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Stable second order boundary conditions for kinetic approximations

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Abstract. We introduce a general framework for applying boundary conditions in the vectorial kinetic scheme of Bouchut [4, 2]. The method ensures entropy stability of the resulting approximation but also high order accuracy.

Keywords: Boundary conditions, Lattice Boltzmann, Entropy stability

1 Introduction

The vectorial kinetic approach is a general method for approximating hyperbolic systems of conservation laws. It has been introduced by Bouchut in [4] and Aregba and Natalini in [2]. It consists in representing any system of conservation laws by a finite set of transport equations coupled through a stiff relaxation term. This representation has several advantages: it allows rigorous mathematical analysis [4, 2, 7]. Associated with time splitting techniques, it leads to the construction of very efficient schemes [3].

We first describe the one-dimensional framework, but it can be generalized to higher dimensions. We consider a system of m conservation laws

$$\partial_t w + \partial_x q(w) = 0, \quad (1)$$

where the unknown conservative variable $w(x, t) \in \mathbb{R}^m$ depends on a space variable $x \in [L, R]$ and a real time variable $t \geq 0$. The system (1) is supplemented with an initial condition and boundary conditions at $x = L$ and $x = R$.

We assume that (1) admits a Lax entropy $s : \mathbb{R}^m \rightarrow \mathbb{R}$, associated to an entropy flux $g : \mathbb{R}^m \rightarrow \mathbb{R}$. This means that s is strictly convex and that $s'q' = g'$. A weak solution w to (1) is admissible if the entropy is decreasing

$$\partial_t s(w) + \partial_x g(w) \leq 0.$$

2 Kinetic approximation

The system of conservation laws is approximated by the following system of $2m$ kinetic equations

$$\partial_t f + \Lambda \partial_x f = \frac{1}{\varepsilon} (f^{eq}(w) - f), \quad (2)$$

where:

– the kinetic vector

$$f(x, t) = \begin{pmatrix} f_1(x, t) \\ f_2(x, t) \end{pmatrix} \in R^{2m}, \quad f_{1,2}(x, t) \in R^m,$$

– the matrix A is defined by (I is the identity matrix of size $m \times m$)

$$\lambda = \begin{pmatrix} \lambda I & 0 \\ 0 & -\lambda I \end{pmatrix}, \quad \lambda > 0,$$

– the parameter $\varepsilon > 0$. The equilibrium f^{eq} is defined below,

– the conservative data are related to the kinetic data thanks to the $m \times 2m$ matrix

$$P = (I, I), \quad \text{and } w = Pf.$$

This kinetic model is consistent with the conservation laws (1) when $\varepsilon \rightarrow 0$ as soon as

$$Pf^{eq}(w) = w, \quad PAf^{eq}(w) = q(w). \quad (3)$$

The consistency conditions (3) lead to a unique possibility for the equilibrium data

$$f^{eq}(w) = \begin{pmatrix} \frac{w}{2} + \frac{q(w)}{2\lambda} \\ \frac{w}{2} - \frac{q(w)}{2\lambda} \end{pmatrix}.$$

For the numerical resolution of (2) we use a Lattice Boltzmann Method (LBM). For a given integer $N > 0$, we define the space step $h = (R - L)/N$, the grid points $x_i = L + ih + h/2$, $0 \leq i < N$ and the time step $\tau = h/\lambda$. The solution is approximated by

$$f_i^n \simeq f(x_i, n\tau).$$

For going from time step $n - 1$ to time step n , we first solve the free transport equation $\partial_t f + A\partial_x f = 0$ exactly, which is possible by simple shift operations, thanks to the choice of the time step. We get

$$f_i^{n,-} = \begin{pmatrix} f_{1,i-1}^{n-1} \\ f_{2,i+1}^{n-1} \end{pmatrix}, \quad w_i^n = Pf_i^{n,-}. \quad (4)$$

Then we apply a relaxation procedure for staying close to equilibrium

$$f_i^n = \omega f^{eq}(w_i^n) + (1 - \omega) f_i^{n,-}. \quad (5)$$

The choice $\omega = 1$ consists in returning to equilibrium at the end of each step. The resulting time marching scheme is first order accurate. The over-relaxation choice $\omega = 2$ results in a second order accurate time scheme [5]. We observe that the LBM is particularly simple and efficient: it is made of independent shift operations followed by independent local relaxations. It is highly parallelizable and the second order extension has no additional cost.

