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Finite Difference formulation of any lattice Boltzmann scheme

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Abstract

Lattice Boltzmann schemes rely on the enlargement of the size of the target problem in order to solve PDEs in a highly parallelizable and efficient kinetic-like fashion, split into a collision and a stream phase. This structure, despite the well-known advantages from a computational standpoint, is not suitable to construct a rigorous notion of consistency with respect to the target equations and to provide a precise notion of stability. In order to alleviate these shortages and introduce a rigorous framework, we demonstrate that any lattice Boltzmann scheme can be rewritten as a corresponding multi-step Finite Difference scheme on the conserved variables. This is achieved by devising a suitable formalism based on operators, commutative algebra and polynomials. Therefore, the notion of consistency of the corresponding Finite Difference scheme allows to invoke the Lax-Richtmyer theorem in the case of linear lattice Boltzmann schemes. Moreover, we show that the frequently-used von Neumann-like stability analysis for lattice Boltzmann schemes entirely corresponds to the von Neumann stability analysis of their Finite Difference counterpart. More generally, the usual tools for the analysis of Finite Difference schemes are now readily available to study lattice Boltzmann schemes. Their relevance is verified by means of numerical illustrations.

Keywords — Lattice Boltzmann methods, Finite Difference multi-step methods, consistency, von Neumann stability analysis, Cayley-Hamilton theorem on the ring of Finite Difference operators

MSC Classification — 76M28, 65M06, 65M12, 15A15

1 Introduction

Lattice Boltzmann schemes are a class of computational methods used to simulate systems of conservation laws under the form of Partial Differential Equations (PDEs). Their basic way of working is the following: instead of taking $N \in \mathbb{N}^*$ PDEs and directly discretize them, a lattice Boltzmann scheme enlarges the size of the problem from N to $q > N$ and treats it in a kinetic-like fashion. This means that the new q variables undergo, at each time step, a local collision phase where different particle distribution functions interact, followed by a lattice-constrained stream phase where no interaction is possible. The advantage of such idiosyncratic approach compared to more traditional numerical methods (*e.g.* Finite Difference, Finite Volume, Finite Elements, *etc.*) is that the local nature of the collision phase allows for massive parallelization of the method and the lattice-constrained stream can be computationally implemented as a pointer shift. Although this way of proceeding is highly beneficial from a computational perspective, it yields a deficient structure to construct a clear and rigorous notion of consistency with respect to the N target equations, as well as a rigorous theory of stability. Indeed, only formal procedures, either based on the Chapman-Enskog expansion [8] or on the equivalent equations by Dubois [15, 17] are currently available to study the consistency of lattice Boltzmann schemes. As far as stability is concerned, most of the studies rely on the linear stability analysis of the eigenvalues of the system, see [4, 37].

In order to bridge the gap between the lattice Boltzmann methods and the traditional approaches known to numerical analysts, the aim of the present contribution is to show that any lattice Boltzmann scheme can be rewritten as a corresponding multi-step Finite Difference scheme on the conserved variables, regardless of the linearity of the equilibria. This is made possible by developing an appropriate formalism based on commutative algebra and therefore yields a proper notion of consistency with respect to the target equations, which is that of Finite Difference schemes (see any standard textbook such as [38]). Furthermore, we confirm that the customary *von Neumann*

analysis used for lattice Boltzmann schemes is equivalent to performing the same analysis on the corresponding Finite Difference scheme and is consequently particularly relevant. The price to pay for passing from an explicit scheme with q variables and utilizing information only at the previous time-step to a method with $N < q$ variables is to increase the number of previous time-steps the new solution depends on, yielding a multi-step Finite Difference scheme.

In the past, few authors have noticed that for some particular lattice Boltzmann schemes, one has a corresponding (sometimes called “equivalent”) Finite Difference formulation on the conserved variables. Despite this, no general theory has been formulated. For instance: Suga [39] derives by direct computations a three-stages Finite Difference scheme from a uni-dimensional three-velocities D_1Q_3 scheme,¹ limiting the computations to a linear framework with one relaxation parameter (SRT). Dellacherie [11] derives a two-stages Finite Difference scheme for the D_1Q_2 lattice Boltzmann scheme. Again, this is limited to one spatial dimension and to a linear framework. A higher level of generality has been reached by the works of Ginzburg and collaborators, see [22] for a recap. They succeeded, using a link formalism, in writing a class of Lattice Boltzmann schemes as Finite Difference schemes [13]. With their highly constrained link structure to be enforced, the resulting Finite Difference scheme with three stages is valid regardless of the spatial dimension and the choice of discrete velocities. The limitations are that the choice of moments is heavily constrained and only the case of one conserved moment is handled. Moreover, the evolution equation of the moving particles can depend on the distribution of the still particles only *via* the conserved moment the equilibria depend upon and the schemes must be two-relaxation time (TRT) models with “magic parameter” equal to one-fourth for any link. The difficulty in establishing a general result comes from the coupling between spatial operators and time shifts. We must mention that during the drafting of the present contribution, an interesting work by Fučík and Straka [21] has been published covering the very same subject and essentially coming to the same conclusion as our paper. Their focus is different than ours since they adopt a purely algorithmic approach rather than a precise algebraic characterization of lattice Boltzmann schemes. We actually provide more insight into the bound on the number of time steps of the corresponding Finite Difference scheme and our formalism, based on polynomials, aims at providing a direct link with the classical tools for the stability analysis and allows to establish a link with the Taylor expansions from [17], as introduced in [1]. In [21], the authors rely on a decomposition of the scheme using an hollow matrix² yielding an equivalent form of the scheme with the diagonal non-equilibrium part, after a finite number of steps of their algorithm. However, to the best of our understanding, the origin of such algorithm is not fully clear. In their work, the spatial shifts of data introduced by the stream phase are taken into account using a rather cumbersome system of indices, whereas we rely on an straightforward algebraic characterization of the stream phase.

Our paper is structured as follows: in Section 2, we introduce – in guise of friendly introduction – the link of our problem with Ordinary Differential Equations (ODEs). The right formalism to make lattice Boltzmann schemes looking very close to a system of ODEs is provided in Section 3 and allows to prove the main results of the work showcased in Section 4. We devote Section 5 to discuss examples, possible simplifications of the problem and particular cases deserving particular attention. In Section 6, we prove the equivalence of the *von Neumann* analysis for lattice Boltzmann and Finite Difference schemes. In Section 7, we show how the well-known tools for Finite Difference schemes can be used to prove convergence theorems for lattice Boltzmann schemes. We corroborate our claim *via* numerical simulations. We eventually conclude in Section 8.

2 The example of Ordinary Differential Equations

Since our way of reducing any lattice Boltzmann scheme to a multi-step Finite Difference scheme has been originally inspired by an analogy with systems of ODEs, let us introduce this way of reasoning with the following example. Consider the system of ODEs of size $q \in \mathbb{N}^*$ with matrix $\mathbf{A} \in \mathcal{M}_q(\mathbb{R})$ given by

$$\begin{cases} \mathbf{y}'(t) &= \mathbf{A}\mathbf{y}(t), & t \geq 0, \\ \mathbf{y}(0) &= \hat{\mathbf{y}} \in \mathbb{R}^q. \end{cases} \quad (1)$$

Transforming a single equation of higher order into a system of first order equations like Equation (1) by considering the companion matrix is a current practice, which unsurprisingly makes the problem more handy from the computational standpoint. Though being the analogous of what we aim at doing of lattice Boltzmann schemes, the other way around, passing from a system of first order to a

¹It is customary to call D_dQ_q a scheme in a d -dimensional space using q discrete velocities.

²Matrix with zero entries on the diagonal.

single equation of higher order, seems to be seldom considered. We proceed like in [10]. By iterating, we have that $\mathbf{y}^{(k)} = \mathbf{A}^k \mathbf{y}$ for $k \in \llbracket 0, q \rrbracket$.³ Let $(\gamma_k)_{k=0}^{k=q} \subset \mathbb{R}$ be $q+1$ real coefficients, then write $\sum_{k=0}^{k=q} \gamma_k \mathbf{y}^{(k)} = (\sum_{k=0}^{k=q} \gamma_k \mathbf{A}^k) \mathbf{y}$. Taking $(\gamma_k)_{k=0}^{k=q}$ as the coefficients of the characteristic polynomial⁴ $\chi_{\mathbf{A}} = \sum_{k=0}^{k=q} \gamma_k X^k$ of \mathbf{A} , by virtue of the Cayley-Hamilton theorem, we deduce the corresponding equation on the first variable y_1 (playing the role of the conserved moment), given by

$$\begin{cases} \sum_{k=0}^{k=q} \gamma_k y_1^{(k)}(t) &= 0, & t \geq 0, \\ y_1(0) &= (\mathbf{A} \hat{\mathbf{y}})_1, \\ &\vdots \\ y_1^{(q-1)}(0) &= (\mathbf{A}^{q-1} \hat{\mathbf{y}})_1. \end{cases} \quad (2)$$

This provides a systematic way of performing the transformation without having to rely on hand computations and substitutions. To give an example, consider

$$\mathbf{A}_I = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 2 & 0 \end{pmatrix}, \quad \text{with} \quad \chi_{\mathbf{A}_I} = X^3 - 3X^2 - 2X + 1.$$

Hence, the corresponding ODE on the first variable is given by $y_1''' - 3y_1'' - 2y_1' + y_1 = 0$.

