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A notion of non-negativity preserving relaxation for a mono-dimensional three velocities scheme with relative velocity

François Dubois [a,b], Benjamin Graille [b,*], S.V. Raghurama Rao [c]

[a] Conservatoire National des Arts et Métiers, LMSSC laboratory, Paris, France
[b] Laboratoire de Mathématiques d'Orsay, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France
[c] Department of Aerospace Engineering, Indian Institute of Science, Bangalore 560 012, India

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ABSTRACT

In this contribution, we study a stability notion for a fundamental linear one-dimensional lattice Boltzmann scheme, this notion being related to the maximum principle. We seek to characterize the parameters of the scheme that guarantee the preservation of the non-negativity of the particle distribution functions. In the context of the relative velocity schemes, we derive necessary and sufficient conditions for the non-negativity preserving property. These conditions are then expressed in a simple way when the relative velocity is reduced to zero. For the general case, we propose some simple necessary conditions on the relaxation parameters and we put in evidence numerically the non-negativity preserving regions. Numerical experiments show finally that no oscillations occur for the propagation of a non-smooth profile if the non-negativity preserving property is satisfied.

1. Introduction

Studying the stability of lattice Boltzmann schemes is a non-trivial problem. Classically for this purpose, the scheme is linearized around a constant state and a von Neumann-Fourier analysis is performed. For this notion of stability, we refer to the work of Sterling and Chen in [21] where some stability results for a 7-velocity hexagonal lattice, a 9-velocity square lattice, and a 15-velocity cubic lattice are proposed; the work of Lallemand and Luo [17] for a 9-velocity square lattice scheme applied to hydrodynamics; the one of Sieber et al. for athermal and thermal models with a larger number of velocities in two space dimensions [20]; the one of Ginzburg et al. [11] extending the Fourier analysis to a wide variety of different two and three-dimensional lattice Boltzmann schemes; the one of Krivovichev [16] for six widely used body force action models; the one of Wissocq et al. [24] for projecting information carried by the lattice Boltzmann eigenvectors on the physical modes.

Instabilities and their interpretation in terms of bulk viscosity have been proposed by Dellar [4]. But no mathematical analysis has been performed.

A new way of improving stability is proposed by Geier [9], who proposed a new generalized lattice Boltzmann scheme with the approach of relative velocities and utilized it for hydrodynamics applications [6]. An attempt to analyze this method for a two-dimensional scalar linear problem has been also proposed [7]. Interesting tentatives have been proposed to enforce stability conditions of multiple-relaxation time lattice Boltzmann schemes with raw or central moments with von Neumann analysis and heuristic selection of wave-number vectors by Golbert et al. [12] and Chávez-Modena et al. [3].

Even if it is a difficult task, it is well known that Fourier method (von Neumann analysis) is a linear approach and in consequence is not relevant for analyzing non-linear hyperbolic equations.

Total variation diminishing schemes, developed for suppressing oscillations in higher-order CFD algorithms [1,23,22], provide an alternative nonlinear stability analysis tool for analyzing the schemes for nonlinear wave propagation. The convergence of such schemes is well established [18]. The underlying stability notion concerns the maximum principle. In brief, if some solution of a partial differential equation is positive on the boundary, it remains positive in all the domain of study [13,10,15]. The lattice Boltzmann schemes do not intrinsically satisfy the property of maximum principle or the associated non-negativity constraint as detailed by Karimi et al. [14]. This notion can be extended to non-linear cases and a first attempt for lattice Boltzmann schemes has been pro-

* Corresponding author.
E-mail address: benjamin.graille@u-psud.fr (B. Graille).

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posed in [2], for the D1Q2 scheme used to simulate scalar non-linear hyperbolic equations.

In this contribution, we propose to investigate the stability in the maximum sense, of a linear mono-dimensional lattice Boltzmann scheme with three velocities. More precisely, we look to a non-negativity constraint for the particle distribution functions in the context of relative velocities. The objective is the description of the parameter sets of the scheme that allow the particle distribution functions to remain non-negative. It is obviously linked with the non-negativity of their equilibrium values but it only coincides with the latter property if all the relaxation parameters are taken to 1. We refer for instance to Servan-Camas et al. [19] where this property is investigated for several schemes used to simulate advection–diffusion equation.

In Section 2, we describe the scheme and the underlying advection model. More precisely, the local relaxation step is written as a linear operator on the particle distribution functions. If all the coefficients of the underlying matrix are nonnegative, the non-negativity of the distribution is maintained during this step. Because the transport step is just a change of locus, the non-negativity is maintained for the whole time step of the scheme. The question is then to find appropriate conditions to handle this property. In Section 3, a necessary and sufficient condition is derived on the parameters to ensure that the scheme has the stability property. In Section 4, we completely describe the classical case where the relative velocity is reduced to zero. In Section 5, the general case is presented, with an analytical study for necessary conditions and a numerical one for a complete description of the stability zones. In Section 6, the presented numerical experiments show the correlation of the positivity constraint for a particle distribution and the presence of oscillations for discontinuous profiles.

2. Description of the framework

2.1. Description of the scheme

In this contribution, we investigate a mono-dimensional 3 velocities linear lattice Boltzmann scheme with relative velocity [6]. Denoting Δx the spatial step, Δt the time step, and $\lambda = \Delta x/\Delta t$ the scheme velocity, this scheme can be described in a generalized d'Humière's framework [5]:

(1) the 3 velocities $c_1 = -1$, $c_2 = 0$, and $c_3 = 1$;
(2) the 3 associated distributions f_1, f_2, and f_3;
(3) the 3 moments ρ, $q(u)$, and $\varepsilon(u)$ given by

$$\rho = \sum_{1\le j\le 3} f_j, \quad q(u) = \lambda \sum_{1\le j\le 3} (c_j - u) f_j, \quad \varepsilon(u) = 3\lambda^2 \sum_{1\le j\le 3} (c_j-u)^2 f_j - 2\lambda^2 \sum_{1\le j\le 3} f_j,$$

where u is a given scalar representing the relative velocity;
(4) the equilibrium value of the 3 moments

$$\rho^{\mathrm{eq}} = \rho, \quad q^{\mathrm{eq}}(u) = \lambda(V-u)\rho, \quad \varepsilon^{\mathrm{eq}}(u) = \lambda^2(3u^2 - 6uV + \alpha)\rho,$$

where V and α are given scalars (without loss of generality, we assume that $V > 0$);
(5) the 2 relaxation parameters s and s' such that the relaxation phase reads

$$q^\star(u) = (1-s) q(u) + s q^{\mathrm{eq}}(u), \quad \varepsilon^\star(u) = (1-s')\varepsilon(u) + s'\varepsilon^{\mathrm{eq}}(u).$$