It is clear that the shift algorithm (4) needs to be adapted at the boundaries, when $i = 0$ or $i = N - 1$. At the left point, the value $f_{1,-1}^{n-1}$ is missing, and at

the right point, the value $f_{2,N}^{n-1}$ is missing. The boundary conditions are given by two “ghost cell” functions b_L and b_R whose role is to reconstruct the missing values from the first and last cell values:

$$f_{1,-1}^{n-1} = b_L(f_{1,0}^{n-1}, f_{2,0}^{n-1}), \quad f_{2,N}^{n-1} = b_R(f_{1,N-1}^{n-1}, f_{2,N-1}^{n-1}).$$

We propose below a general strategy to apply the boundary conditions on the kinetic scheme. We shall test it on the very simple transport conservation law at constant velocity v . In this case, we thus have $m = 1$ and

$$q(w) = vw. \tag{6}$$

Let us explicit the kinetic model in this case. We find

$$P = (1, 1), \quad w = f_1 + f_2, \quad f^{eq}(w) = \begin{pmatrix} w(\frac{1}{2} + \frac{v}{2\lambda}) \\ w(\frac{1}{2} - \frac{v}{2\lambda}) \end{pmatrix}.$$

The chosen entropy and entropy flux are

$$s(w) = \frac{w^2}{2}, \quad g(w) = v \frac{w^2}{2}.$$

3 Entropy stability and boundary conditions

3.1 Stability analysis

For constructing the kinetic model we follow [4, 7]. We assume that it is possible to find convex kinetic entropies s_k such that

$$s(w) = \min_{w=f_1+f_2} s_1(f_1) + s_2(f_2) = s_1(f_1^{eq}) + s_2(f_2^{eq}). \tag{7}$$

For the simple transport equation (6) that we consider, we can take

$$s_1(f_1) = \frac{\lambda}{\lambda + v} (f_1)^2, \quad s_2(f_2) = \frac{\lambda}{\lambda - v} (f_2)^2.$$

These two kinetic entropies are convex under the sub-characteristic condition

$$|v| < \lambda.$$

For a general system of conservation laws with a Lax entropy, it is also possible to compute s_k . The practical calculations can be done thanks to the Legendre transform [7, 8].

Once the consistency (3) and the kinetic entropy property (7) are ensured, the lattice Boltzmann scheme (4-5) is entropy dissipative for $\omega \in [1, 2]$. Indeed, the shift step (4) preserves the kinetic entropy exactly and the relaxation step (5) makes it decrease, by design. This reasoning has to be adapted at the boundaries.

For establishing the entropy dissipative kinetic boundary condition, we assume that the initial condition is constant outside an interval $[a, b] \subset]L, R[$

$$w(x, 0) = \bar{w}, \quad \text{if } x < a \text{ or } x > b.$$

Without loss of generality, we can assume that $s(\bar{w}) = 0$ and $g(\bar{w}) = 0$, because the properties of the entropy are not modified by the addition of affine functions. Then the boundary entropy condition simply states that, in the shift step (4), the kinetic entropy that enters the domain should be smaller than the kinetic entropy that leaves the domain. We obtain

$$s_1(b_L(f_1, f_2)) \leq s_2(f_2), \quad s_2(b_R(f_1, f_2)) \leq s_1(f_1). \quad (8)$$

