Simulation of strong nonlinear waves with vectorial lattice Boltzmann schemes

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17 November 2013 *

\textbf{Abstract.} We show that an hyperbolic system with a mathematical entropy can be discretized with vectorial lattice Boltzmann schemes with the methodology of kinetic representation of the dual entropy. We test this approach for the shallow water equations in one and two space dimensions. We obtain interesting results for a shock tube, reflection of a shock wave and unstationary two-dimensional propagation. This contribution shows the ability of vectorial lattice Boltzmann schemes to simulate strong nonlinear waves in unstationary situations.

\textbf{Keywords:} hyperbolic conservation laws, entropy, shock wave, shallow water equations.
\textbf{PACS numbers:} 02.70.Ns, 05.20.Dd, 47.10.+g, 47.11.+j.

\begin{small}
\textsuperscript{*} Contribution submitted to \textit{International Journal of Modern Physics C}, presented at the 22th International Conference on the Discrete Simulation of Fluid Dynamics, Yerevan, Armenia, 15-19 July 2013. Edition 02 January 2014.
\end{small}
Introduction

- 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 [2] and Elton et al. [10]). With the lattice Boltzmann methods described *e.g.* by Lallemand and Luo [18], first tentative were proposed by d’Humières [14], Alexander *et al.* [1] among others. A D1Q2 entropic scheme for the one-dimensional viscous Burgers equation has been developed by Boghosian *et al.* [3]. The extension for gas dynamics equations and in particular shock tubes problems is studied in the works of Philippi *et al.* [20], Nie, Shan and Chen [19], Karlin and Asinari [15], Chikatamarla and Karlin [6].

- In this contribution, we experiment the ability of lattice Boltzmann schemes to approach weak entropy solutions of hyperbolic equations. It is well known that a first order hyperbolic equation exhibits shock waves. In order to enforce the uniqueness, the notion of mathematical entropy has been proposed by Godunov [13] and Friedrichs-Lax [12]. A mathematical entropy is a strictly convex function of the conserved variables satisfying *ad hoc* differential constraints to ensure a complementary conservation law for regular solutions (see *e.g.* our book with Després [8]). The gradient of the entropy defines the so-called “entropy variables”. The Legendre-Fenchel-Moreau duality for convex functions allows us to define the dual of the entropy; it is a convex function of the entropy variables.

- We start from the mathematical framework developed by Bouchut [5] making the link between the finite volume method and kinetic models in the framework of the BGK approximation. The key notion is the representation of the dual entropy with the help of convex functions associated with the discrete velocities of the lattice. If we suppose that a single distribution of particles is present, our previous contribution [9] shows that the Burgers equation can be simulated. We have shown also that the approach can be extended to the nonlinear wave equation but is not compatible with the system of shallow water equations.

- In section 1, we develop vectorial lattice Boltzmann schemes with kinetic representation of the dual entropy. This framework is applied in section 2 for the approximation of one-dimensional shallow water equations and in section 3 for the two-dimensional case. Stationary and unstationary two-dimensional simulations are presented in section 4.

1) Dual entropy vectorial lattice Boltzmann schemes

- In order to treat complex physics with particle like methods, a classical idea is to multiply the number of particle distributions, as proposed by Khobalatte and Perthame [17], Shan and Chen [21], Bouchut [4], Dellar [7], Wang *et al.* [22]. We follow here the idea of dual entropy decomposition with vectorial particle distributions proposed by Bouchut [5]. We consider an hyperbolic system composed by $N$ conservation laws with space described by a point in $x \in \mathbb{R}^d$. The unknowns are the conserved variables $W \in \mathbb{R}^N$. 