In this formalism, the moments are defined as polynomial functions of discrete velocities and the discrete distribution functions. Indeed, introducing the one variable polynomials $P_1(X) = 1$, $P_2(X) = \lambda X$, and $P_3(X) = \lambda^2(3X^2 - 2)$ relative to an abstract indeterminate X, the three moments read

$$\rho = \sum_{1\le j\le 3} f_j P_1(c_j - u), \quad q(u) = \sum_{1\le j\le 3} f_j P_2(c_j - u), \quad \varepsilon(u) = \sum_{1\le j\le 3} f_j P_3(c_j - u).$$

The equilibrium values are chosen such that the equilibrium distributions do not depend on the relative velocity u. Indeed, we have:

$$f_j^{\mathrm{eq}} = \frac{1}{6}\rho\left(2 + 3c_jV + (3c_j^2 - 2)\alpha\right), \quad 1 \le j \le 3.$$

Note that this scheme can be used (see e.g. [8]) to simulate a scalar transport equation with constant velocity λV given by

$$\partial_t \rho + \lambda V \partial_x \rho = 0.$$

This advection equation is a first-order asymptotic limit as the space and time steps tend to zero with a fixed ratio $\lambda \equiv \Delta x/\Delta t$. We are not interested in this contribution in the second-order asymptotic expansion and refer to the relative velocity schemes of Février et al. [6] for the same.

With the notation $x_k = k\Delta x$, $k \in \mathbb{Z}$, and $t^n = n\Delta t$, $n \in \mathbb{N}$, one time step of the scheme reads

$$f_j(t^n + \Delta t, x_k + c_j\Delta t) = f_j(t^{n+1}, x_{k+j}) = f_j^\star(t^n, x_k), \quad 1 \le j \le 3.$$

Note that the scheme does not depend on the relative velocity u in the case where the relaxation parameters are identical, i.e., $s = s'$. The two moments $q(u)$ and $\varepsilon(u)$ depend on u but the particle distribution functions remain identical at each time iteration. In that case, for all values of u, the scheme yields the standard BGK scheme.

2.2. A notion of non-negativity preserving relaxation

In this contribution, we are concerned with the *non-negativity of the particle distribution functions*. We propose the following definition of stability through non-negativity preserving relaxation.

Definition 1 *(Non-negativity preserving relaxation).* The relaxation phase is said to be *non-negativity preserving* if

$$\forall j \;\; f_j \ge 0 \Rightarrow \forall i \;\; f_i^\star \ge 0. \qquad (1)$$

This property can be viewed as referring to a weak maximum principle for schemes. Indeed, it is always possible, by adding a constant, to assume that all the particle distribution functions are initially non-negative. If the scheme ensures that this property of non-negativity remains as time marches, each particle distribution function is then bounded, as their total sum is conserved. Moreover, as the transport step consists simply in exchanging the position of the particle distribution functions, we focus on the relaxation step.

In other words, if ρ is conserved during the relaxation step (and periodic boundary conditions are used for compact space set), the sum of ρ over all the space points x_k, $k \in \mathbb{Z}$, is constant. Then the particle distribution functions verify a maximum principle

$$(\forall k \in \mathbb{Z}, \forall j \;\; f_j(0, x_k) \ge 0) \Rightarrow (\forall k \in \mathbb{Z}, \forall n \in \mathbb{N}, \forall j 0 \le f_j(t^n, x_k) \le \bar\rho)$$

with

$$\bar\rho = \sum_{k\in\mathbb{Z}} \sum_j f_j(0, x_k).$$

Note that the property of non-negativity preserving relaxation is automatically satisfied if the equilibrium values of the distribution functions are non-negative and if the relaxation parameters verify $s = s' \in (0, 1]$. This result does not depend on the relative velocity u (as the equilibrium values of the distribution functions do not depend on u). We will recover this result in the following.

2.3. Matrix notation for the relaxation step

We use a matrix notation for the relaxation step as it can be read as a multiplication by a matrix. As this step is local in space, we omit the dependency on time and space. We define the vector of the distribution functions $\mathtt{f}$

$$\mathtt{f} = (f_1 \;\; f_2 \;\; f_3)^T.$$

One relaxation step then reads

$$\mathtt{f}^\star = \mathtt{R}(u)\mathtt{f},$$

where the matrix $\mathtt{R}(u)$ is defined by

$$\mathtt{R}(u) = \mathtt{M}^{-1}\mathtt{T}(-u)(\mathtt{I} + \mathtt{S}(\mathtt{T}(u)\mathtt{E}\mathtt{T}(-u) - \mathtt{I}))\mathtt{T}(u)\mathtt{M},$$

with

$$\mathtt{M} = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \lambda^2 & -2\lambda^2 & \lambda^2 \end{pmatrix}, \quad \mathtt{T}(u) = \begin{pmatrix} 1 & 0 & 0 \\ -\lambda u & 1 & 0 \\ 3\lambda^2 u^2 & -6\lambda u & 1 \end{pmatrix},$$
$$\mathtt{S} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s' \end{pmatrix}, \quad \mathtt{E} = \begin{pmatrix} 1 & 0 & 0 \\ V\lambda & 0 & 0 \\ \alpha\lambda^2 & 0 & 0 \end{pmatrix}, \quad \mathtt{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The coefficients of the matrix $\mathtt{M}$ are obtained by the relations $\mathtt{M}_{k,j} = P_k(c_j)$, $1 \le k, j \le 3$ and those of the matrix $\mathtt{T}(u)$ by the change of basis formula: $\mathtt{T}(u)_{k,l}$ is the coefficient of the l^{th}-element $P_l(c_j)$ in the definition of $P_k(c_j - u)$ according to

$$P_k(c_j - u) = \sum_{1 \le l \le 3} \mathtt{T}(u)_{k,l} P_l(c_j), \quad 1 \le j \le 3.$$

The matrix $\mathtt{M}$ is then the change of basis that transforms the vector $\mathtt{f}$ into the vector $\mathtt{m}(0) = (\rho, q(0), \varepsilon(0))^T$:

$$\mathtt{m}(0) = \mathtt{M}\mathtt{f}, \quad \mathtt{m}(u) = \mathtt{T}(u)\mathtt{M}\mathtt{f}.$$

The matrix $\mathtt{T}(u)$ can then be viewed as the change of basis matrix from the classical moments without relative velocity toward the moments with relative velocity.

2.4. Remark on the choice of the moments

Note that the last moment $\varepsilon(u)$ that is chosen in this contribution is not the energy but a moment that is orthogonal to the two first ones, ρ and $q(u)$. In this section, we show that all the results of the contribution would be identical by choosing the last moment as the energy: the relaxation matrix $\mathtt{R}(u)$ would still be the same.

We consider two schemes with two different choices of polynomials: the moments of the first scheme are defined by (P_1, P_2, P_3) while the moments of the second scheme by $(\hat{P}_1, \hat{P}_2, \hat{P}_3)$. The first moment is the same in both schemes to be able to simulate the same transport equation. We then have $\hat{P}_1 = P_1$. We define $\mathtt{C}$ the change of basis matrix associated to the tranformation $\mathtt{M}$ into $\hat{\mathtt{M}}$:

$$\hat{\mathtt{M}} = \mathtt{C}\mathtt{M}.$$

The first line of $\mathtt{C}$ is then $(1, 0, 0)$.