3.2 First order stable boundary conditions

We consider the simple transport case $q(w) = vw$. We assume that $\bar{w} = 0$ and $v > 0$. It is then mandatory to impose $w = 0$ at the left boundary. A condition is missing at the right boundary. As in [6] we apply a null boundary condition on the flux error y , defined by

$$y = \lambda f_1 - \lambda f_2 - q(f_1 + f_2) = (\lambda - v)f_1 - (\lambda + v)f_2.$$

This quantity vanishes when $f_k = f_k^{eq}$. The boundary conditions are thus

$$f_1 + f_2 = 0 \text{ at } x = L, \quad \lambda f_1 - \lambda f_2 - q(f_1 + f_2) = 0 \text{ at } x = R.$$

This allows to deducing the ghost cell functions b_L and b_R

$$b_L(f_1, f_2) = -f_2, \quad b_R(f_1, f_2) = \frac{\lambda - v}{\lambda + v} f_1. \quad (9)$$

The kinetic entropy condition (8) is then satisfied, because $v > 0$.

The boundary conditions (9) are thus stable. However, we have observed that the right outgoing condition is only first order accurate, even when $\omega = 2$.

3.3 Stabilized second order boundary conditions

As proposed in [6] we replace the right Dirichlet boundary condition by a Neumann boundary condition, because it was experimentally observed a better second order accuracy with $w(L, t) = 0$, $\partial_x y(R, t) = 0$. The spatial derivative is approximated by

$$\partial_x y(R, n\tau) \simeq \frac{y_{N-1}^n - y_{N-2}^n}{h} = 0.$$

But with this approximation, the right ghost cell boundary function now depends on the kinetic data in cell $N - 1$ and cell $N - 2$:

$$f_{2,N}^{n-1} = b_R(f_{1,N-1}^{n-1}, f_{2,N-1}^{n-1}, f_{1,N-2}^{n-1}, f_{2,N-2}^{n-1}). \quad (10)$$

It is then generally not possible to ensure directly (8). We thus propose the following nonlinear correction at the right boundary:

- Compute $f_{2,N}^{n-1}$ with formula (10).
- If the right entropy inequality is not satisfied, i.e. if $s_2(f_{2,N}^{n-1}) > s_1(f_{1,N-1}^{n-1})$, then replace $f_{2,N}^{n-1}$ by the closest value $\tilde{f}_{2,N}^{n-1}$ such that

$$s_2(\tilde{f}_{2,N}^{n-1}) = s_1(f_{1,N-1}^{n-1}).$$

This construction ensures the decrease of entropy, with a minimal adjustment. It is expected that it will remain a second order accurate approximation. Similar ideas are exposed for instance in [1] (see also included references) in the FV framework.

4 Extension to higher dimension

The above construction can be extended to higher dimensions. Let us comment a two-dimensional example. We solve the transport equation

$$\partial_t w + \nabla \cdot q(w) = 0, \quad q_i(w) = v_i w.$$

The unknown $w(x_1, x_2, t)$ depends on a two-dimensional variable (x_1, x_2) in a square $\Omega \subset \mathbb{R}^2$. The velocity vector $v = (v_1, v_2)^T$. In this case, we can consider the D2Q4 model with four kinetic unknowns f_k , $1 \leq k \leq 4$. The kinetic velocities are (λ is a positive parameter)

$$c_1 = \lambda \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad c_2 = \lambda \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \quad c_3 = \lambda \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad c_4 = \lambda \begin{pmatrix} 0 \\ -1 \end{pmatrix}.$$

The kinetic equations read

$$\partial_t f_k + c_k \cdot \nabla f_k = \frac{1}{\varepsilon} (f_k^{eq} - f_k).$$

The equilibrium is given by

$$f_k^{eq}(w) = \frac{w}{4} + \frac{v \cdot c_k w}{2\lambda^2}, \quad w = \sum_{k=1}^4 f_k.$$

We also define the flux error by

$$y = \begin{pmatrix} \lambda(f_1 - f_2) - v_1(f_1 + f_2) \\ \lambda(f_3 - f_4) - v_2(f_3 + f_4) \\ \lambda^2(f_1 + f_2 - f_3 - f_4) \end{pmatrix}.$$

As in the D1Q2 model, the flux error vanishes when $f = f^{eq}$. The kinetic entropy is given by

$$\Sigma(f) = \frac{1}{\lambda + 2v_1} f_1^2 + \frac{1}{\lambda - 2v_1} f_2^2 + \frac{1}{\lambda + 2v_2} f_3^2 + \frac{1}{\lambda - 2v_2} f_4^2.$$

Its convexity implies the sub-characteristic condition $2 \max(|v_1|, |v_2|) < \lambda$.