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(i.e. \(W^k \in \mathbb{R}\)). The nonlinear physical fluxes: \(F_\alpha(W) \in \mathbb{R}^N\) (with \(1 \leq \alpha \leq d\)) are given regular functions. The system is of first order:

\[
\partial_t W^k + \sum_{\alpha=1}^d \partial_\alpha F_\alpha^k(W) = 0, \quad 1 \leq k \leq N.
\]

We suppose that a mathematical entropy \(\eta(W)\) is given with the associated entropy fluxes \(\zeta_\alpha(W)\) for \(0 \leq \alpha \leq d\):

\[
d\zeta_\alpha(W) \equiv d\eta(W) \cdot dF_\alpha(W), \quad 1 \leq \alpha \leq d.
\]

The entropy variables \(\varphi_k \equiv \frac{\partial \eta(W)}{\partial W^k}\) are defined as the jacobian of the entropy:

\[
d\eta(W) \equiv \sum_{k=1}^N \varphi_k dW^k.
\]

The dual entropy \(\eta^*(\varphi)\) and the so-called “dual entropy fluxes” \(\zeta_\alpha^*(\varphi)\) satisfy

\[
\eta^*(\varphi) = \varphi \cdot W - \eta(W), \quad \zeta_\alpha^*(\varphi) \equiv \varphi \cdot F_\alpha(W) - \zeta_\alpha(W).
\]

They can be differentiated without difficulty (see e.g. [8]):

\[
d\eta^*(\varphi) \equiv \sum_k d\varphi_k W^k, \quad d\zeta_\alpha^*(\varphi) \equiv \sum_k d\varphi_k F_\alpha^k(W).
\]

- With Bouchut [5], we introduce \(N\) particle distributions \(f_j^k\) (for \(1 \leq k \leq N\)) and \(q\) velocities (\(0 \leq j \leq q - 1\)). The conserved moments \(W^k\) are simply the first discrete integral of these distribution:

\[
W^k = \sum_{j=0}^{q-1} f_j^k, \quad 1 \leq k \leq N.
\]

We suppose that the particle distributions \(f_j^k\) are solution of the Boltzmann equations with discrete velocities:

\[
\partial_t f_j^k + v_j^\alpha \partial_\alpha f_j^k = Q_j^k, \quad 0 \leq j \leq q - 1, \quad 1 \leq k \leq N
\]

We suppose \(\sum_j Q_j^k = 0\) in order to enforce the conservation laws (1). The nonequilibrium fluxes take the natural form \(\Phi_\alpha^k \equiv \sum_j v_j^\alpha f_j^k\) and we have a system of \(N\) conservation laws:

\[
\partial_t W^k + \sum_\alpha \partial_\alpha F_\alpha^k = 0, \quad 1 \leq k \leq N.
\]

- In the following, we call the “Perthame-Bouchut hypothesis” the fact that the dual mathematical entropy \(\eta^*(\varphi)\) can be is decomposed into \(q\) scalar potentials \(h_j^\varphi\). The potentials \(h_j^\varphi\) are supposed to be regular convex functions of the entropy variables \(\varphi\) and satisfy the two identities

\[
\sum_{j=0}^{q-1} h_j^\varphi(\varphi) \equiv \eta^*(\varphi), \quad \sum_{j=0}^{q-1} v_j^\alpha h_j^\varphi(\varphi) \equiv \zeta_\alpha^*(\varphi), \quad \forall \varphi.
\]
The equilibrium fluxes \((f_{eq})^k_j\) are easy to derive from the potentials \(h_j^*\): and we have
\[
(f_{eq})^k_j = \frac{\partial h_j^*}{\partial \varphi_k}, \quad \sum_{j=0}^{q-1} (f_{eq})^k_j = W^k, \quad 1 \leq k \leq N
\]

- We introduce the Legendre dual of the convex potentials \(h_j^*\):

\[
h_j(f_j, f_{j1}^2, \ldots, f_{jN}^N) \equiv \sup_{\varphi} \left( \left[ \sum_{k=1}^{N} \varphi_k f_j^k \right] - h_j^*(\varphi) \right), \quad 0 \leq j \leq q - 1.
\]

We observe that each function \(h_j(\bullet)\) is a convex function of \(N\) variables. The so-called “microscopic entropy”
\[
H(f) \equiv \sum_{j=0}^{q-1} h_j(f_j^1, f_j^2, \ldots, f_j^N).
\]

It is a convex function in the domain where the \(h_j^*\)’s are convex.