3 Algebraic form of lattice Boltzmann schemes

Now that the reader is familiar – through a simple example – with the main idea and the final aim of the present contribution, we introduce the general framework of lattice Boltzmann schemes and the right formalism to treat them almost as systems of ODEs.

3.1 Spatial and temporal discretization

We set the problem in any spatial dimension $d = 1, 2, 3$ considering the whole space \mathbb{R}^d , because we are not interested in studying boundary conditions. The space is discretized by a d -dimensional lattice $\mathcal{L} := \Delta x \mathbb{Z}^d$ of constant step $\Delta x > 0$ in all direction. The time is uniformly discretized with step $\Delta t > 0$. The discrete instants of time shall be indexed by the integer indices $n \in \mathbb{N}$ so that the corresponding time is $t^n = n\Delta t$. We finally introduce the so-called lattice velocity $\lambda > 0$ defined by $\lambda := \Delta x / \Delta t$. Observe that the developing theory is totally discrete and thus fully independent from the scaling between Δx and Δt .

3.2 Discrete velocities and shift operators

The first choice to be made when devising a lattice Boltzmann scheme concerns the discrete velocities $(\mathbf{e}_j)_{j=1}^{j=q} \subset \mathbb{R}^d$ with $q \in \mathbb{N}^*$, which are multiples of the lattice velocity, namely $\mathbf{e}_j = \lambda \mathbf{c}_j$ for any $j \in \llbracket 1, q \rrbracket$ with $(\mathbf{c}_j)_{j=1}^{j=q} \subset \mathbb{Z}^d$. Therefore, particles are stuck to move – at each time step – on the lattice \mathcal{L} . We denote the distribution density of the particles moving with velocity \mathbf{e}_j by f_j for every $j \in \llbracket 1, q \rrbracket$. The shift operators associated with the discrete velocities are an important element of the following analysis.

Definition 1 (Shift operator). *Let $\mathbf{z} \in \mathbb{Z}^d$, then the associated shift operator on the lattice \mathcal{L} , denoted $T_{\Delta x}^{\mathbf{z}}$, is defined in the following way. Take $f : \mathcal{L} \rightarrow \mathbb{R}$ be any function defined on the lattice,⁵ then the action of $T_{\Delta x}^{\mathbf{z}}$ is*

$$(T_{\Delta x}^{\mathbf{z}} f)(\mathbf{x}) = f(\mathbf{x} - \mathbf{z} \Delta x), \quad \forall \mathbf{x} \in \mathcal{L}.$$

We also introduce $\mathcal{T}_{\Delta x}^d := \{T_{\Delta x}^{\mathbf{z}} \text{ with } \mathbf{z} \in \mathbb{Z}^d\} \cong \mathbb{Z}^d$.

The shift yields information sought in the upwind direction with respect to the considered velocity. Let us introduce the natural binary operation between shifts.

Definition 2 (Product). *Let the “product” $\circ : \mathcal{T}_{\Delta x}^d \times \mathcal{T}_{\Delta x}^d \rightarrow \mathcal{T}_{\Delta x}^d$ be the binary operation defined as $T_{\Delta x}^{\mathbf{z}} \circ T_{\Delta x}^{\mathbf{w}} = T_{\Delta x}^{\mathbf{z}+\mathbf{w}}$, for any $\mathbf{z}, \mathbf{w} \in \mathbb{Z}^d$.*

³We shall consistently use the notation $\llbracket a, b \rrbracket := \{a, a+1, \dots, b\}$ for $a, b \in \mathbb{Z}$ and $a < b$.

⁴In the whole work, the indeterminate of any polynomial shall be denoted by X .

⁵The function could take values in any ring, see [30].

Henceforth, the product \circ is understood whenever no ambiguity is possible. This operation provides an algebraic structure to the shifts, directly inherited from that of \mathbb{Z}^d .

Proposition 1. $(\mathcal{T}_{\Delta x}^d, \circ)$ forms an Abelian group.

Moreover, there is only “one movement” for each Cartesian direction which “generates” the shifts. More precisely

$$\begin{aligned} \text{for } d = 1, \text{ let } x &:= T_{\Delta x}^1, \text{ then } \mathcal{T}_{\Delta x}^d = \langle \{x\} \rangle, \\ \text{for } d = 2, \text{ let } x &:= T_{\Delta x}^{(1,0)}, y := T_{\Delta x}^{(0,1)}, \text{ then } \mathcal{T}_{\Delta x}^d = \langle \{x, y\} \rangle, \\ \text{for } d = 3, \text{ let } x &:= T_{\Delta x}^{(1,0,0)}, y := T_{\Delta x}^{(0,1,0)}, z := T_{\Delta x}^{(0,0,1)}, \text{ then } \mathcal{T}_{\Delta x}^d = \langle \{x, y, z\} \rangle, \end{aligned} \quad (3)$$

where $\langle \cdot \rangle$ is the customary notation for the generating set of a group. We can add one more binary operation, which is non-internal to $\mathcal{T}_{\Delta x}^d$. This yields the cornerstone of this work, namely the set of Finite Difference operators, finite combinations of weighted shifts operators *via* a sum. It is defined as follows, see Chapter 3 of [30].

Definition 3 (Finite Difference operators). *The set of Finite Difference operators on the lattice \mathcal{L} is defined as*

$$\mathcal{D}_{\Delta x}^d := \mathbb{R}\mathcal{T}_{\Delta x}^d = \left\{ \sum_{T \in \mathcal{T}_{\Delta x}^d} \alpha_T T, \text{ where } \alpha_T \in \mathbb{R} \text{ and } \alpha_T = 0 \text{ a.e.}^6 \right\},$$

the group ring (or group algebra) of $\mathcal{T}_{\Delta x}^d$ over \mathbb{R} . The sum $+$: $\mathcal{D}_{\Delta x}^d \times \mathcal{D}_{\Delta x}^d \rightarrow \mathcal{D}_{\Delta x}^d$ the product⁶ \circ : $\mathcal{D}_{\Delta x}^d \times \mathcal{D}_{\Delta x}^d \rightarrow \mathcal{D}_{\Delta x}^d$ of two elements are defined by

$$\begin{aligned} \left(\sum_{T \in \mathcal{T}_{\Delta x}^d} \alpha_T T \right) + \left(\sum_{T \in \mathcal{T}_{\Delta x}^d} \beta_T T \right) &= \sum_{T \in \mathcal{T}_{\Delta x}^d} (\alpha_T + \beta_T) T, \\ \left(\sum_{T \in \mathcal{T}_{\Delta x}^d} \alpha_T T \right) \circ \left(\sum_{H \in \mathcal{T}_{\Delta x}^d} \beta_H H \right) &= \sum_{T, H \in \mathcal{T}_{\Delta x}^d} \alpha_T \beta_H T \circ H. \end{aligned}$$

Furthermore, the product of $\sigma \in \mathbb{R}$ with elements of $\mathcal{D}_{\Delta x}^d$ is given by

$$\sigma \left(\sum_{T \in \mathcal{T}_{\Delta x}^d} \alpha_T T \right) = \sum_{T \in \mathcal{T}_{\Delta x}^d} (\sigma \alpha_T) T.$$

With the two binary operations, $\mathcal{D}_{\Delta x}^d$ behaves closely to \mathbb{Z} , \mathbb{R} or \mathbb{C} as stated by the following result, see [30].

Proposition 2 (Ring of Finite Difference operators). $(\mathcal{D}_{\Delta x}^d, +, \circ)$ is a commutative ring.⁷

Observe that $(\mathcal{D}_{\Delta x}^d, +, \circ)$ is not a field: not every element of $\mathcal{D}_{\Delta x}^d$ has multiplicative inverse, take for example the centered approximation of the derivative along x : $(T_{\Delta x}^{-1} - T_{\Delta x}^1)/(2\Delta x)$ and see for instance the concept of indefinite sum in the calculus of Finite Differences [33, 32]. The elements having inverse are called “units” and divide all the other elements. It can be easily seen that the units are the product of a non-zero real number and a shift in $\mathcal{T}_{\Delta x}^d$. Indeed $(\alpha T_{\Delta x}^z)^{-1} = (1/\alpha) T_{\Delta x}^{-z}$ for any $\alpha \in \mathbb{R} \setminus \{0\}$ and $z \in \mathbb{Z}^d$. The inverse of a unit shall also be denoted by a bar.