We summarize two boundary condition strategies in Table 1 ((n_1, n_2) is the normal vector to the considered boundary):

Boundary conditions	Entropy stable	Second order accurate
Inflow border	Exact solution on w $y_3 = 0$	Exact solution on w
Outflow border	$y_1 n_1 + y_2 n_2 = 0$ $y_3 = 0$	Neumann on $v_1 y_1 + v_2 y_2$
Corner inflow/inflow	Exact solution on w $y_3 = 0$	Exact solution on w $y_3 = 0$
Corner inflow/outflow	Exact solution on w $v_1 y_1 + v_2 y_2 = 0$ $y_3 = 0$	Exact solution on w Neumann on $v_1 y_1 + v_2 y_2$
Corner outflow/outflow	$y_1 = 0$ $y_2 = 0$ $y_3 = 0$	Neumann on $v_1 y_1 + v_2 y_2$ $y_3 = 0$

Table 1. Two different boundary condition strategies for the D2Q4 model. Left: It is possible to prove that this boundary condition is entropy dissipative, but first order accurate. Right: second order boundary condition, but not stable for long time simulations. By projecting this second-order boundary condition on the space of the decreasing entropy boundary conditions, we obtain stability and second-order accuracy.

5 Numerical results

5.1 D1Q2 model

For our tests, the initial data is the compact support function

$$w(x, 0) = \begin{cases} 0 & \text{if } r(x) > 1, \\ (1 - r(x)^2)^5 & \text{otherwise,} \end{cases}$$

where $r(x) = \frac{|x-x_0|}{\sigma}$, with $\sigma = 0.2$. We consider several test cases corresponding to different initial positions x_0 of the peak: in test case 1, $x_0 = -1/2$; in test case 2, $x_0 = 0$ and in test case 3, $x_0 = 1/2$. In Figure 1 we check the accuracy and the stability of the second order boundary condition.

5.2 D2Q4 model

We choose a square geometry, aligned with the kinetic velocities: $\Omega = [0, 1] \times [0, 1]$. We initialize w with a compact support function

$$w(x_1, x_2, t) = \begin{cases} 0 & \text{if } r(x_1, x_2) > 1, \\ (1 - r(x_1, x_2)^2)^5 & \text{otherwise.} \end{cases}$$

with $r(x_1, x_2) = \frac{\sqrt{(x_1-x_{1,0})^2 + (x_2-x_{2,0})^2}}{\sigma}$ and $\sigma = 0.4$. We consider several test cases in Table 5.2, corresponding to different initial positions of the peak and several velocities (v_1, v_2) .

We first check in Figure 2 the second order accuracy and the instability of the boundary condition described in the second column of Table 1. Finally, we check in Figure 2 the improvement given by the projection strategy.

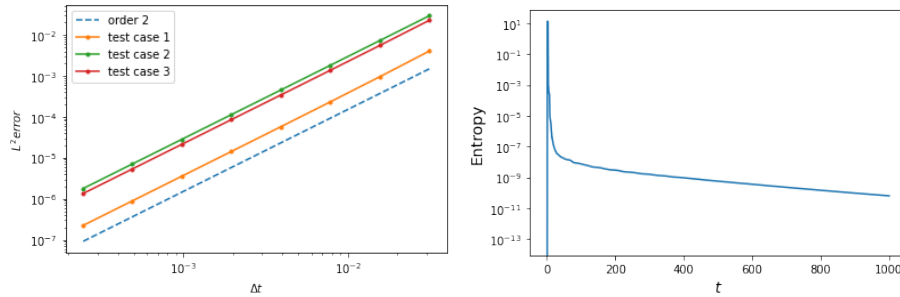


Fig. 1. Second order boundary condition for the D1Q2 model (Dirichlet on w at the left boundary and Neumann on y at the right boundary). Left: error rates in the L^2 norm for the three test cases. Second order is achieved for all the tests. Right: entropy evolution for test case 1. Once the peak has entered the domain, the entropy decreases.