- We can establish a “H-theorem” for the continuous dynamics relative to time and space, in a way similar to the maximal entropy approach developed by Karlin and his co-workers [16]. Under a BGK type hypothesis

\[
Q_k^j \equiv \frac{1}{\tau} \left( (f_{eq})^k_j - f_j^k \right)
\]

we have
\[
\partial_t H(f) + \sum_{\alpha} \partial_{\alpha} \left( \sum_j v_j^\alpha h_j(f_j^*) \right) \leq 0.
\]

- To establish this result, we derive the microscopic entropy relative to time:

\[
\frac{\partial H}{\partial t} = \sum_{jk} \frac{\partial h_j}{\partial f_j^k} \frac{\partial f_j^k}{\partial t} = \sum_{jk} \frac{\partial h_j}{\partial f_j^k} v_j^\alpha \partial_{\alpha} f_j^k = \sum_{jk} \frac{\partial h_j}{\partial f_j^k} Q_j^k - \sum_{jk} \frac{\partial h_j}{\partial f_j^k} \left( \sum_{j=0}^{q-1} v_j^\alpha h_j \right).
\]

Then
\[
\frac{\partial H}{\partial t} + \partial_{\alpha} \left( \sum_j v_j^\alpha h_j \right) = \frac{1}{\tau} \sum_{jk} \frac{\partial h_j}{\partial f_j^k} \left( (f_{eq})^k_j - f_j^k \right) \leq \frac{1}{\tau} \sum_{jk} \frac{\partial h_j}{\partial f_j^k} \left( (f_{eq})^k_j - f_j^k \right)
\]

by convexity of the potentials \(h_j^*\). This last expression is equal to
\[
\frac{1}{\tau} \sum_{jk} \varphi_k \left[ (f_{eq})^k_j - f_j^k \right]
\]

due to Legendre duality:
\[
\frac{\partial h_j}{\partial f_j^k} (f_{eq}) = \varphi_k.
\]

In consequence,
\[
\frac{\partial H}{\partial t} + \partial_{\alpha} \left( \sum_j v_j^\alpha h_j \right) \leq \sum_k \varphi_k \sum_j \left[ (f_{eq})^k_j - f_j^k \right] = 0
\]

by construction of the values \(f_{eq}\) at equilibrium. The H-theorem is proven. \(\square\)

2) “D1Q3Q2” lattice Boltzmann scheme for shallow water

- We apply the previous ideas to the shallow water equations in one space dimension
\[
\partial_t \rho + \partial_x q = 0, \quad \partial_t q + \partial_x \left( \frac{q^2}{\rho} + \frac{p_0}{\rho_0^\gamma} \rho^\gamma \right) = 0.
\]
Velocity $u$, pressure $p$ and sound velocity $c > 0$ are given through the expressions:

$$u = \frac{q}{\rho}, \quad p = \frac{p_0}{\rho_0} \rho^\gamma, \quad c^2 = \frac{\gamma p}{\rho} = \frac{\gamma}{\rho_0} \rho^\gamma - 1.$$

The entropy $\eta$ and the entropy flux $\zeta$ can be explicited without difficulty (see e.g. [9]):

$$\eta = \frac{1}{2} \rho u^2 + \frac{p}{\gamma - 1}, \quad \zeta = \eta u + p u.$$

Then the entropy variables $\varphi = (\theta \equiv \partial_\rho \eta, \beta \equiv \partial_q \eta)$ can be related to usual ones:

$$\theta = \frac{c^2}{\gamma - 1} - \frac{u^2}{2}, \quad \beta = u.$$

Thanks to (2), the dual entropy $\eta^*$ and the dual entropy flux $\zeta^*$ can be explicited: $\eta^* = p$ and $\zeta^* = pu$. We observe that $p = K (\theta + \beta^2 / 2^2)$ with $K = p_0 / c_0^4$ when $\gamma = 2$.

- We model this system with a kinetic approach and a D1Q3 stencil. We have to find the particle components of the entropy variables, id est (still unknown) convex functions $h^*_j$ satisfying the Perthame-Bouchut hypothesis (4), that now can be written under the form:

$$(5) \quad h^*_+(\theta, \beta) + h^*_0(\theta, \beta) + h^*_-(\theta, \beta) = p, \quad \lambda h^*_+(\theta, \beta) - \lambda h^*_-(\theta, \beta) = pu,$$

where $\lambda \equiv \frac{\Delta x}{\Delta t}$ is the numerical velocity of the mesh. We use a simple quadratic function as in our previous contribution [9]. We suggest when $\gamma = 2$:

$$h^*_0 = h^*_0(\theta) = \frac{a}{2} K \theta^2,$$

with the introduction of a parameter $a$ that has to be precised for real computations. With this choice (6), the resolution of the system (5) with unknowns $h^*_\pm$ is easy:

$$(7) \quad h^*_\pm(\theta, \beta) = \frac{K}{2} \left( \frac{\theta^2}{\lambda} + \frac{\beta^2}{2} \right) \left( 1 \pm \frac{\beta}{\lambda} \right) - \frac{a K}{4} \theta^2.$$