Proposition 2. *We assume that the equilibrium values of the distribution functions are the same, that is* $\hat{\mathtt{E}} = \mathtt{C}\mathtt{E}\mathtt{C}^{-1}$, *and that the relaxation parameters are the same, that is* $\hat{\mathtt{S}} = \mathtt{S}$. *Then, we have* $\hat{\mathtt{R}}(u) = \mathtt{R}(u)$ *for all* (s, s') *iff*

$$\hat{P}_2 \in \mathrm{Span}(P_1, P_2), \quad \hat{P}_3 \in \mathrm{Span}(P_1, P_3), \quad \text{in } \mathbb{R}[X]/X(X-1)(X+1).$$

In a practical way, the exact choice of the moments has no influence on the precise computation of the matrix $\mathtt{R}(u)$ even in the relative velocity framework. If for example, we use on one hand the matrix proposed previously in this contribution $\mathtt{M}$ and on the other hand the favorite moment matrix of one of us, $\hat{\mathtt{M}}$, with

$$\mathtt{M} = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \lambda^2 & -2\lambda^2 & \lambda^2 \end{pmatrix}, \quad \hat{\mathtt{M}} = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \lambda^2/2 & 0 & \lambda^2/2 \end{pmatrix},$$

we just change the definition of the third moment named "energy" in this contribution. We observe that

$$\mathtt{C} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \lambda^2/3 & 0 & 1/6 \end{pmatrix}.$$

The equilibrium matrices $\mathtt{E}$ and $\hat{\mathtt{E}}$

$$\mathtt{E} = \begin{pmatrix} 1 & 0 & 0 \\ V\lambda & 0 & 0 \\ \alpha\lambda^2 & 0 & 0 \end{pmatrix}, \quad \hat{\mathtt{E}} = \begin{pmatrix} 1 & 0 & 0 \\ V\lambda & 0 & 0 \\ \lambda^2 \dfrac{\alpha+2}{6} & 0 & 0 \end{pmatrix}$$

are linked by $\hat{\mathtt{E}} = \mathtt{C}\mathtt{E}\mathtt{C}^{-1}$ in order to maintain identical the equilibrium distribution functions. Then we maintain unchanged the relaxation coefficients because $\mathtt{S} = \hat{\mathtt{S}}$.

Proof. First, we immediately obtain the following relations by identifying the coefficients of $\hat{\mathtt{M}}$ and of $\mathtt{M}$:

$$\hat{P}_k(c_j) = \sum_{1 \le l \le 3} \mathtt{C}_{k,l} P_l(c_j), \quad 1 \le j \le 3.$$

We deduce that

$$\hat{\mathtt{T}}(u) = \mathtt{C}\mathtt{T}(u)\mathtt{C}^{-1}.$$

We have

$$\begin{aligned} \hat{\mathtt{R}}(u) &= \hat{\mathtt{M}}^{-1}\hat{\mathtt{T}}(-u)(\mathtt{I} + \hat{\mathtt{S}}(\hat{\mathtt{T}}(u)\hat{\mathtt{E}}\hat{\mathtt{T}}(-u) - \mathtt{I}))\hat{\mathtt{T}}(u)\hat{\mathtt{M}} \\ &= \mathtt{M}^{-1}\mathtt{T}(-u)\mathtt{C}^{-1}(\mathtt{I} + \mathtt{S}(\mathtt{C}\mathtt{T}(u)\mathtt{E}\mathtt{T}(-u)\mathtt{C}^{-1} - \mathtt{I}))\mathtt{C}\mathtt{T}(u)\mathtt{M} \\ &= \mathtt{M}^{-1}\mathtt{T}(-u)(\mathtt{I} + \mathtt{C}^{-1}\mathtt{S}\mathtt{C}(\mathtt{T}(u)\mathtt{E}\mathtt{T}(-u) - \mathtt{I}))\mathtt{T}(u)\mathtt{M}. \end{aligned}$$

Then

$$\hat{\mathtt{R}}(u) - \mathtt{R}(u) = \mathtt{M}^{-1}\mathtt{T}(-u)\mathtt{C}^{-1}(\mathtt{S}\mathtt{C} - \mathtt{C}\mathtt{S})\mathtt{T}(u)(\mathtt{E} - \mathtt{I})\mathtt{M}.$$

As the matrices $\mathtt{M}$, $\mathtt{T}(u)$, $\mathtt{T}(-u)$, and $\mathtt{C}$ are invertible, the condition $\hat{\mathtt{R}}(u) = \mathtt{R}(u)$ is equivalent to $(\mathtt{S}\mathtt{C} - \mathtt{C}\mathtt{S})\mathtt{T}(u)(\mathtt{E} - \mathtt{I}) = 0$. Denoting

$$\mathtt{C} = \begin{pmatrix} 1 & 0 & 0 \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{pmatrix},$$

a straightforward calculation yields

$$(\mathtt{S}\mathtt{C} - \mathtt{C}\mathtt{S})\mathtt{T}(u)(\mathtt{E} - \mathtt{I}) = (s - s') \begin{pmatrix} 0 & 0 & 0 \\ c_{23}\lambda^2(\alpha - 6V) & c_{23}6\lambda u & -c_{23} \\ c_{32}\lambda V & -c_{32} & 0 \end{pmatrix}.$$

Then the property $\hat{\mathrm{R}}(u) = \mathrm{R}(u)$ for all values of s and s' is equivalent to $c_{23} = c_{32} = 0$, that ends the proof. □

2.5. Positivity of the $\mathrm{R}(\mathrm{u})$ *matrix*

The velocity V being fixed, we propose to give a full description of the sets

$$\Omega^{V,u} = \{(s, s', \alpha) \in \mathbb{R}^3 \ \text{ such that } \ \mathrm{R}(u) \ \text{ is a non-negative matrix}\}, \quad u \in \mathbb{R}.$$

The relaxation phase is non-negativity preserving in the sense of the Definition 1, for given V and u, if and only if the parameters (s, s', α) are in $\Omega^{V,u}$. Indeed, the non-negativity of the matrix $\mathrm{R}(u)$ imposes that all the distributions f_α, $\alpha \in \{-, 0, +\}$, remain non-negative if they are so at the initial time. These sets are first described by a set of nine inequalities that can be joined into just one. Numerical illustrations are then given to visualize it in the characteristic cases including single relaxation time, multiple relaxation time and relative velocity scheme.

In this contribution, we assume that $V \geq 0$ without loss of generality as

$$\Omega^{-V,-u} = \Omega^{V,u}.$$

This last property is obvious after some algebra or after remarking that the transformation just exchanges the f_1 and f_3 values (corresponding to the velocities $\pm\lambda$).