Remark 1. One can see $\mathcal{D}_{\Delta x}^d$ as the ring of Laurent polynomials of d variables over the field \mathbb{R} , where the indeterminates are x, y and z . For example, for $d = 1$, the identification $\mathcal{D}_{\Delta x}^d = \mathbb{R}[x, x^{-1}] = \mathbb{R}[x, \bar{x}]$ holds. This automatically implies that $\mathcal{D}_{\Delta x}^d$ is more than a commutative ring, namely a unique factorization domain.

Remark 2. The reals \mathbb{R} can be identified with the subring $\mathbb{R} \cong \{\alpha T_{\Delta x}^0 : \alpha \in \mathbb{R}\}$.

3.3 Lattice Boltzmann algorithm: collide and stream

Any lattice Boltzmann scheme consists in an algorithm made up of two phases: a local collision phase performed on each site of the lattice and a stream phase, where particles are exchanged between different sites of the lattice. Let us introduce each of them.

⁶Which interestingly corresponds to the discrete convolution product.

⁷It also an (Hopf) algebra over \mathbb{R} and can also be viewed as a free module where the scalars belong to \mathbb{R} and the basis are the elements of the group $\mathcal{T}_{\Delta x}^d$.

3.3.1 Collision phase

We adopt the point of view of the multiple-relaxation-times (MRT) schemes, where it is customary to consider the collision written as a diagonal relaxation in the moments basis, see [12]. For this reason, we introduce a change of basis called moment matrix $\mathbf{M} \in \text{GL}_q(\mathbb{R})$. The entries of \mathbf{M} can depend on Δx and/or on Δt but cannot be a function of the space and time variables. Gathering the distributions into $\mathbf{f} = (f_1, \dots, f_q)^\top$, the moments are recovered by $\mathbf{m} = \mathbf{M}\mathbf{f}$. We also introduce

- the matrix $\mathbf{I} \in \text{GL}_q(\mathbb{R})$ which is the identity matrix of size q ;
- the matrix $\mathbf{S} \in \mathcal{M}_q(\mathbb{R})$ is the relaxation matrix which is a singular with $\text{rank}(\mathbf{S}) = q - N$, where $N \in \llbracket 1, q - 1 \rrbracket$ is the number of conserved moments:

$$\mathbf{S} = \text{diag}(0, \dots, 0, s_{N+1}, \dots, s_q),$$

where the first N entries are zero⁸ and correspond to the conserved moments, the following $q - N$ are such that $s_i \in]0, 2]$ for $i \in \llbracket N + 1, q \rrbracket$, see [15].

- We employ the notation $\mathbf{m}^{\text{eq}|n}(\mathbf{x}) = \mathbf{m}^{\text{eq}}(m_1^n(\mathbf{x}), \dots, m_N^n(\mathbf{x}))$ for $\mathbf{x} \in \mathcal{L}$, where $\mathbf{m}^{\text{eq}} : \mathbb{R}^N \rightarrow \mathbb{R}^q$ are possibly non-linear functions of the conserved moments. Since these equilibria are then multiplied by \mathbf{S} , the first N components do not need to be defined.

The collision phase reads, denoting by \star any post-collision state

$$\mathbf{m}^{n,\star}(\mathbf{x}) = (\mathbf{I} - \mathbf{S})\mathbf{m}^n(\mathbf{x}) + \mathbf{S}\mathbf{m}^{\text{eq}|n}(\mathbf{x}), \quad \forall \mathbf{x} \in \mathcal{L}. \quad (4)$$

In the collision phase Equation (4), the entries of \mathbf{S} can depend on Δx or Δt , but not on space and time. The equilibria are allowed to follow the same dependencies plus those on space and time and can also depend on some “external variable” like in the case of vectorial schemes [23].

3.3.2 Stream phase

The stream phase is diagonal in the space of the distributions. It can be written as

$$\mathbf{f}^{n+1}(\mathbf{x}) = (\text{diag}(T_{\Delta x}^{c_1}, \dots, T_{\Delta x}^{c_q})\mathbf{f}^{n,\star})(\mathbf{x}), \quad \forall \mathbf{x} \in \mathcal{L}, \quad (5)$$

where for the first time, the matrices have entries in a commutative ring, see [19] and [6], instead than in the field \mathbb{R} . The set $\mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$ of square matrices of size q with entries belonging to $\mathcal{D}_{\Delta x}^d$ forms a ring under the usual operations between matrices. Even if $\mathcal{D}_{\Delta x}^d$ is commutative from Proposition 2, $\mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$ is not commutative for $q \geq 2$, as for real matrices and matrices of first-order differential operators [17].

3.3.3 Monolithic scheme

The stream phase Equation (5) can be rewritten in a non-diagonal form in the space of moments as done by [17, 20] by introducing the matrix $\mathbf{T} := \mathbf{M}\text{diag}(T_{\Delta x}^{c_1}, \dots, T_{\Delta x}^{c_q})\mathbf{M}^{-1} \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$ and merged with the collision phase Equation (4) to obtain the scheme

$$\mathbf{m}^{n+1}(\mathbf{x}) = \mathbf{A}\mathbf{m}^n(\mathbf{x}) + \mathbf{B}\mathbf{m}^{\text{eq}|n}(\mathbf{x}), \quad \forall \mathbf{x} \in \mathcal{L}, \quad (6)$$

where $\mathbf{A} := \mathbf{T}(\mathbf{I} - \mathbf{S}) \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$ and $\mathbf{B} := \mathbf{T}\mathbf{S} \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$. In the sequel, we shall not indicate the spatial variable $\mathbf{x} \in \mathcal{L}$ for the sake of readability.

We observe that the operators $(T_{\Delta x}^{c_j})_{j=1}^{j=q} \subset \mathcal{T}_{\Delta x}^d \subset \mathcal{D}_{\Delta x}^d$ are the eigenvalues of the matrix \mathbf{T} . However, they are not the eigenvalues of the matrix \mathbf{A} . Indeed, it is general false that the eigenvalues of \mathbf{A} belong to the space $\mathcal{D}_{\Delta x}^d$. It is interesting to interpret the lattice Boltzmann scheme under the form Equation (6) as discrete-time linear control system with matrices on a commutative ring [6]. The moments are the state of the system evolving *via* the matrix \mathbf{A} , whereas the equilibria are the control *via* \mathbf{B} being a feedback observing only a part of the state, namely the conserved moments.

We introduce our example of choice, which shall be used through the whole paper.

Example 1 (D_1Q_3 scheme with one conserved moment). *Consider the D_1Q_3 scheme with one conserved moment [18] by taking $d = 1$, $q = 3$ and $N = 1$. We have $c_1 = 0$, $c_2 = 1$ and $c_3 = -1$ with $\mathbf{S} = \text{diag}(0, s, p)$ and*

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \lambda & -\lambda \\ -2\lambda^2 & \lambda^2 & \lambda^2 \end{pmatrix}, \quad \mathbf{T} = \begin{pmatrix} \frac{1}{3}(\mathbf{x} + 1 + \bar{\mathbf{x}}) & \frac{1}{2\lambda}(\mathbf{x} - \bar{\mathbf{x}}) & \frac{1}{6\lambda^2}(\mathbf{x} - 2 + \bar{\mathbf{x}}) \\ \frac{\lambda}{3}(\mathbf{x} - \bar{\mathbf{x}}) & \frac{1}{2}(\mathbf{x} + \bar{\mathbf{x}}) & \frac{1}{6\lambda}(\mathbf{x} - \bar{\mathbf{x}}) \\ \frac{\lambda^2}{3}(\mathbf{x} - 2 + \bar{\mathbf{x}}) & \frac{\lambda}{2}(\mathbf{x} - \bar{\mathbf{x}}) & \frac{1}{6}(\mathbf{x} + 2 + \bar{\mathbf{x}}) \end{pmatrix},$$

⁸This is not always the case in literature but shall be used consistently in this paper. We put them at the beginning for the sake of presentation.

taking $s, p \in]0, 2]$ and where x has been introduced in Equation (3). It can be used to simulate the non-linear conservation law $\partial_t m_1 + \partial_x m_2^{eq} = 0$ under the acoustic scaling $\Delta t \sim \Delta x$. The matrices A and B are

$$A = \begin{pmatrix} \frac{1}{3}(x+1+\bar{x}) & \frac{(1-s)}{2\lambda}(x-\bar{x}) & \frac{(1-p)}{6\lambda^2}(x-2+\bar{x}) \\ \frac{\lambda}{3}(x-\bar{x}) & \frac{(1-s)}{2}(x+\bar{x}) & \frac{(1-p)}{6\lambda}(x-\bar{x}) \\ \frac{\lambda^2}{3}(x-2+\bar{x}) & \frac{\lambda(1-s)}{2}(x-\bar{x}) & \frac{(1-p)}{6}(x+2+\bar{x}) \end{pmatrix},$$

$$B = \begin{pmatrix} 0 & \frac{s}{2\lambda}(x-\bar{x}) & \frac{p}{6\lambda^2}(x-2+\bar{x}) \\ 0 & \frac{s}{2}(x+\bar{x}) & \frac{p}{6\lambda}(x-\bar{x}) \\ 0 & \frac{\lambda s}{2}(x-\bar{x}) & \frac{p}{6}(x+2+\bar{x}) \end{pmatrix}.$$

4 Main result of the paper

With a new way of writing any lattice Boltzmann scheme using Definition 3 and thanks to Proposition 2, which provides the ideal setting to generalize the Cayley-Hamilton theorem, we can proceed like in Section 2 to prove the main result of the paper: any lattice Boltzmann can be viewed as a multi-step Finite Difference scheme on the conserved variables.