- From the previous potentials (6) and (7), it is possible to derive the entire distribution at equilibrium. Observe first that with a vectorial lattice Boltzmann scheme, it is necessary to use two families $f$ and $g$ of particle distributions, one relative to mass conservation and the other to momentum conservation. We have in this case

$$(8) \quad f_{j0}^{eq} = \frac{\partial h^*_j}{\partial \theta}, \quad g_{j0}^{eq} = \frac{\partial h^*_j}{\partial \beta}.$$
The relaxation step of the scheme is particularly simple when all the relaxation parameters are equal to a constant value \( \tau \) as proposed in the BGK hypothesis. When a general MRT scheme is used, we follow the rule \( [18] \) of the moments \( m^*_\ell \) after relaxation:

\[
m^*_\ell = m_\ell + s_\ell \left( m^\text{eq}_\ell - m_\ell \right).
\]

- We have tested the previous ideas for a Riemann problem (a shock type tube). We have chosen the following numerical data and parameters:

\[
\gamma = 2, \quad \frac{\rho_\ell}{\rho_0} = 2, \quad \frac{\rho_r}{\rho_0} = 0.5, \quad q_\ell = q_r = 0, \quad \frac{\lambda}{c_0} = 8, \quad a = 0.15, \quad s_j \equiv 1.8.
\]

The numerical results are displayed on Fig. 1. The rarefaction wave (on the left) and the shock wave (on the right) are correctly captured.

![Figure 1. Riemann problem for shallow water equations. Density (blue, top) and velocity (pink, bottom) fields computed with the D1Q3Q2 lattice Boltzmann scheme with 80 mesh points and compared to the exact solution.](image)

3) "D2Q5Q4Q4" vectorial lattice Boltzmann scheme

- We study now the two-dimensional shallow water equations

\[
\begin{aligned}
\partial_t \rho + \partial_x (\rho u) + \partial_y (\rho v) &= 0 \\
\partial_t (\rho u) + \partial_x (\rho u^2 + \frac{p_0}{\rho_0^2} \rho^2) + \partial_y (\rho u v) &= 0 \\
\partial_t (\rho v) + \partial_x (\rho u v) + \partial_y (\rho v^2 + \frac{p_0}{\rho_0^2} \rho^2) &= 0.
\end{aligned}
\]

We have three conservation laws in two space dimensions. We extend the previous D1Q3Q2 vectorial lattice Boltzmann scheme into a D2Q5Q4Q4 scheme. The D2Q5 stencil is associated to the following velocities:

\[
v_0 = (0, 0), \quad v_1 = (\lambda, 0), \quad v_2 = (0, \lambda), \quad v_3 = (-\lambda, 0), \quad v_4 = (0, -\lambda).
\]

We have now three particle distributions: \( f \in \text{D2Q5} \), \( g_x \in \text{D2Q4} \) and \( g_y \in \text{D2Q4} \). The natural question is to find an intrinsic method to determine the equilibrium values \( f^\text{eq}_j \) for \( 0 \leq j \leq 4 \) and \( (g^\text{eq}_{xj}, g^\text{eq}_{yj}) \) for \( 1 \leq j \leq 4 \). As in the one-dimensional case, a key
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point is to be able to explicit the dual entropy. In this two-dimensional case, the entropy variables \( \varphi \in \mathbb{R}^3 \) can be written as

\[
\varphi = (\theta , u , v), \quad \theta = \frac{\partial \eta}{\partial \rho} = \frac{c^2}{\gamma - 1} - \frac{u^2 + v^2}{2}.
\]

We have now as suggested in (9):

\[
\eta^*(\theta , u , v) \equiv p = \frac{\rho_0}{2c_0^2} \left( \theta + \frac{1}{2}(u^2 + v^2) \right)^2.
\]