3. Positivity of the iterative matrix

The nine inequalities obtained from the matrix $\mathrm{R}(u)$ can be combined neatly into one formula.

The inequalities are

$$\begin{cases} R_{0,0} &= Vsu - \dfrac{Vs}{2} - Vs'u + \dfrac{\alpha s'}{6} + su - \dfrac{s}{2} - s'u - \dfrac{s'}{6} + 1 \geqslant 0, \\ R_{0,1} &= Vsu - \dfrac{Vs}{2} - Vs'u + \dfrac{\alpha s'}{6} + \dfrac{s'}{3} \geqslant 0, \\ R_{0,2} &= Vsu - \dfrac{Vs}{2} - Vs'u + \dfrac{\alpha s'}{6} - su + \dfrac{s}{2} + s'u - \dfrac{s'}{6} \geqslant 0, \\ R_{1,0} &= -2Vsu + 2Vs'u - \dfrac{\alpha s'}{3} - 2su + 2s'u + \dfrac{s'}{3} \geqslant 0, \\ R_{1,1} &= -2Vsu + 2Vs'u - \dfrac{\alpha s'}{3} - \dfrac{2s'}{3} + 1 \geqslant 0, \\ R_{1,2} &= -2Vsu + 2Vs'u - \dfrac{\alpha s'}{3} + 2su - 2s'u + \dfrac{s'}{3} \geqslant 0, \\ R_{2,0} &= Vsu + \dfrac{Vs}{2} - Vs'u + \dfrac{\alpha s'}{6} + su + \dfrac{s}{2} - s'u - \dfrac{s'}{6} \geqslant 0, \\ R_{2,1} &= Vsu + \dfrac{Vs}{2} - Vs'u + \dfrac{\alpha s'}{6} + \dfrac{s'}{3} \geqslant 0, \\ R_{2,2} &= Vsu + \dfrac{Vs}{2} - Vs'u + \dfrac{\alpha s'}{6} - su - \dfrac{s}{2} + s'u - \dfrac{s'}{6} + 1 \geqslant 0. \end{cases} \tag{2}$$

We prove now that the previous nine inequalities can be written in a much more lucid way.

Proposition 3. *We introduce the reduced parameters* $\overline{u}$ *and* γ *according to*

$$\overline{u} = 2u(s - s'), \quad \gamma = \frac{s'}{6}(1 - \alpha) - u(s - s')V. \tag{3}$$

Then the nine previous inequalities $R_{i,j} \geq 0$ *displayed in (2) are equivalent to*

$$\max(s' - 1, |\overline{u}|) \leq 2\gamma \leq \min(2 - s - |\overline{u} - sV|, s - |\overline{u} + sV|, s' - |sV|). \tag{4}$$

Proof. Consider first the two inequalities associated with $R_{0,0}$ and $R_{2,2}$:

$$\begin{cases} Vsu - Vs'u + \dfrac{\alpha s'}{6} - \dfrac{s}{2} - \dfrac{s'}{6} + 1 \geqslant \dfrac{Vs}{2} - su + s'u \\ Vsu - Vs'u + \dfrac{\alpha s'}{6} - \dfrac{s}{2} - \dfrac{s'}{6} + 1 \geqslant -\dfrac{Vs}{2} + su - s'u. \end{cases}$$

They can be synthesized in the following form:

$$\left| \frac{\overline{u}}{2} - \frac{Vs}{2} \right| \leq 1 - \frac{s}{2} - \left(\frac{s'}{6}(1 - \alpha) + u(s' - s)V\right) = 1 - \frac{s}{2} - \gamma$$

and we can write this relation as

$$2\gamma \leq 2 - s - |\overline{u} - sV|. \tag{5}$$

Write now the inequalities (2) associated with $R_{0,1}$ and $R_{2,1}$:

$$\begin{cases} Vsu - Vs'u + \dfrac{\alpha s'}{6} + \dfrac{s'}{3} \geqslant \dfrac{Vs}{2} \\ Vsu - Vs'u + \dfrac{\alpha s'}{6} + \dfrac{s'}{3} \geqslant -\dfrac{Vs}{2}. \end{cases}$$

In other words, $|\frac{Vs}{2}| \leq -\gamma + \frac{s'}{2}$. Then

$$2\gamma \leq s' - |sV|. \tag{6}$$

We now focus on the inequalities (2) associated with $R_{0,2}$ and $R_{2,0}$:

$$\begin{cases} Vsu - Vs'u + \dfrac{\alpha s'}{6} + \dfrac{s}{2} - \dfrac{s'}{6} \geqslant \dfrac{Vs}{2} + su - s'u \\ Vsu - Vs'u + \dfrac{\alpha s'}{6} + \dfrac{s}{2} - \dfrac{s'}{6} \geqslant -\dfrac{Vs}{2} - su + s'u \end{cases}$$

We have $|\frac{Vs}{2} + su - s'u| \leq Vsu - Vs'u + \frac{\alpha s'}{6} + \frac{s}{2} - \frac{s'}{6} = \frac{s}{2} - \gamma$. In consequence,

$$2\gamma \leq s - |\overline{u} + sV|. \tag{7}$$

Considering the inequalities with $R_{1,0}$ and $R_{1,2}$, we have

$$\begin{cases} -Vsu + Vs'u - \dfrac{\alpha s'}{6} + \dfrac{s'}{6} \geqslant su - s'u \\ -Vsu + Vs'u - \dfrac{\alpha s'}{6} + \dfrac{s'}{6} \geqslant -su + s'u \end{cases}$$

and $|\frac{1}{2}\overline{u}| \leq -Vsu + Vs'u - \frac{\alpha s'}{6} + \frac{s'}{6} = \gamma$. In consequence,

$$|\overline{u}| \leq 2\gamma. \tag{8}$$

The last inequality $R_{1,1} \geq 0$ can be written as $-Vsu + Vs'u - \frac{\alpha s'}{6} - \frac{s'}{3} + \frac{1}{2} \geqslant 0$ and this inequality is equivalent to $\gamma - \frac{s'}{2} + \frac{1}{2} \geqslant 0$. In other terms,

$$s' - 1 \leq 2\gamma. \tag{9}$$

4. The particular case $u = 0$

In this section, we suppose that the relative velocity u is reduced to zero. Then the necessary and sufficient conditions for non-negativity preserving relaxation can be written as

$$\max(s' - 1, 0) \leq \frac{s'}{3}(1 - \alpha) \leq \min(2 - s - |sV|, s - |sV|, s' - |sV|). \tag{10}$$

