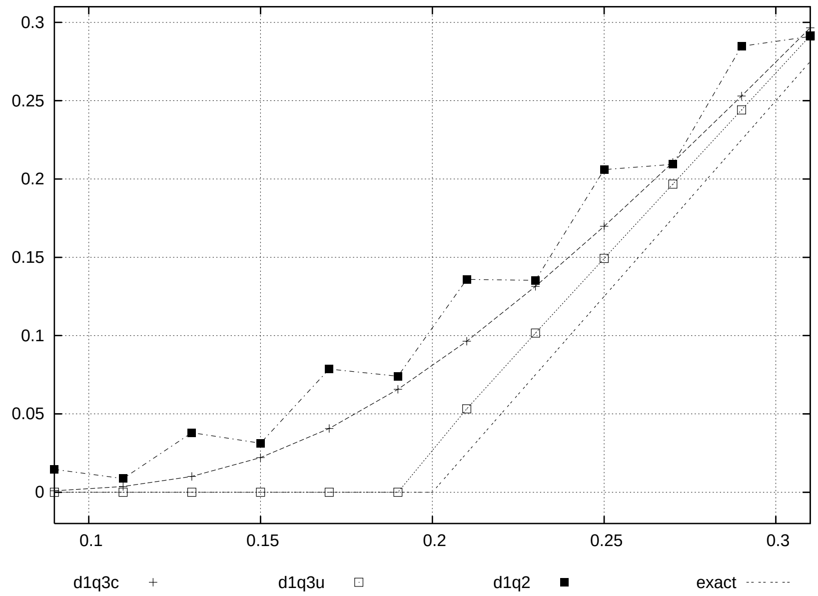

Figure 13. Zoom of Figure 12 at the foot of the rarefaction.

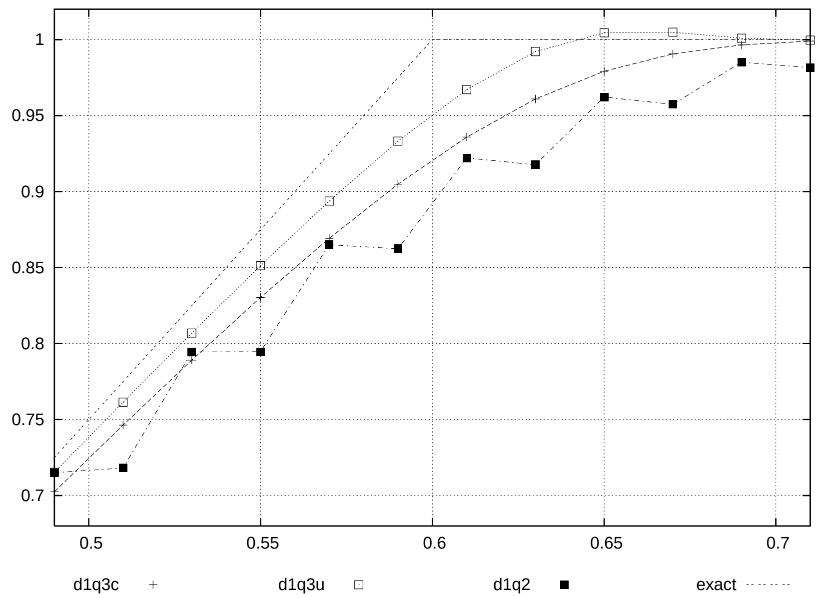

Figure 14. Zoom of Figure 12 at the top of the rarefaction.

7) Systems of conservation laws

• The extension of the previous ideas from scalar equation to hyperbolic systems is a difficult task. We first consider the example of one-dimensional linear acoustics to fix the ideas. We recall that we can write this physical model as an hyperbolic system of first order :

$$\partial_t \begin{pmatrix} \rho \\ q \end{pmatrix} + \partial_\alpha \begin{pmatrix} q \\ c_0^2\, \rho \end{pmatrix} = 0\,. \tag{41}$$

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

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

The entropy variables are the gradients of the entropy (42) relative to the conserved variables $(\rho,\, q)$ and we have

(43) $$\varphi = \Big(\rho\,,\frac{q}{c_0^2}\Big)\,.$$

The associated entropy flux $\zeta(W)$ is easy to determine and $\zeta(W) = \rho\, q$. The dual entropy $\eta^*(\varphi) \equiv \varphi {\scriptstyle\bullet} W - \eta(W)$ and the dual entropy flux $\zeta^*(\varphi) \equiv \varphi {\scriptstyle\bullet} F(W) - \zeta(W)$ can be evaluated without difficulty and we obtain

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

all is quadratic in this system !