In order to determine the equilibrium distributions, we search convex functions \( h^*_j(\theta , u , v) \) for \( 0 \leq j \leq 4 \) such that the first set of Perthame-Bouchut conditions (4) are satisfied:

\[
\sum_{j=0}^{4} h^*_j(\theta , u , v) \equiv \eta^*(\theta , u , v).
\]

Then

\[
f^\text{eq}_j = \frac{\partial h^*_j}{\partial \theta}, \quad g^\text{eq}_{xj} = \frac{\partial h^*_j}{\partial u}, \quad g^\text{eq}_{yj} = \frac{\partial h^*_j}{\partial v}.
\]

We have also to take into account the dual entropy fluxes \( \zeta_\alpha \) in order to represent correctly the first order terms of the model (1) or (9) in our case. With second set of Perthame-Bouchut conditions (4):

\[
\sum_{j=0}^{4} v^2_j h^*_j(\theta , u , v) \equiv \eta^* u, \quad \sum_{j=0}^{4} v^2_j h^*_j(\theta , u , v) \equiv \eta^* v.
\]

For the D2Q5 stencil, the conditions of (11) (12) take the form

\[
\begin{align*}
\sum_{j=0}^{4} h^*_0(\theta) + h^*_1 + h^*_2 + h^*_3 &\equiv p, \quad \lambda \left(h^*_1 - h^*_3\right) \equiv pu, \quad \lambda \left(h^*_2 - h^*_4\right) \equiv pv.
\end{align*}
\]

We mimic for shallow water in two space dimensions what we have done for the one-dimensional case (6) and we suggest here to set

\[
h^*_0(\theta) = \frac{a}{2} K \theta^2
\]

as previously. Because this function \( h^*_0 \) does not depend explicitly on the variables \( u \) and \( v \), we are not defining a D1Q5Q5Q5 scheme but simply a D1Q5Q4Q4 vectorial lattice Boltzmann scheme! The positive parameter \( a \) has to be fixed at best. Nevertheless, we have still a lot of degrees of freedom. We suggest moreover to cut into two part the first relation of (13):

\[
\begin{align*}
h^*_1 + h^*_3 &= \frac{1}{2} \left(p - h^*_0\right), \quad h^*_2 + h^*_4 &= \frac{1}{2} \left(p - h^*_0\right).
\end{align*}
\]

We have now a set of 5 independent equations (6) (13) and (14) with 5 unknowns \( h^*_j \). The end of the algebraic resolution of the system (6), (13) and (14) is completely elementary.

When the potentials \( h^*_j \) are known, the computation of the equilibrium values is easy. With the 5+4+4=13 particle distributions, we can construct 13 moments for the D2Q5Q4Q4 lattice Boltzmann scheme. We suggest the following 5 moments associated with the distribution \( f_j \):

\[
\begin{align*}
\rho &= f_0 + f_1 + f_2 + f_3 + f_4, \quad J_{x,\rho} = \lambda \left(f_1 - f_3\right), \quad J_{y,\rho} = \lambda \left(f_2 - f_4\right),
\end{align*}
\]

\[
\begin{align*}
\varepsilon_\rho &= f_1 + f_2 + f_3 + f_4 - 4 f_0, \quad XX_\rho = f_1 - f_2 + f_3 - f_4.
\end{align*}
\]
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For the 8 moments relative to the distributions \( g_{xj} \) and \( g_{yj} \), we have chosen
\[
\begin{align*}
q_x &= g_{x1} + g_{x2} + g_{x3} + g_{x4}, \\
f_{xx} &= \lambda (g_{x1} - g_{x3}), \\
XX_u &= g_{x1} - g_{x2} + g_{x3} - g_{x4}, \\
f_{xy} &= \lambda (g_{x2} - g_{x4}),
\end{align*}
\]
and
\[
\begin{align*}
q_y &= g_{y1} + g_{y2} + g_{y3} + g_{y4}, \\
f_{yx} &= \lambda (g_{y1} - g_{y3}), \\
XX_v &= g_{y1} - g_{y2} + g_{y3} - g_{y4}, \\
f_{yy} &= \lambda (g_{y2} - g_{y4}).
\end{align*}
\]