Proposition 4. *To fix the ideas, we suppose that the advection velocity* V *is positive:*

$$V \geq 0. \tag{11}$$

The case $V \leq 0$ *follows directly. When* $u = 0$*, the reduced stability conditions*

$$\max(s' - 1, 0) \leq \min(2 - s - |sV|, s - |sV|, s' - |sV|) \tag{12}$$

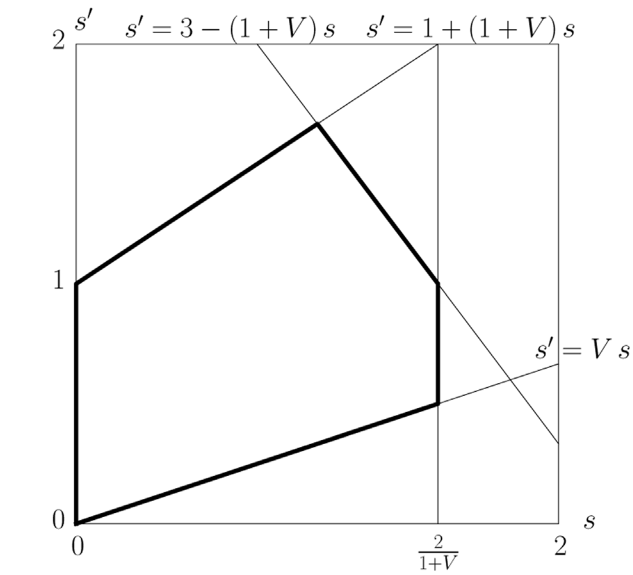

Fig. 1. Necessary and sufficient stability regions described by the inequalities (12) for a null relative velocity u. Illustration proposed for $V = \frac{2}{3}$.

are equivalent to the following conditions for the relaxation parameters

$$\begin{cases} 0 \le s, s' \le 2 \\ s' \ge sV \\ s \le \dfrac{2}{1+V} \\ s' \le \min(3-(1+V)s,\, 1+(1-V)s) \end{cases} \tag{13}$$

joined with a natural Courant type condition for explicit schemes

$$V \le 1 \tag{14}$$

for the advection velocity.

Of course, the conditions (10) have still to be imposed for the equilibrium parameter α when the pair s, s' is given. In particular,

$$\alpha \le 1 \tag{15}$$

and

$$s' \le \frac{3}{\alpha+2}. \tag{16}$$

Fig. 1 illustrates the necessary and sufficient stability region described by the inequalities (12) in the case $V = 2 = 3$.

Proof. We first observe that $0 \le \max(s'-1, 0) \le |s\ V| \le \min(2-s, s)$.

Then $0 \le s \le 2$. Secondly, we have $|s\ V| \le s'$ and because both s and V are positive, we have $0 \le s\ V \le s'$. We have also $s\ V \le s$ and (14) is established. Moreover, $s \ge 0$ and $|s\ V| \le 2-s$ implies $s \le \frac{2}{1+V}$. Due to the positivity of the parameter s, we deduce from (10) a new set of inequalities: $s'-1 \le \max(s'-1, 0) \le \min(2-s-s\ V, s-s\ V)$. Then $s' \le \min(3-(1+V)s, 1+(1-V)s)$. Moreover, $s' \le 3-(1+V)s \le 2$ because $V \ge 0$.

Conversely, if the relations (13) and (14) are satisfied, we have $s'-1 \le 2-s-s\ V$, $s'-1 \le s-s\ V$ and $s'-1 \le s'-s\ V$. Then $s'-1 \le \min(2-s-s\ V, s-s\ V, s'-s\ V)$. Moreover, $0 \le 2-s-s\ V$, $0 \le s-s\ V$ because $V \le 1$ and $0 \le s'-s\ V$. Thus $0 \le \min(2-s-s\ V, s-s\ V, s'-s\ V)$. Finally the inequalities (12) are established and the proposition is proven. □

5. The general case

We analyse the general case of non-zero u in this section, with suitable illustrations of the stability region for various ranges of the parameters.

5.1. Necessary conditions for stability

In this subsection, we prove the following proposition.

Proposition 5. *We suppose that the necessary and sufficient non-negativity preserving relaxation conditions (4) are satisfied as*

$$\max(s'-1, |\overline{u}|) \le 2\gamma \le \min(2-s-|\overline{u}-sV|, s-|\overline{u}+sV|, s'-|sV|)$$

with the notations (3):

$$\overline{u} = 2u(s-s'), \quad \gamma = \frac{s'}{6}(1-\alpha) - u(s-s')V.$$

We suppose also that the advection velocity V is non-negative. Then, the point (s, s') satisfies the following inequalities

$$\begin{cases} 0 \le sV \le s' \le 2, \\ 0 \le sV \le 1, \\ 0 \le s \le 2, \\ s' \le \min(2-sV, s+1, 3-s), \\ s \le \dfrac{2}{1+V}. \end{cases} \tag{17}$$

With these necessary stability conditions, the parameter $\overline{u}$ has been eliminated. We have also, necessarily

$$V \le 1 \tag{18}$$

and

$$|\overline{u}| \le \frac{1}{2}. \tag{19}$$

Proof. We start from the inequalities (4). Then we have

$$0 \le |\overline{u}| \le \max(s'-1, |\overline{u}|) \le \min(2-s-|\overline{u}-sV|, s-|\overline{u}$$
$$+sV|, s'-|sV|) \le s'-|sV|$$

and $s' \ge |s\ V| \ge s\ V$.

We have the triangular inequality $|sV| \le |\overline{u}-sV| + |\overline{u}|$. Then from the general stability conditions (4), we deduce $|\overline{u}-sV| + |\overline{u}| \le 2-s$ and $|s\ V| \le 2-s$. In a similar way, $|sV| \le |\overline{u}+sV| + |\overline{u}|$, $|\overline{u}+sV| + |\overline{u}| \le s$ from (4) and finally $|s\ V| \le 2-s$. We put together the two inequalities and we have $0 \le |s\ V| \le \min(s, 2-s)$.

In consequence, we have $0 \le s \le 2$ and the third point is proven. Since we made the choice of $V \ge 0$ then $s \ge 0$. The first inequality of the two first points are established. From $s\ V \le s$ we have $V \le 1$ and the relation (18) is true. Moreover, $s\ V \le 2-s$ and the last inequality of (17) is true.

Consider now the inequalities $s'-1 \le 2\gamma \le \min(2-s-|\overline{u}-sV|, s-|\overline{u}+sV|)$. We deduce $s'-1+|\overline{u}-sV| \le 2-s$ and $s'-1+|\overline{u}+sV| \le s$. Due to the positvity of the absolute values, we have also $s' \le 3-s$ and $s' \le s+1$. A part of the fifth inequality of (17) is proven.

Finally, due to the triangular inequality, $sV = |sV| \le \frac{1}{2}|\overline{u}-sV| + \frac{1}{2}|\overline{u}+sV|$.

We add this inequality with the two following ones: $s'-1+|\overline{u}-sV| \le 2-s$ and $s'-1+|\overline{u}+sV| \le s$. Then $s'-1+sV \le \frac{1}{2}(2-s+s) = 1$ and $s' \le 2-s\ V$. The fifth inequality of (17) is completely established. Because $s\ V \ge 0$, we have also $s' \le 2$ and the first inequality of (17) is also established. □

We illustrate the zones of necessary stability in Fig. 2 for five particular velocities : $V = 0, \frac{1}{4}, \frac{1}{3}, \frac{1}{2}$ and 1.