4.1 Characteristic polynomial and Cayley-Hamilton theorem

Polynomials with coefficients in $\mathcal{D}_{\Delta x}^d$ and matrices with entries in $\mathcal{D}_{\Delta x}^d$ play a central role in what we are going to develop.

Definition 4 (Characteristic polynomial). *Let \mathcal{R} be a commutative ring and $C \in \mathcal{M}_r(\mathcal{R})$ for some $r \in \mathbb{N}^*$. The characteristic polynomial of C , denoted $\chi_C \in \mathcal{R}[X]$, is given by $\chi_C := (-1)^r \det(C - XI)$, where $\det(\cdot)$ is the determinant and I is the $r \times r$ identity matrix.*

The naive computation of the characteristic polynomial χ_C using its definition *via* the determinant could be computationally expensive, especially when dealing with symbolic computations like in our case. For this reason, we employed the Faddeev-Leverrier algorithm [25] which is of polynomial complexity, generally lower than that of the pivot method. The process is detailed in Algorithm 1

Algorithm 1 Faddeev-Leverrier algorithm for the computation of the characteristic polynomial of a square matrix on a commutative ring \mathcal{R} .

Input: $C \in \mathcal{M}_r(\mathcal{R})$

Set $D = C$

for $k \in \llbracket 1, r \rrbracket$ **do**

if $k > 1$ **then**

 Compute $D = C(D + \gamma_{r-k+1}I)$

end if

 Compute $\gamma_{r-k} = -\frac{\text{tr}(D)}{k}$

end for

Output: the coefficients $(\gamma_k)_{k=0}^{k=r} \subset \mathcal{R}$ of the characteristic polynomial $\chi_C = \sum_{k=0}^{k=r} \gamma_k X^k$

and only uses matrix-matrix multiplications and the computation of the trace, denoted by $\text{tr}(\cdot)$.

Example 2. *Coming back to Example 1, it is easy to show either by manual computations or by using Algorithm 1 that $\chi_A = X^3 + \gamma_2 X^2 + \gamma_1 X + \gamma_0$ with*

$$\begin{aligned} \gamma_2 &= p(x+4+\bar{x})/6 + s(x+\bar{x})/2 - (x+1+\bar{x}), \\ &= -(1-p)(x+4+\bar{x})/6 - (1-s)(x+\bar{x})/2 - (x+1+\bar{x})/3, \\ \gamma_1 &= ps(x+1+\bar{x})/3 - p(5x+2+5\bar{x})/6 - s(x+2+\bar{x})/2 + (x+1+\bar{x}), \\ &= (-p(1-s)/3 - (p+s-2)/2)(x+\bar{x}) + 2((1-s) - s(1-p) - (p+s-2)), \\ \gamma_0 &= -(1-p)(1-s). \end{aligned}$$

We see that $\gamma_0 = 0$ if either s or p are equal to one, this shall be discussed in Section 5.2. On the other hand $\gamma_1 = 0$ if we have $s = p = 1$.

A central result used in this work is the Cayley-Hamilton theorem for matrices over a commutative ring, see [6] for the proof, generalizing the same result holding for matrices on a field utilized in Section 2.

Theorem 3 (Cayley-Hamilton). *Let \mathcal{R} be a commutative ring and $\mathbf{C} \in \mathcal{M}_r(\mathcal{R})$ for some $r \in \mathbb{N}^*$. Then $\chi_{\mathbf{C}}$ is a monic polynomial in the ring $\mathcal{R}[X]$ in the indeterminate X , under the form $\chi_{\mathbf{C}} = X^r + \gamma_{r-1}X^{r-1} + \dots + \gamma_1X + \gamma_0$ with $(\gamma_k)_{k=0}^{k=r} \subset \mathcal{R}$. Then⁹ $\mathbf{C}^r + \gamma_{r-1}\mathbf{C}^{r-1} + \dots + \gamma_1\mathbf{C} + \gamma_0\mathbf{I} = \mathbf{0}$.*

This result states that any square matrix with entries in a commutative ring verifies its characteristic equation.

4.2 Corresponding Finite Difference schemes

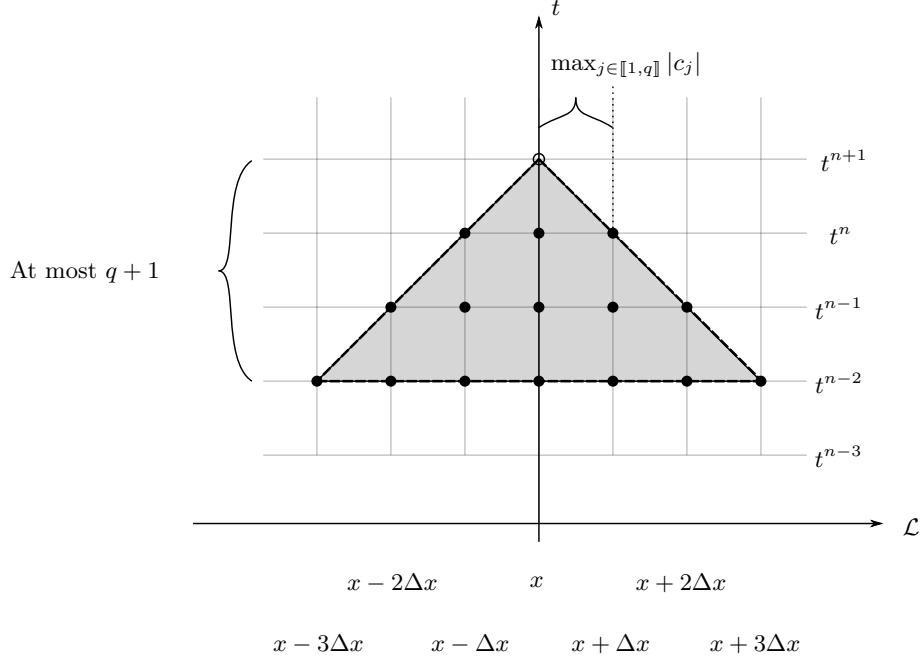


Figure 1: Maximal space-time domain of dependence of the corresponding Finite Difference scheme for $N = 1$ (full black points inside the grey area) by virtue of Proposition 4 in the case of $d = 1$. The maximal space-time slopes are determined by the maximal shift of the considered scheme whereas the number of involved time-steps is at most $q + 1$.

The previous Theorem 3 is the key for proving the following results, whose backbone is essentially the same than in Section 2.

4.2.1 One conserved moment

We first analyze the case of one conserved moment, namely $N = 1$, to keep the presentation as simple as possible. We shall eventually deal with $N > 1$ once the principles are established.

Proposition 4 (Corresponding Finite Difference scheme for $N = 1$). *Let $N = 1$, then the lattice Boltzmann scheme Equation (6) corresponds to a multi-step explicit Finite Difference scheme on the conserved moment m_1 under the form*

$$m_1^{n+1} = - \sum_{k=0}^{q-1} \gamma_k m_1^{n+1-q+k} + \left(\sum_{k=0}^{q-1} \left(\sum_{\ell=0}^k \gamma_{q+\ell-k} \mathbf{A}^\ell \right) \mathbf{B} \mathbf{m}^{eq|n-k} \right)_1,$$

where $(\gamma_k)_{k=0}^{k=q} \subset \mathcal{D}_{\Delta x}^d$ are the coefficients of $\chi_{\mathbf{A}} = \sum_{k=0}^{k=q} \gamma_k X^k$, the characteristic polynomial of \mathbf{A} .

This result means that the conserved moment satisfies an explicit multi-step Finite Difference scheme with at most q steps, thus involving $q + 1$ discrete time instants, see Figure 1. The maximal size of spatial influence at each past time step can be deduced by looking at Algorithm 1, derived from the Newton's identities.