• We approach the system (41) 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 $\varphi {\scriptstyle\bullet} M_j$ introduced in (12) are given according to

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

The identities (13) take now the form

(46) $$\left\{ \begin{array}{ll} h_+^*\big(\varphi \bullet M_+\big) + h_0^*\big(\varphi \bullet M_0\big) + h_-^*\big(\varphi \bullet M_-\big) & \equiv \eta^*(\varphi) \\ \lambda\, h_+^*\big(\varphi \bullet M_+\big) - \lambda\, h_-^*\big(\varphi \bullet M_-\big) & \equiv \zeta^*(\varphi)\,. \end{array} \right.$$

We search a possible solution of system (46) 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 (46) leads to

(47) $$\left\{ \begin{array}{lll} h_+^*\Big(\rho + \dfrac{\lambda\, q}{c_0^2}\Big) & = & \dfrac{c_0^2}{4\,\lambda^2}\Big(\rho + \dfrac{\lambda\, q}{c_0^2}\Big)^2 \\ h_0^*(\rho) & = & \dfrac{1}{2}\Big(1 - \dfrac{c_0^2}{\lambda^2}\Big)\,\rho^2 \\ h_-^*\Big(\rho - \dfrac{\lambda\, q}{c_0^2}\Big) & = & \dfrac{c_0^2}{4\,\lambda^2}\Big(\rho - \dfrac{\lambda\, q}{c_0^2}\Big)^2\,. \end{array} \right.$$

The functions proposed in (47) are convex under the stability condition :

$$|\, c_0 \,| \leq \lambda\,.$$

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.* [25]). A microscopic entropy $H(f) = h_+(f_+) + h_0(f_0) + h_-(f_-)$ can be easily derived from (47) with the following contributors :

$$h_+\big(f_+\big) = \frac{\lambda^2}{c_0^2}\, f_+^2\,, \quad h_0\big(f_0\big) = \frac{1}{2\Big(1 - \dfrac{c_0^2}{\lambda^2}\Big)}\, f_0^2\,, \quad h_-\big(f_-\big) = \frac{\lambda^2}{c_0^2}\, f_-^2\,.$$

The particle distribution $f_j^{\rm eq}$ at equilibrium is a direct consequence of relations (17) and (47) and we have

$$f_+^{\rm eq} \,=\, \frac{c_0^2}{2\,\lambda^2}\,\Big(\rho+\frac{\lambda\,q}{c_0^2}\Big)\,,\quad f_0^{\rm eq} \,=\, \frac{1}{2}\Big(1-\frac{c_0^2}{\lambda^2}\Big)\,\rho\,,\quad f_-^{\rm eq} \,=\, \frac{c_0^2}{2\,\lambda^2}\,\Big(\rho-\frac{\lambda\,q}{c_0^2}\Big)\,. \qquad (48)$$

In terms of moments, the relations (48) reduce to $m_3^{\rm eq} \,=\, c_0^2\,\rho$ as used classically since the work [24] of Lallemand and Luo !

• In the case of shallow water equations at one space dimension we can apply the program presented above for the linear acoustic model and try to represent the dual entropy with the help of a D1Q3 particle distribution. More precisely, we consider the one-dimensional system of conservation laws due to A. Barré de Saint Venant :

$$\left\{ \begin{array}{ll} \partial_t\rho+\partial_x q & =0 \\ \partial_t q+\partial_x\Big(\dfrac{q^2}{\rho}+k\,\rho^\gamma\Big) & =0 \end{array} \right. \qquad (49)$$

where $k>0$ and $\gamma>1$ are given positive constants. We introduce velocity u, pressure p and sound velocity $c>0$ according to the relations

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

Then the entropy η and the entropy flux ζ satisfy

$$\eta\,=\,\frac{1}{2}\rho\,u^2+\frac{p}{\gamma-1}\,,\quad \zeta\,=\,\eta\,u+p\,u\,; \qquad (50)$$

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 :

$$\eta^*\,=\,K\left(\alpha+\frac{\beta^2}{2}\right)^{\frac{\gamma}{\gamma-1}}\,,\quad \zeta^*\,=\,K\left(\alpha+\frac{\beta^2}{2}\right)^{\frac{\gamma}{\gamma-1}}\beta\,,\quad K=k\left(\frac{\gamma-1}{\gamma\,k}\right)^{\frac{\gamma}{\gamma-1}}\,. \qquad (51)$$