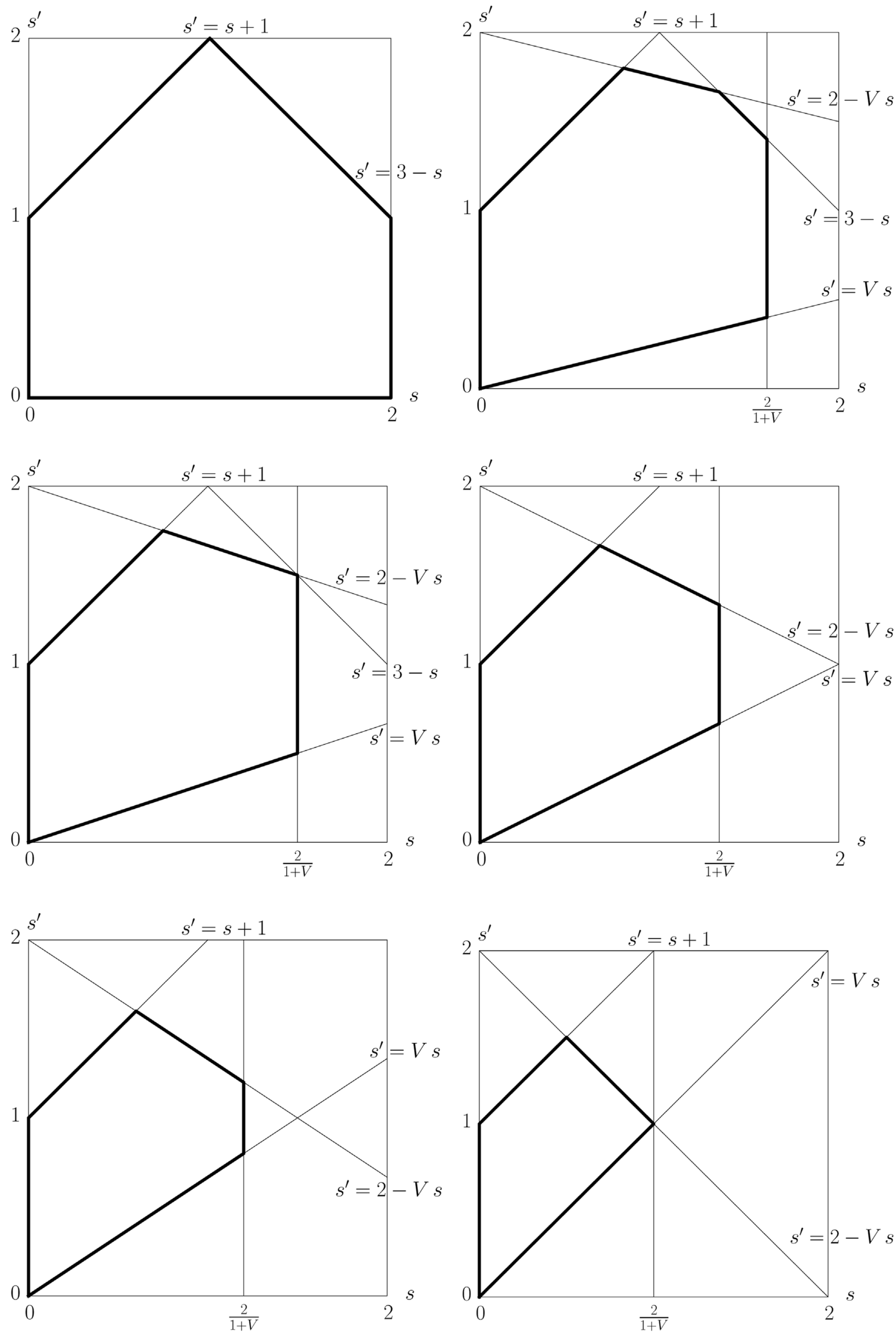

Fig. 2. Necessary stability regions described by the inequalities (17) for $V = 0$, $V = \frac{1}{4}$ [first line, from left to right], $V = \frac{1}{3}$, $V = \frac{1}{2}$ [second line, from left to right], and for $V = \frac{2}{3}$, $V = 1$ [third line, from left to right].