It is interesting to observe that also the non-conserved moments satisfy a Finite Difference numerical scheme, see the following proof. However, these schemes would depend on the conserved moment *via* the equilibria and are therefore not independent from the rest of the system.

⁹Sometimes, we shall indulge to the notation $\chi_{\mathbf{C}}(\mathbf{C}) = \mathbf{0}$.

Proof. Let $n \in \mathbb{N}$. Then for any $k \in \mathbb{N}$, applying Equation (6) recursively we have

$$\mathbf{m}^{n+1} = \mathbf{A}^k \mathbf{m}^{n-(k-1)} + \sum_{\ell=0}^{k-1} \mathbf{A}^\ell \mathbf{B} \mathbf{m}^{\text{eq}|^{n-\ell}}.$$

We perform a temporal shift in order to fix the first term on the right hand side regardless of the value of k . Introduce $\tilde{n} := n - (k - 1)$, therefore

$$\mathbf{m}^{\tilde{n}+k} = \mathbf{A}^k \mathbf{m}^{\tilde{n}} + \sum_{\ell=0}^{k-1} \mathbf{A}^\ell \mathbf{B} \mathbf{m}^{\text{eq}|\tilde{n}+k-1-\ell}.$$

This holds true, in particular, for any $k \in \llbracket 0, q \rrbracket$. We can then consider the coefficients $(\gamma_k)_{k=0}^{k=q}$ of the characteristic polynomial $\chi_{\mathbf{A}} = \sum_{k=0}^{k=q} \gamma_k X^k$ of \mathbf{A} and write

$$\sum_{k=0}^q \gamma_k \mathbf{m}^{\tilde{n}+k} = \left(\sum_{k=0}^q \gamma_k \mathbf{A}^k \right) \mathbf{m}^{\tilde{n}} + \sum_{k=0}^q \gamma_k \left(\sum_{\ell=0}^{k-1} \mathbf{A}^\ell \mathbf{B} \mathbf{m}^{\text{eq}|\tilde{n}+k-1-\ell} \right).$$

Applying the Cayley-Hamilton Theorem 3 by virtue of Proposition 2, we know that $\sum_{k=0}^{k=q} \gamma_k \mathbf{A}^k = \mathbf{0}$. Using the monicity of the characteristic polynomial and coming back by setting $\tilde{n} + q = n + 1$ gives

$$\mathbf{m}^{n+1} = - \sum_{k=0}^{q-1} \gamma_k \mathbf{m}^{n+1-q+k} + \sum_{k=0}^q \gamma_k \left(\sum_{\ell=0}^{k-1} \mathbf{A}^\ell \mathbf{B} \mathbf{m}^{\text{eq}|^{n-q+k-\ell}} \right).$$

The last sum can start from $k = 1$. Performing a change of indices in the last double sum yields the result.

$$\mathbf{m}^{n+1} = - \sum_{k=0}^{q-1} \gamma_k \mathbf{m}^{n+1-q+k} + \sum_{k=0}^{q-1} \left(\sum_{\ell=0}^k \gamma_{q+\ell-k} \mathbf{A}^\ell \right) \mathbf{B} \mathbf{m}^{\text{eq}|^{n-k}}. \quad (7)$$

□

Example 3. We come back to Example 1. Using Proposition 4, we have the corresponding Finite Difference scheme given by

$$\begin{aligned} m_1^{n+1} = & -\frac{p}{6}(x+4+\bar{x})m_1^n - \frac{s}{2}(x+\bar{x})m_1^n + (x+1+\bar{x})m_1^n - \frac{ps}{3}(x+1+\bar{x})m_1^{n-1} \\ & + \frac{p}{6}(5x+2+5\bar{x})m_1^{n-1} + \frac{s}{2}(x+2+\bar{x})m_1^{n-1} - (x+1+\bar{x})m_1^{n-1} \\ & + (1-p)(1-s)m_1^{n-2} + \frac{s}{2\lambda}(x-\bar{x})m_2^{\text{eq}|^n} - \frac{s(1-p)}{2\lambda}(x-\bar{x})m_2^{\text{eq}|^{n-1}} \\ & + \frac{p}{6\lambda^2}(x-2+\bar{x})m_3^{\text{eq}|^n} + \frac{p(1-s)}{6\lambda^2}(x-2+\bar{x})m_3^{\text{eq}|^{n-1}}. \end{aligned} \quad (8)$$

One can easily check its consistency – under the acoustic scaling – with the target conservation law.

Remark 3. One could think of allowing \mathbf{M} and/or \mathbf{S} to depend on the space and time variables. This would imply to consider weights made up of functions instead of the real numbers in Definition 3. However, $\mathcal{D}_{\Delta x}^d$ would no longer be commutative, because the multiplication by a function does not commute with shifts (not shift-invariant according to [35]). For example, take $\mathbf{z} \in \mathbb{Z}^d$ and a function $g : \mathcal{L} \rightarrow \mathbb{R}$, then

$$\begin{aligned} ((T_{\Delta x}^{\mathbf{z}} \circ (gT_{\Delta x}^{\mathbf{0}})) f)(\mathbf{x}) &= g(\mathbf{x} - \mathbf{z}\Delta x) f(\mathbf{x} - \mathbf{z}\Delta x), \\ ((gT_{\Delta x}^{\mathbf{0}}) \circ T_{\Delta x}^{\mathbf{z}}) f(\mathbf{x}) &= g(\mathbf{x}) f(\mathbf{x} - \mathbf{z}\Delta x), \end{aligned}$$

for every $\mathbf{x} \in \mathcal{L}$ and for any function $f : \mathcal{L} \rightarrow \mathbb{R}$. The right-hand sides are not equal in general, except if g is constant.

4.2.2 Several conserved moments and vectorial schemes

Consider now to deal with multiple conservation laws, namely $N > 1$. We select a conserved moment and we consider the other conserved moments as “slave” variables as the equilibria have been until so far, for $N = 1$, because they imply variables that we eventually want to keep. In particular, we utilize different polynomials for different conserved moments to obtain the Finite

Difference schemes. To formalize this concept, for any square matrix $\mathbf{C} \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$, consider $\mathbf{C}_I := (\sum_{i \in I} \mathbf{e}_i \otimes \mathbf{e}_i) \mathbf{C} (\sum_{i \in I} \mathbf{e}_i \otimes \mathbf{e}_i) \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$ for any $I \subset \llbracket 1, q \rrbracket$, corresponding to the matrix where only the rows and columns of indices I are conserved and the remaining ones are set to zero. We can also consider the matrix $\mathbf{C}[I] \in \mathcal{M}_{|I| \times |I|}(\mathcal{D}_{\Delta x}^d)$ obtained by keeping only the rows and the columns indexed in I . A useful corollary of Theorem 3 and of the Laplace formula for the determinant is the following.

Corollary 5. *Let $\mathbf{C} \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$ and $I \subset \llbracket 1, q \rrbracket$, then one has that $\chi_{\mathbf{C}_I} = X^{q-|I|} \chi_{\mathbf{C}[I]}$. Moreover, the polynomial $\chi_{\mathbf{C}[I]}$ annihilates \mathbf{C}_I .*

This means that the characteristic polynomial of \mathbf{C}_I is directly linked to that of the smaller matrix $\mathbf{C}[I]$, which is thus faster to compute, and that the latter is an annihilator for the first matrix.

For any conserved moment indexed by $i \in \llbracket 1, N \rrbracket$ we introduce the matrix $\mathbf{A}_i := \mathbf{A}_{\{i\} \cup \llbracket N+1, q \rrbracket}$ and $\mathbf{A}_i^\diamond := \mathbf{A}_{\llbracket 1, N \rrbracket \setminus \{i\}}$. Notice that we have the decomposition $\mathbf{A} = \mathbf{A}_i + \mathbf{A}_i^\diamond$. Indeed, we “save” the conserved moments other than the i^{th} by placing them into \mathbf{A}_i^\diamond , which shall not participate in the computation of the characteristic polynomial. With this notations, we have generated a family of problems from Equation (6) under the form

$$\mathbf{m}^{n+1} = \mathbf{A}_i \mathbf{m}^n + \mathbf{A}_i^\diamond \mathbf{m}^n + \mathbf{B} \mathbf{m}^{\text{eq}|n}, \quad i \in \llbracket 1, N \rrbracket. \quad (9)$$

It is useful to stress that the term $\mathbf{A}_i \mathbf{m}^n$ in Equation (9) does not involve any conserved moment other than the i^{th} . Conversely, $\mathbf{A}_i^\diamond \mathbf{m}^n$ does not involve any function except the conserved moments other than the i^{th} . Then, the corresponding Finite Difference schemes come under the form stated by the following Proposition.