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

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

The unknown convex functions h_j^* satisfy the identities (46) and take now the form

$$\left\{ \begin{array}{ll} h_+^*(\varphi_+)+h_0^*(\varphi_0)+h_-^*(\varphi_-) & =\,K\left(\alpha+\dfrac{\beta^2}{2}\right)^{\frac{\gamma}{\gamma-1}} \\ \lambda\,h_+^*(\varphi_+)-\lambda\,h_-^*(\varphi_-) & =\,K\left(\alpha+\dfrac{\beta^2}{2}\right)^{\frac{\gamma}{\gamma-1}}\beta\,. \end{array} \right. \qquad (52)$$

• We prove in the following that the system of equations (52) where the unknowns are the convex functions h_j^* has no solution. In order to establish this property, we introduce the equilibrium distributions $f_j^{\rm eq}$ according to (17). We differentiate the relations (52) relatively to α and β. We obtain

$$(53) \qquad \left\{ \begin{array}{ll} f_+^{\rm eq}(\alpha + \lambda\,\beta) + f_0^{\rm eq}(\alpha) + f_-^{\rm eq}(\alpha - \lambda\,\beta) & = \rho \\ \lambda\, f_+^{\rm eq}(\alpha + \lambda\,\beta) - \lambda\, f_-^{\rm eq}(\alpha - \lambda\,\beta) & = \rho\, u \\ \lambda^2\, f_+^{\rm eq}(\alpha + \lambda\,\beta) + \lambda^2\, f_-^{\rm eq}(\alpha - \lambda\,\beta) & = \rho\, u^2 + p\,. \end{array} \right.$$

and we are supposed to determine an increasing function $f_0^{\rm eq}$ of **only one** real variable such that

$$(54) \qquad f_0^{\rm eq}\Big(\frac{c^2}{\gamma - 1} - \frac{u^2}{2} \Big) \,\equiv\, \rho - \frac{1}{\lambda^2} \big(\rho\, u^2 + p \big)\,.$$

Due to the elementary calculus $\frac{{\rm d}c^2}{{\rm d}\rho} = \gamma\, k\, (\gamma - 1) \rho^{\gamma - 2} = (\gamma - 1) \frac{c^2}{\rho}$, we differentiate the relation (54) relative to ρ and independently relatively to u. We obtain

$$(55) \qquad \frac{c^2}{\rho}\, \big(f_0^{\rm eq}\big)'(\alpha) + \frac{1}{\lambda^2} \big(u^2 + c^2 \big) = 1\,, \quad -u\, \big(f_0^{\rm eq}\big)'(\alpha) + \frac{2\, \rho\, u}{\lambda^2} = 0\,.$$

We extract the derivative $(f_0^{\rm eq})'(\alpha)$ from the second equation of (55) and report the result in the first equation. We deduce

$$u^2 + 3\, c^2 = \lambda^2$$

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

• As a summary of this section, the generalization of what have been done in this contribution for the Burgers equation is absolutely nontrivial and mathematically impossible for the familiar nonlinear system of Saint-Venant equations. One idea is to keep the approach as a possible approximation of systems of conservation laws.

8) Conclusion and perspectives

• We first propose a summary of the algebraic work that has to be done in order to determine in which domain a given lattice Boltzmann scheme is stable in the sense proposed by Bouchut [3]. If very interesting results are computed with a very good lattice Boltzmann scheme in the framework proposed by d'Humières [11], we first determine the conserved variables $W_k \equiv \sum_j M_{kj}\, f_j$. Then the convective fluxes follow the relation $F_{\alpha k}(W) \,\equiv\, \sum_j M_{kj}\, v_j^\alpha\, f_j^{\rm eq}$. First it is necessary to have a kinetic decomposition of the entropy and the associated entropy flux of the type $\eta(W) = \sum_j h_j(f_j^{\rm eq})$ and $\zeta_\alpha(W) = \sum_j v_j^\alpha\, h_j(f_j^{\rm eq})$. 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 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 "s" parameters of the lattice Boltzmann scheme. It remains open for as 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 observe that the situation for systems is very tricky ! Progress could result from t he use of a **vectorial** particle distribution as initially proposed by Khobalatte and Perthame in [23] and developed by Bouchut [2] 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, as suggested by He, Chen and Doolen [19], Dellar [9] and used by Peng, Shu and Chew [27] 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.

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