Test case	$x_{1,0}$	$x_{2,0}$	v_1	v_2
1	0.5	0.5	0.8	0
2	-0.4	0.5	0.8	0
3	0.4	0.5	-0.8	0
4	0	0.5	0.8	0
5	$-\sqrt{2}/4$	$-\sqrt{2}/4$	$\sqrt{2}/2$	$\sqrt{2}/2$
6	$\sqrt{2}/4$	$\sqrt{2}/4$	$-\sqrt{2}/2$	$-\sqrt{2}/2$
7	0	0	$\sqrt{2}/2$	$\sqrt{2}/2$

Table 2. Parameters of the test cases for the D2Q4 model.

6 Conclusion

In this short paper, we have described a general strategy for imposing boundary conditions on a vectorial kinetic approximation. The difficulty is that the number of necessary boundary conditions is different between the kinetic model and the approximated conservation laws. With our method, it is possible to rigorously stabilize boundary schemes that are accurate but slightly unstable. In future works, we will extend the approach to nonlinear systems of conservation laws and more complex boundary geometries.

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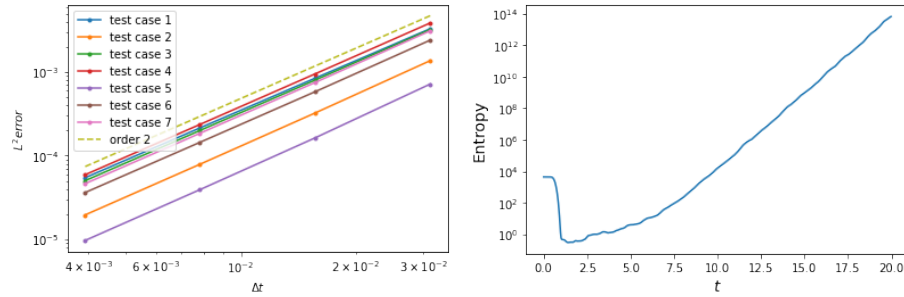


Fig. 2. Second order boundary condition for the D2Q4 model, without entropy limiting. Left: error rates in the L^2 norm for the test cases of Table 5.2. Second order is achieved for all the tests for short times. Right: entropy evolution for test case 1. The scheme is unstable on the long time.

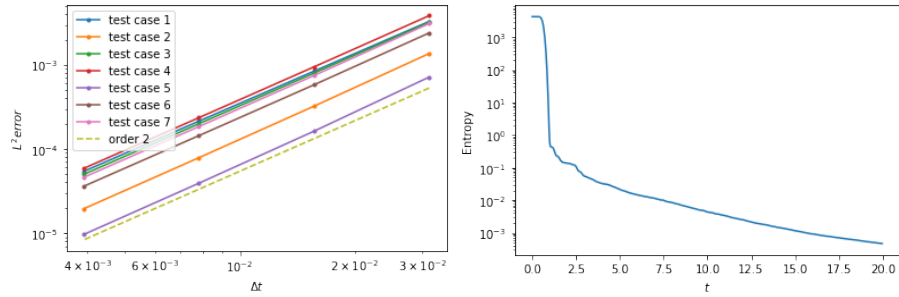


Fig. 3. Second order boundary condition for the D2Q4 model, with entropy limiting. Left: error rates in the L^2 norm for the test cases of Table 5.2. Second order is achieved for all the tests. Right: entropy evolution for test case 1. The scheme is now stable thanks to the entropy limiting procedure.

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