- The value at equilibrium of the previous moments can be explicited, taking into account that the three moments \( \rho, q_x \) and \( q_y \) are at equilibrium. We have:
\[
\begin{align*}
J_{\text{eq} x, \rho} &= \rho u = q_x, \\
\varepsilon_{\rho} &= (1 - \frac{5}{2} a^2) \rho + \frac{5}{4} \rho_0 (u^2 + v^2), \\
XX_{\rho} &= 0,
\end{align*}
\]
We have also
\[
\begin{align*}
f_{\text{eq} xx} &= \rho u^2 + p, \\
f_{\text{eq} xy} &= \rho u v, \\
f_{\text{eq} yx} &= \rho u v, \\
f_{\text{eq} yy} &= \lambda (g_{y2} - g_{y4}),
\end{align*}
\]

The multiple relaxation time algorithm can be implemented without difficulty. It is just necessary to write a relation of the type \([\Box]\) for the 10 moments that are not at equilibrium.

Our present choice is the BGK variant of the scheme, with all parameters \( s_\ell \) supposed to be equal. The boundary conditions of wall constraint, supersonic inflow or supersonic outflow are treated with an easy adaptation of the usual methods of bounce-back and “anti-bounce-back”.

4) First test cases

- We propose two bidimensional test cases for the shallow water equations: a stationary shock reflexion and a classical unstationary forward facing step first proposed by Emery [11] for gas dynamics. The first test case is a the reflexion of an incident shock wave of angle \(-\pi/4\) issued from a “left” state into a new shock of angle \(\text{atan}(4/3)\) due to the physical nature of the “top” state (in green on the left picture of Fig. 2) and the “right” state (in indigo). The exact solution is determined through the use of Rankine Hugoniot relations. We have chosen
\[
\begin{align*}
\rho_\ell = 1, & \quad u_\ell = 1.59497132403753, \quad v_\ell = 0, \\
\rho_t = 1.17150636388320, & \quad u_t = 1.47822089880855, \quad v_t = -0.116750425228984, \\
\rho_r = 1.38196199044604, & \quad u_r = 1.33228286727232, \quad v_r = 0.
\end{align*}
\]

The stationary result of the vectorial lattice Boltzmann scheme for this first test case can be compared with the pure finite volume approach with the Godunov [13] scheme solving a discontinuity at each interface at each time step. We have used three meshes of \(35 \times 20, 70 \times 40\) and \(140 \times 80\) grid points. The iso-values of density are presented on Fig. 2. The numerical results are similar.
The second test case (Emery [11]) is purely unstationary. At time equal zero, a small step is created inside a flow at Froude number equal to 3. A strong shock wave separates from the wall and various nonlinear waves occur and interact. Our present experiment (Fig. 3 and 4) shows the ability of a vectorial lattice Boltzmann scheme to approach such a flow. We have refined the mesh, using three families of meshes: 120 × 40, 240 × 80 and 480 × 120. We have used $\lambda = 80$, $a = 0.05$, $s_j = 1.8$ for all $j$ to achieve experimental stability. The time step is very small (due to the high value of $\lambda = \frac{\Delta x}{\Delta t}$) and in consequence the computation relatively slow.
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Figure 4. Emery test case for the shallow water equations, mesh $480 \times 120$, $t = 4$, density profile, D2Q5Q4Q4 vectorial lattice Boltzmann scheme (top) and Godunov scheme (bottom).

- We present our results for the finer mesh, at adimensionalized time equal to $1/2$ (Fig. 3) and 4 (Fig. 4). The results show the ability for the vectorial scheme based on the decomposition of the dual entropy to capture such flows. Nevertheless, the Godunov scheme, well known of being only of order one, gives better unstationary result compared to the new approach.

Conclusion
- We have extended the methodology of kinetic decomposition of the dual entropy previously studied for 1D problems into a general framework of vectorial lattice Boltzmann schemes for systems of conservation laws in several space dimensions, in the spirit of Bouchut [5]. The key point is to decompose the dual entropy of the system into convex potentials satisfying the Perthame-Bouchut hypothesis. Our first choices show that the system of shallow water equations can be solved numerically without major difficulty. Nevertheless, our first numerical experiments show that the resulting scheme contains a lot of numerical viscosity. Future work is necessary to reduce this effect.

Acknowledgments
- The author thanks François Bouchut for an enlightening discussion during the elaboration of this work.
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