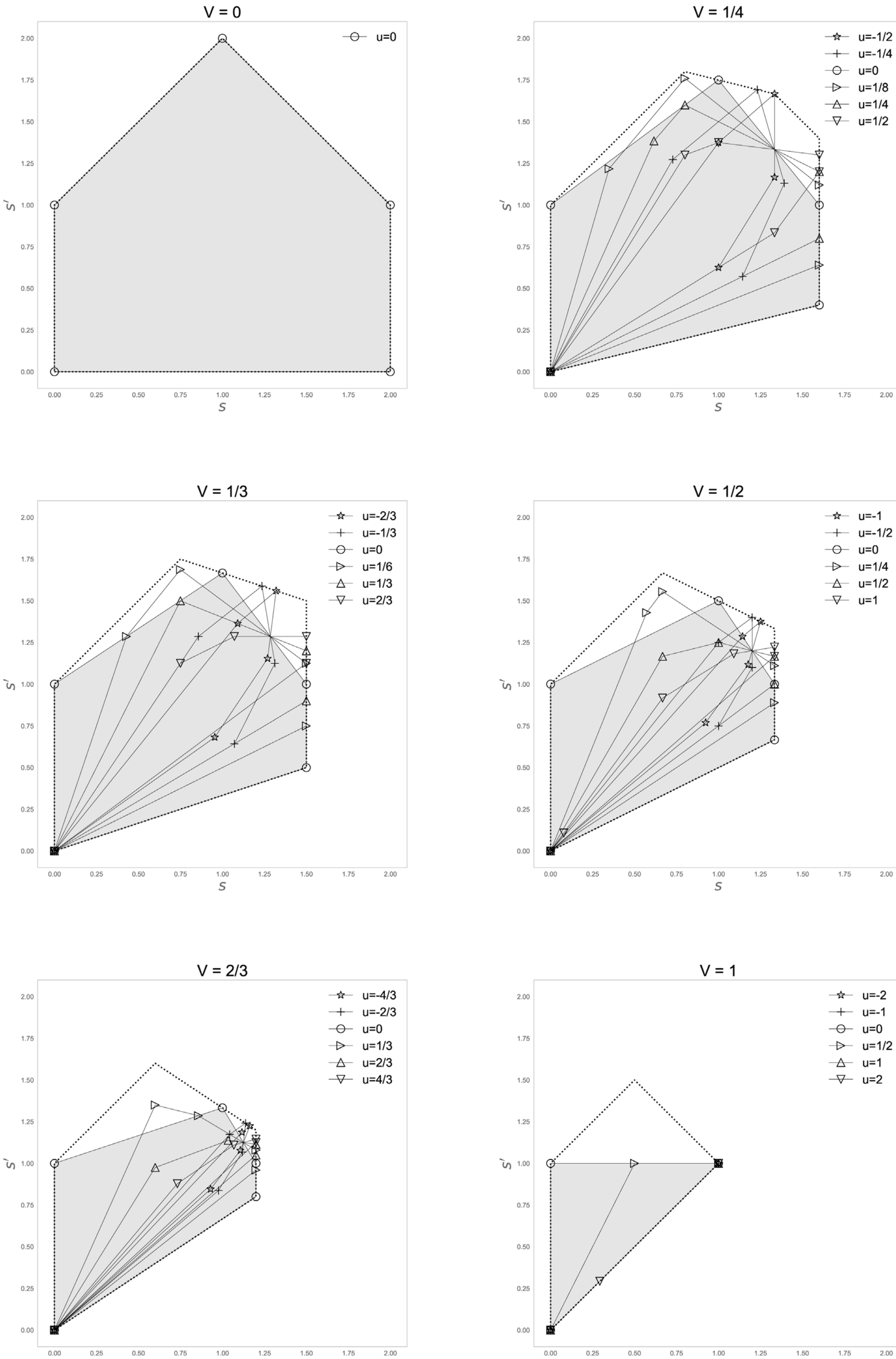

Fig. 3. Numerical study of necessary and sufficient stability regions.

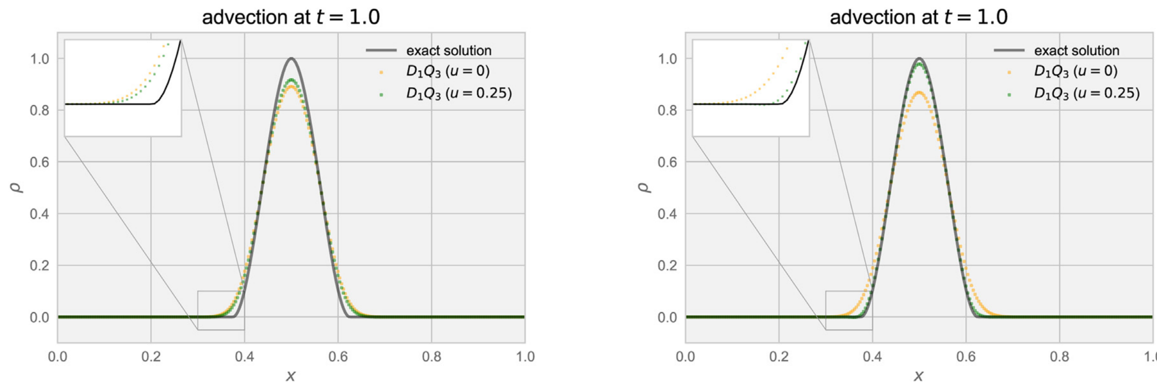

Fig. 4. Smooth profile with a continuous derivative. The parameters for the D1Q3 are tuned in order to have (left) or not (right) the non-negativity property.

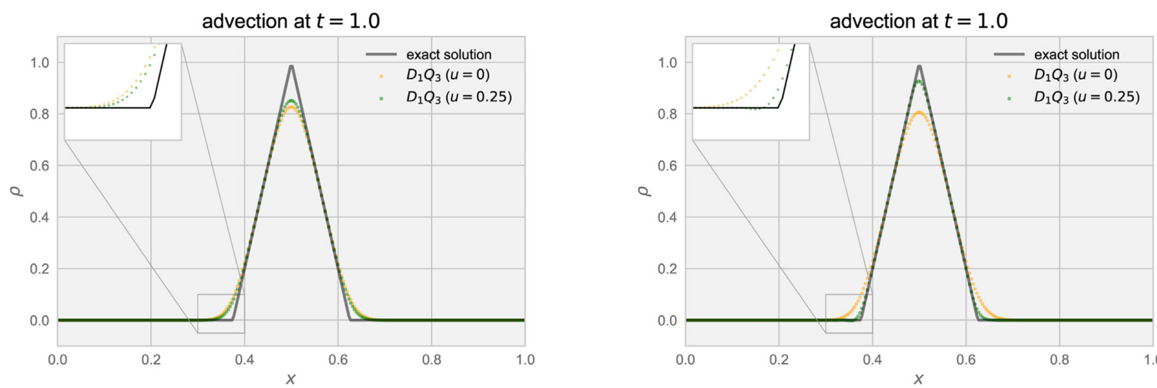

Fig. 5. Continuous profile. The parameters for the D1Q3 are tuned in order to have (left) or not (right) the non-negativity property.

5.2. Numerical study of necessary and sufficient conditions for stability

We now illustrate the necessary and sufficient stability regions for $V=0$, $V=\frac{1}{4}$, $V=\frac{1}{3}$, $V=\frac{1}{2}$, $V=\frac{2}{3}$ and $V=1$ for various ranges of u in Fig. 3. Each figure represents the projection of the set $\Omega^{V,u}$ onto the two-dimensional plane $(s, s') \in \mathbb{R}^2$ given by the external inequalities of (4):

$$\max(s' - 1, |\overline{u}|) \leq \min(2 - s - |\overline{u} - sV|, s - |\overline{u} + sV|, s' - |sV|).$$

Indeed, if (s, s') verifies (4), there exists always a value of α such that $(s, s', \alpha) \in \Omega^{V,u}$. The figures were obtained by following the straight edges of the domain, which can be written as an intersection of half-planes.

For each value of V, the necessary and sufficient stability regions given by the relations (4) are displayed for several values of the relative velocity: $u \in \{-2V, -V, 0, V/2, V, 2V\}$. In dotted line, the necessary stability region of the Proposition 5 is added for comparison. The particular value $u=0$ is enhanced by filling the region in gray.

Some analysis can be drawn from these figures:

- the stability region changes with the relative velocity;
- the maximal value of the first relaxation parameter s is obtained (not only) for $u=0$;
- the stability region is not clearly more favorable (larger or including greater value of s) for $u=V$;
- the segment corresponding to $s=s' \in (0, 1]$ is always in the stability region.

To conclude this section, this notion of stability allows a large set of values for the relaxation parameters. If the scheme is used to simulate the hyperbolic advection equation without second-order operators, we can try to minimize the numerical diffusion while maintaining this stability property. This task is complicated and out of the scope of the paper as the numerical second-order term reads as a non-linear formula that links all the parameters s, α, and V.

6. Numerical illustrations

In this section, we illustrate the stability property with numerical simulations involving the D1Q3 model, with and without relative velocity, used to simulate the linear advection equation. The stability is demonstrated for the parameters chosen according to the analysis presented in the previous sections. Oscillations are seen whenever the parameters go beyond the stability limits presented, as highlighted in the results.