Proposition 6 (Corresponding Finite Difference scheme for $N \geq 1$). *Let $N \geq 1$, then the lattice Boltzmann scheme Equation (6) rewritten as Equation (9) corresponds to the multi-step explicit Finite Difference schemes on the conserved moments m_1, \dots, m_N under the form*

$$\begin{aligned} m_i^{n+1} = & - \sum_{k=0}^{q-N} \gamma_{i,k} m_i^{n-q+N+k} + \left(\sum_{k=0}^{q-N} \left(\sum_{\ell=0}^k \gamma_{i,q+1-N+\ell-k} \mathbf{A}_i^\ell \right) \mathbf{A}_i^\diamond \mathbf{m}^{n-k} \right)_i \\ & + \left(\sum_{k=0}^{q-N} \left(\sum_{\ell=0}^k \gamma_{i,q+1-N+\ell-k} \mathbf{A}_i^\ell \right) \mathbf{B} \mathbf{m}^{\text{eq}|n-k} \right)_i, \end{aligned}$$

for any $i \in \llbracket 1, N \rrbracket$ where $(\gamma_{i,k})_{k=0}^{q+1-N} \subset \mathcal{D}_{\Delta x}^d$ are the coefficients of the characteristic polynomial $\chi_{\mathbf{A}_i} = X^{N-1} \sum_{k=0}^{q+1-N} \gamma_{i,k} X^k$ of \mathbf{A}_i .

This Proposition states that for each conserved moment, the corresponding Finite Difference scheme has at most $q - N$ steps, thus involves $q - N + 1$ discrete times. This result encompasses and generalizes Proposition 4. The proof is the same than that of Proposition 4 by taking advantage of Corollary 5. We show in another contribution [1] that the result of Proposition 6 is the right one to bridge between the consistency analysis of Finite Difference schemes and the Taylor expansions on the lattice Boltzmann schemes for $N \geq 1$ proposed by [17].

Example 4 ($D_1 Q_3$ for two conservation laws). *Consider the $D_1 Q_3$ scheme [3] with $d = 1$, $q = 3$ and $c_1 = 0$, $c_2 = 1$ and $c_3 = -1$*

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \lambda & -\lambda \\ 0 & \lambda^2 & \lambda^2 \end{pmatrix}, \quad \mathbf{S} = \text{diag}(0, 0, p), \quad \text{with } p \neq 1, \quad (10)$$

thus having $N = 2$. This scheme can be used to simulate the system of conservation laws $\partial_t m_1 + \partial_x m_2 = 0$ and $\partial_t m_2 + \partial_x m_3^{\text{eq}} = 0$ under the acoustic scaling $\Delta t \sim \Delta x$. Using Proposition 6 we have

$$\begin{aligned} m_1^{n+1} = & m_1^n + \frac{1}{2}(1-p)(x + \bar{x})m_1^n - \frac{1}{2}(1-p)(x + \bar{x})m_1^{n-1} + \frac{(x - \bar{x})}{2\lambda} m_2^n \\ & - \frac{(1-p)(x - \bar{x})}{2\lambda} m_2^{n-1} + \frac{p(x - 2 + \bar{x})}{2\lambda^2} m_3^{\text{eq}|n}, \\ m_2^{n+1} = & \frac{1}{2}(2-p)(x + \bar{x})m_2^n - (1-p)m_2^{n-1} + \frac{p(x - \bar{x})}{2\lambda} m_3^{\text{eq}|n}. \end{aligned}$$

One could remark that the linear part is different from one scheme to the other, since we have used different polynomials for each conserved moment.

4.3 Initialization schemes

In the corresponding Finite Difference schemes in Proposition 4 and Proposition 6, the only remaining freedom is to devise the initialization schemes for the multi-step schemes at regime, analogously to Equation (2) in Section 2. This is the counter-part of the freedom of choice on the initial data for the original lattice Boltzmann scheme, which are not necessarily taken at equilibrium, see [27]. By applying Equation (6) to the initial data as many times as needed, one progressively obtains the initialization schemes, as function of the initial datum. It is worthwhile observing that the choice of initial datum does not play any role in the previous procedure and does not influence the stability analysis of Section 6. It only comes into play during the consistency analysis of the numerical method, which is not investigated in this paper, in particular, as far as time boundary layers are concerned, see [40, 34].

5 Examples, simplifications and particular cases

Now that the main results of the paper, namely Proposition 4 and Proposition 6, have been stated and proved, we can analyze and comment some particular cases which deserve a closer look. More examples are available in the Appendices.

Example 5 (ODEs). *To illustrate some basic peculiarities that easily transpose to lattice Boltzmann schemes, we introduce the following matrices extending the discussion of Section 2.*

$$\mathbf{A}_{II} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad \mathbf{A}_{III} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 2 & 0 \\ 1 & 2 & 1 \end{pmatrix}, \quad \mathbf{A}_{IV} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & -2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

For \mathbf{A}_{II} , we have $\chi_{\mathbf{A}_{II}} = X^3 - 5X^2 + 8X - 4$, corresponding to $y_1''' - 5y_1'' + 8y_1' - 4y_1 = 0$. However, contrarily to \mathbf{A}_I in Section 2, the characteristic polynomial $\chi_{\mathbf{A}_{II}}$ does not correspond to the minimal polynomial $\mu_{\mathbf{A}_{II}} = X^2 - 3X + 2$. Thus in this case, we could use the latter to obtain Equation (2) having $y_1'' - 3y_1' + 2y_1 = 0$. This phenomenon is studied in Section 5.1. It indicates that we can achieve a more compact corresponding ODE by using the annihilating polynomial of smallest degree on every variable. This does not change the core of the strategy.

For \mathbf{A}_{III} , we obtain $\chi_{\mathbf{A}_{III}} = X^3 - 4X^2 + 4X - 1$, corresponding to $y_1''' - 4y_1'' + 4y_1' - y_1 = 0$. However, by inspecting \mathbf{A}_{III} , one notices that the first two equations do not depend on the last variable y_3 . For this reason, we could have considered the matrix $\mathbf{A}_{III}[\{1,2\}]$ obtained from \mathbf{A}_{III} by removing the last row and column. In this case $\chi_{\mathbf{A}_{III}[\{1,2\}]} = X^2 - 3X + 1$, corresponding to the equation $y_1'' - 3y_1' + y_1 = 0$. This kind of situation for lattice Boltzmann schemes is investigated in Section 5.2. It is interesting to observe once more that $\chi_{\mathbf{A}_{III}[\{1,2\}]}$ divides $\chi_{\mathbf{A}_{III}}$. This shows that an initial inspection of the matrix can yield a reduction of the size of the problem that can be achieved by a simple trimming operation, which eliminates some variable from the problem but treats the remaining ones as usual.

Finally, consider \mathbf{A}_{IV} . In this case the characteristic polynomial and the minimal polynomial coincide $\chi_{\mathbf{A}_{IV}} = X^3 - X^2 - 4X + 4$ corresponding to the equation $y_1''' - y_1'' - 4y_1' + 4y_1 = 0$. However, if we take the polynomial $\nu_{\mathbf{A}_{IV}} = X^2 - 3X + 2$ such that $\nu_{\mathbf{A}_{IV}}$ divides $\chi_{\mathbf{A}_{IV}} = \mu_{\mathbf{A}_{IV}}$ and such that

$$\nu_{\mathbf{A}_{IV}}(\mathbf{A}_{IV}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 12 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

we see that it annihilates the first row, thus can be used instead of the other polynomials to yield Equation (2). This gives $y_1'' - 3y_1' + 2y_1 = 0$. The question is elucidated for lattice Boltzmann schemes in Section 5.3 and show that asking for the annihilation of the whole matrix is too much to achieve a restatement of the equation focusing only on the first variable. This strategy is different from the previous one because not all the lines of the matrix are treated in the same way.

Let us transpose these observations to actual lattice Boltzmann schemes. A question which might arise concerns the possibility of performing better than the characteristic polynomial, in terms of number of steps in the resulting Finite Difference scheme. There are cases, which seem quite rare according to our experience (we succeeded in finding only one special case where this happens), where the answer is positive. This phenomenon has also been discussed by [21], without envisioning a systematic way of guaranteeing the minimality of the Finite Difference scheme obtained by their algorithm.

5.1 Minimal reductions in terms of time-steps

The first idea to obtain a simpler scheme is to use the minimal polynomial of \mathbf{A} (or its submatrices, if needed) as done for \mathbf{A}_{II} in Example 5.