The parameters chosen for the simulations are the following:

	V	u	s	s'	α
Left (stable)	0.25	0.0	1.6	1.3	0.3076923076923076
	0.25	0.25	1.6	1.3	−0.17548076923076938
Right (unstable)	0.25	0.0	1.9	1.4	0.14285714285714302
	0.25	0.25	1.9	1.4	−0.10491071428571441

Moreover, all the simulations are performed for the same space range [0, 1] with periodic boundary conditions, with the same space step $\Delta x = 1/128$, the same time step $\Delta t = \Delta x$, such that $\lambda = 1$, until the final time $t = 1$.

For the left figures, the parameters are chosen in order to satisfy the stability property. We observe numerically also a maximum principle (the conserved moment ρ remains in the interval [0, 1] corresponding to the initial condition), even if it is not formally the stability notion that we investigate. For the right figures, the parameters are chosen in order to break the stability property.

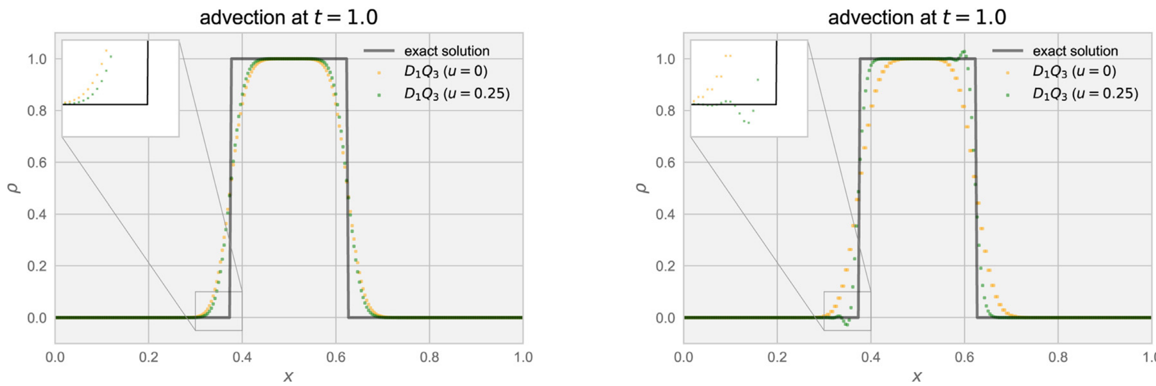

Fig. 6. Discontinuous profile. The parameters for the D1Q3 are tuned in order to have (left) or not (right) the non-negativity property.

The initial conditions are built from the polynomial functions $\phi_0(X) = 1$, $\phi_1(X) = X$, and $\phi_2(X) = X(3 - X^2)/2$ by

$$\rho_k(x) = \begin{cases} \frac{1}{2}\left[1 + \phi_k\left(\frac{2x - 3\ell}{\ell}\right)\right] & \text{if} \ell \qquad \leq x \leq 2\ell, \\ \frac{1}{2}\left[1 + \phi_k\left(\frac{5\ell - 2x}{\ell}\right)\right] & \text{if} 2\ell \qquad \leq x \leq 3\ell, \\ 0 & \text{otherwise,} \end{cases}$$

with ℓ=0.125, for $0 \leq k \leq 2$. For Fig. 4, we choose $\rho(0, x) = \rho_2(x)$ to have a smooth initial condition, for Fig. 5, $\rho(0, x) = \rho_1(x)$ to have a continuous initial condition, and for Fig. 6, $\rho(0, x) = \rho_0(x)$ to have a discontinuous initial condition.

If the profile is smooth (Fig. 4), we have observed that no numerical oscillations occur even if the non-negativity property of the matrix is not satisfied. If the profile is just continuous (Fig. 5), small negative values of the macroscopic quantity are observed when our non-negativity property is not satisfied. Last but not least, classical oscillations are visible for discontinuous profiles (Fig. 6) if our non-negativity property is not satisfied. These oscillations are eliminated when the non-negativity property of the matrix is realized.

7. Conclusion

In this contribution, we have investigated a stability property for a classical mono-dimensional linear three velocities lattice Boltzmann scheme with relative velocity. This property ensures that non-negativity of the initial particle distribution functions continues to remain the same in time. We then give a necessary and sufficient condition to describe the stability region. The case without relative velocity is completely described and simpler necessary conditions are given for the general case. We finally propose some numerical simulations that illustrate the stability property: even if the stability notion that we investigate is not exactly a constraint of convexity, a numerical maximum principle is observed if the parameters are inside the stability region whereas numerical oscillations appear (in particular for the non-smooth profiles) if the parameters are outside.

Moreover, relative velocities modify the stability array in a non-trivial manner. For instance, intuition might have suggested that the stability region for the relative velocity equal to the advection velocity contains all the others but it is really not the case. For a given advection velocity, relative velocities cannot be used to increase the value of the first relaxation parameter, the one involved in the numerical diffusion operator.

In order to focus on fundamental aspects, we have assumed periodic boundary conditions in this contribution. Of course, the possibility of including more realistic boundary conditions and the associated source terms is an important task for a future work.

The non-negativity of the relaxation matrix could be extended to nonlinear schemes. The theoretical study will then be much more technical and has not been performed. Nevertheless, numerical experiments for the Burgers equation show that the behavior of the D1Q3 scheme, and in particular the appearance or absence of oscillations, is analogous to the linear case.

Authors' contribution

ASG credited for code development, simulations; data curation; formal analysis; validation; visualization; roles/writing – original draft; writing – review & editing. DVP contributed for conceptualization; code development, formal analysis; validation; supervision; roles/writing – original draft; writing – review & editing.

Conflict of interest

None declared.

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François Dubois (61 years old) University Professor, Member of Structural Mechanics and Coupled Systems Laboratory, Conservatoire National des Arts et Métiers, Paris (since 1994), Associated to Mathematics Laboratory, Université Paris-Saclay (since 2003).

B. Graille (43 years old) is an Associate Professor (Maître de conférences habilité à diriger des recherches) in the Laboratory of mathematics of the University Paris-Saclay, France, since 2005. His research interests include developing and investigating the lattice Boltzmann methods, developing hydrodynamics models from the kinetic theory.

S.V. Raghurama Rao is an Associate Professor in the Department of Aerospace Engineering, Indian Institute of Science, Bangalore. His education includes B.E. (Mechanical Engineering) from National Institute of Technology, Surat, M.Sc.(Engg.) & Ph.D. degrees from Indian Institute of Science, postdoctoral fellowships from Université Pierre et Marie Curie, Paris, France and Fraunhofer Institut für Techno-und Wirtschaftsmathematik, Kaiserslautern, Germany, before becoming a faculty member at Indian Institute of Science. His research interests include developing CFD algorithms, kinetic theory based numerical methods, Lattice Boltzmann methods, meshless algorithms, aerodynamic shape optimization and algorithms for turbulence simulations.