Definition 5 (Minimal polynomial). *Let \mathcal{R} be a commutative ring and $\mathbf{C} \in \mathcal{M}_r(\mathcal{R})$ for some $r \in \mathbb{N}^*$. We define the minimal polynomial of \mathbf{C} , denoted $\mu_{\mathbf{C}}$ as being the monic polynomial in $\mathcal{R}[X]$ of smallest degree, thus under the form*

$$\mu_{\mathbf{C}} = X^{\deg(\mu_{\mathbf{C}})} + \omega_{\deg(\mu_{\mathbf{C}})-1} X^{\deg(\mu_{\mathbf{C}})-1} + \dots + \omega_1 X + \omega_0,$$

with $(\omega_k)_{k=0}^{k=\deg(\mu_{\mathbf{C}})} \subset \mathcal{R}$ such that

$$\mathbf{C}^{\deg(\mu_{\mathbf{C}})} + \omega_{\deg(\mu_{\mathbf{C}})-1} \mathbf{C}^{\deg(\mu_{\mathbf{C}})-1} + \dots + \omega_1 \mathbf{C} + \omega_0 \mathbf{I} = \mathbf{0}.$$

The characteristic and the minimal polynomial for problems set of a commutative ring are linked by a divisibility property.

Lemma 7. *Let \mathcal{R} be a commutative ring and $\mathbf{C} \in \mathcal{M}_r(\mathcal{R})$ for some $r \in \mathbb{N}^*$, then $\mu_{\mathbf{C}}$ divides $\chi_{\mathbf{C}}$. Therefore, we also have $\deg(\mu_{\mathbf{C}}) \leq \deg(\chi_{\mathbf{C}})$.*

Proof. The proof is standard and works the same than that of Lemma 10. \square

Unfortunately, the minimal polynomial cannot be mechanically computed by something like Algorithm 1 as for the characteristic polynomial. The same reduction of Proposition 4 with $\deg(\mu_{\mathbf{A}})$ instead of q and ω_k instead of γ_k is possible. It can be observed that for Example 1, the minimal and the characteristic polynomial of the matrix \mathbf{A} coincide. We have been unable to find an example of lattice Boltzmann scheme where the minimal polynomial does not match the characteristic polynomial.

5.2 Relaxation on the equilibrium

Secondly, a more careful look at relaxation matrix allows us to write it as $\mathbf{S} = \text{diag}(0, \dots, 0, s_{N+1}, \dots, s_{N+Q}, 1, \dots, 1)$, where $s_i \in]0, 1[\cup]1, 2]$ for $i \in \llbracket N+1, N+Q \rrbracket$ for some $Q \in \mathbb{N}$ and the last $q - Q - N$ relaxation parameters are equal to one, meaning that the corresponding moments exactly relax on their respective equilibrium. Without loss of generality, we have decided to put them at the end of \mathbf{S} . The fact of considering some relaxation rates equal to one is used in the so-called “regularization” models, see [9] and references therein, showing the enhancement of the stability features of the schemes.

In terms of matrix structure, the consequence is that the last $q - N - Q$ columns of \mathbf{A} are zero, analogously to \mathbf{A}_{III} in Example 5. We can therefore employ the following decomposition of \mathbf{A} : $\mathbf{A} = \mathbf{A}_{\llbracket 1, N+Q \rrbracket} + \mathbf{A}_{\llbracket N+Q+1, q \rrbracket}$ similarly to Equation (9). We shall consider the characteristic polynomial of $\mathbf{A}_{\llbracket 1, N+Q \rrbracket}$ (if $N = 1$, otherwise the characteristic polynomials of its submatrices), whereas we know that the second matrix does not involve the last $q - N - Q$ moments (indeed, non conserved) because the corresponding columns are zero. Therefore, Proposition 4 and Proposition 6 are still valid using $N+Q$ instead of q and the matrix $\mathbf{A}_{\llbracket 1, N+Q \rrbracket}$ instead of \mathbf{A} . The corresponding Finite Difference scheme for each conserved moment shall therefore have at most $Q+1$ steps instead of $q+1$.

Example 6. *We come back to Example 1 taking $p = 1$ and $s \neq 1$, thus having $Q = 1$ and $N = 1$. Following the procedure described before gives $\chi_{\mathbf{A}_{\llbracket 1, 2 \rrbracket}} = X^2 + \gamma_1 X + \gamma_0$ with $\gamma_1 = -(1-s)(x + \bar{x})/2 - (x+1+\bar{x})/3$ and $\gamma_0 = (1-s)(x+4+\bar{x})/6$ and the corresponding scheme*

$$\begin{aligned} m_1^{n+1} &= \frac{(1-s)}{2}(x+\bar{x})m_1^n + \frac{1}{3}(x+1+\bar{x})m_1^n - \frac{(1-s)}{6}(x+4+\bar{x})m_1^{n-1} \\ &\quad + \frac{s}{2\lambda}(x-\bar{x})m_2^{eq|n} + \frac{1}{6\lambda^2}(x-2+\bar{x})m_3^{eq|n} + \frac{(1-s)}{6\lambda^2}(x-2+\bar{x})m_3^{eq|n-1}. \end{aligned}$$

Unsurprisingly, this is Equation (8) setting $p = 1$, obtained treating a smaller problem.

Observe that the fact of taking all the relaxation rates equal to one, relaxing on the equilibria, is the core mechanism of the relaxation schemes [5]. In this case, there is nothing to do since the original lattice Boltzmann scheme is already in the form of a Finite Difference scheme on the conserved moments. Our way of proposing a corresponding Finite Difference scheme using characteristic polynomials is flawlessly compatible with this setting.

5.3 A different reduction strategy

The third idea is to proceed as for \mathbf{A}_{IV} in Example 5, namely looking for a polynomial which does not annihilate the whole matrix \mathbf{A} . To simplify the presentation, we limit ourselves to $N = 1$, namely one conserved moment. We sketch this strategy to account for previous results on the subject [13, 22]. Nevertheless, we shall justify its limited interest at the end of the Section.

Example 7 (Link scheme with magic parameter). *Consider the so-called link scheme by [13, 22] defined for any spatial dimension $d = 1, 2, 3$ considering $q = 1 + 2W$ with $W \in \mathbb{N}^*$ with $\mathbf{c}_1 = \mathbf{0}$ and any $\mathbf{c}_{2j} = -\mathbf{c}_{2j+1} \neq \mathbf{0}$ for $j \in \llbracket 1, W \rrbracket$. The system is taken with all the so-called “magic parameters” equal to one-fourth, therefore $\mathbf{S} = \text{diag}(0, s, 2 - s, s, 2 - s, \dots) \in \mathcal{M}_{1+2W}(\mathbb{R})$ for $s \neq 1$ and*

$$\mathbf{M} = \left(\begin{array}{c|cc|cc|cc} 1 & 1 & 1 & \cdots & \cdots & 1 & 1 \\ \hline 0 & \lambda & -\lambda & 0 & 0 & 0 & 0 \\ 0 & \lambda^2 & \lambda^2 & 0 & 0 & 0 & 0 \\ \hline \vdots & 0 & 0 & \ddots & \ddots & 0 & 0 \\ \vdots & 0 & 0 & \ddots & \ddots & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & \lambda & -\lambda \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & \lambda^2 \end{array} \right) \in \mathcal{M}_{1+2W}(\mathbb{R}),$$

The claim in [22] is that the corresponding Finite Difference scheme is the two-steps scheme

$$\begin{aligned} m_1^{n+1} = (2 - s)m_1^n - (1 - s)m_1^{n-1} + s \left(\sum_{\ell=1}^W \frac{(T_{\Delta x}^{\mathbf{c}_{2\ell}} - T_{\Delta x}^{-\mathbf{c}_{2\ell}}) m_{2\ell}^{eq|n}}{2\lambda} \right) \\ + \frac{(2 - s)}{2} \left(\sum_{\ell=1}^W \frac{(T_{\Delta x}^{\mathbf{c}_{2\ell}} - 2 + T_{\Delta x}^{-\mathbf{c}_{2\ell}}) m_{2\ell+1}^{eq|n}}{\lambda^2} \right). \end{aligned} \quad (11)$$

This is true regardless of the choice of d and W . By direct inspection of the corresponding Finite Difference scheme Equation (11), we can say that this reduction has been achieved using the polynomial $\nu_{\mathbf{A}} = X^2 - (2 - s)X + (1 - s)$. However, it can be easily shown that this polynomial does not annihilate the entire matrix \mathbf{A} as the minimal and characteristic polynomials do: it only does so for the first row.

Indeed, we have seen for ODEs in Example 5 that we might try just to annihilate the first row of the problem. Thus, we define the polynomial annihilating all the first row of the matrix \mathbf{A} , except the very first element.

Definition 6. We call $\nu_{\mathbf{A}} \in \mathcal{D}_{\Delta x}^d[X]$ “minimal polynomial annihilating most of the first row” (MPAMFR) of \mathbf{A} the monic polynomial of minimal degree under the form

$$\nu_{\mathbf{A}} = X^{\deg(\nu_{\mathbf{A}})} + \psi_{\deg(\nu_{\mathbf{A}})-1} X^{\deg(\nu_{\mathbf{A}})-1} + \dots + \psi_1 X + \psi_0,$$

with $(\psi_k)_{k=0}^{k=\deg(\nu_{\mathbf{A}})} \subset \mathcal{D}_{\Delta x}^d$ such that for every $j \in \llbracket 2, q \rrbracket$

$$(\mathbf{A}^{\deg(\nu_{\mathbf{A}})})_{1j} + \psi_{\deg(\nu_{\mathbf{A}})-1} (\mathbf{A}^{\deg(\nu_{\mathbf{A}})-1})_{1j} + \dots + \psi_1 (\mathbf{A})_{1j} = 0.$$

By seeing the coefficients of this unknown polynomial as the unknowns of a linear system, the problem of finding $\nu_{\mathbf{A}}$ can be rewritten in terms of matrices.¹⁰ Let $K \in \llbracket 1, \deg(\mu_{\mathbf{A}}) \rrbracket$ and construct the matrix of variable size

$$\mathbf{V}_K = \left(\begin{array}{ccc} (\mathbf{A})_{12} & \cdots & (\mathbf{A}^K)_{12} \\ \vdots & & \vdots \\ (\mathbf{A})_{1,Q+1} & \cdots & (\mathbf{A}^K)_{1,Q+1} \end{array} \right) \in \mathcal{M}_{Q \times K}(\mathcal{D}_{\Delta x}^d). \quad (12)$$

Therefore, we want to find the smallest $K \in \llbracket 1, \deg(\mu_{\mathbf{A}}) \rrbracket$ such that $\ker(\mathbf{V}_K) \neq \{\mathbf{0}\}$, that is, the smallest $K \in \llbracket 1, \deg(\mu_{\mathbf{A}}) \rrbracket$ such that \mathbf{V}_K is not injective. Since the kernel of the “minimal” \mathbf{V}_K shall be a $\mathcal{D}_{\Delta x}^d$ -module of dimension 1, we can chose a monic polynomial by always taking $\psi_K = 1$. On the other hand, it should be observed that the zero order coefficient ψ_0 remains free. This underdetermination comes from the fact that we do not request that $\nu_{\mathbf{A}}$ annihilates the whole first row.

¹⁰The same procedure is used to find the minimal polynomial, since we do not have a definition like Definition 4.

Proposition 8. Let $N = 1$, then the lattice Boltzmann scheme (6) can be rewritten as a Finite Difference scheme on the conserved moment m_1 under the form

$$m_1^{n+1} = - \sum_{k=1}^{\deg(\nu_{\mathbf{A}})-1} \psi_k m_1^{n+1-\deg(\nu_{\mathbf{A}})+k} + \left(\sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k (\mathbf{A}^k)_{11} \right) m_1^{n+1-\deg(\nu_{\mathbf{A}})} + \left(\sum_{k=0}^{\deg(\nu_{\mathbf{A}})-1} \left(\sum_{\ell=0}^k \psi_{\deg(\nu_{\mathbf{A}})+\ell-k} \mathbf{A}^\ell \right) \mathbf{B} \mathbf{m}^{\text{eq}} |^{n-k} \right)_1, \quad (13)$$

where $(\psi_k)_{k=1}^{k=\deg(\nu_{\mathbf{A}})} \subset \mathcal{D}_{\Delta x}^d$ are the coefficients of $\nu_{\mathbf{A}} = \sum_{k=0}^{k=\deg(\nu_{\mathbf{A}})} \psi_k X^k$.

The proof can be found in the Appendices. Looking at Equation (13), we see that we do not need the value of ψ_0 to reduce the scheme, neither to reduce \mathbf{A} nor to deal with the equilibria through \mathbf{B} . Changing time indices and putting everything on the left hand side

$$\begin{aligned} \sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k m_1^{\tilde{n}+k} - \left(\sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k (\mathbf{A}^k)_{11} \right) m^{\tilde{n}} &= \sum_{k=0}^{\deg(\nu_{\mathbf{A}})} \tilde{\psi}_k m_1^{\tilde{n}+k}, \\ &= \sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k \left(\sum_{\ell=0}^{k-1} \mathbf{A}^\ell \mathbf{B} \mathbf{m}^{\text{eq}} |^{\tilde{n}+k-1-\ell} \right)_1, \\ &= \sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \tilde{\psi}_k \left(\sum_{\ell=0}^{k-1} \mathbf{A}^\ell \mathbf{B} \mathbf{m}^{\text{eq}} |^{\tilde{n}+k-1-\ell} \right)_1, \end{aligned}$$

where we have defined

$$\tilde{\psi}_k = \begin{cases} \psi_k, & k \in \llbracket 1, \deg(\nu_{\mathbf{A}}) \rrbracket, \\ - \sum_{\ell=1}^{\deg(\nu_{\mathbf{A}})} \psi_\ell (\mathbf{A}^\ell)_{11}, & k = 0. \end{cases}$$

This generates a polynomial, which is indeed $\nu_{\mathbf{A}}$ but with a precise choice of ψ_0 . We will soon give a precise characterization of this particular polynomial.

Definition 7. We call $\tilde{\nu}_{\mathbf{A}} \in \mathcal{D}_{\Delta x}^d[X]$ “minimal polynomial annihilating the first row” (MPAFR) of \mathbf{A} the monic polynomial of minimal degree under the form

$$\tilde{\nu}_{\mathbf{A}} = X^{\deg(\tilde{\nu}_{\mathbf{A}})} + \tilde{\psi}_{\deg(\tilde{\nu}_{\mathbf{A}})-1} X^{\deg(\tilde{\nu}_{\mathbf{A}})-1} + \dots + \tilde{\psi}_1 X^1 + \tilde{\psi}_0,$$

such that for every $j \in \llbracket 1, q \rrbracket$

$$(\mathbf{A}^{\deg(\tilde{\nu}_{\mathbf{A}})})_{1j} + \tilde{\psi}_{\deg(\tilde{\nu}_{\mathbf{A}})-1} (\mathbf{A}^{\deg(\tilde{\nu}_{\mathbf{A}})-1})_{1j} + \dots + \tilde{\psi}_1 (\mathbf{A})_{1j} + \tilde{\psi}_0 = 0. \quad (14)$$

Compared to Definition 6, we are just asking the property to hold also for the very first element of the first row, namely for $j = 1$. This polynomial is $\nu_{\mathbf{A}}$ for a particular choice of ψ_0 . It has been deduced from the reduction of the lattice Boltzmann scheme.

Lemma 9. The polynomial of degree $\deg(\nu_{\mathbf{A}})$ given by

$$\tilde{\nu}_{\mathbf{A}} = X^{\deg(\nu_{\mathbf{A}})} + \psi_{\deg(\nu_{\mathbf{A}})-1} X^{\deg(\nu_{\mathbf{A}})-1} + \dots + \psi_1 X - \sum_{l=1}^{\deg(\nu_{\mathbf{A}})} \psi_l (\mathbf{A}^l)_{11},$$

where $(\psi_k)_{k=1}^{k=\deg(\nu_{\mathbf{A}})} \subset \mathcal{D}_{\Delta x}^d$ are the coefficients of a MPAMFR $\nu_{\mathbf{A}}$ of \mathbf{A} being $\nu_{\mathbf{A}} = \sum_{k=0}^{k=\deg(\nu_{\mathbf{A}})} \psi_k X^k$, is the MPAFR $\tilde{\nu}_{\mathbf{A}}$ of \mathbf{A} .

Proof. We are only left to check Equation (14) for $j = 1$. □

So in order to reduce the lattice Boltzmann scheme to a Finite Difference scheme using the new strategy, considering a MPAMFR or the MPAFR is exactly the same thing. Moreover, the MPAFR (but not the more general MPAMFR) can be linked to the minimal/characteristic polynomial.¹¹

Lemma 10. Let $\mu_{\mathbf{A}} \in \mathcal{D}_{\Delta x}^d[X]$ be the minimal polynomial of \mathbf{A} , then $\tilde{\nu}_{\mathbf{A}}$ exists and divides the minimal polynomial $\mu_{\mathbf{A}}$. Moreover $\deg(\tilde{\nu}_{\mathbf{A}}) = \deg(\nu_{\mathbf{A}}) \leq \deg(\mu_{\mathbf{A}})$.

¹¹The principle is the same than the one linking the characteristic and the minimal polynomial through divisibility.

The proof is given in the Appendices. We now show how this discussion allows to account for Example 7 and more specifically for Equation (11).

Example 8. We come back to Example 7. We introduce the notations $A_\ell := T_{\Delta x}^{c_{2\ell}} + T_{\Delta x}^{c_{2\ell+1}}$, the “average” on the ℓ^{th} link and $D_\ell := T_{\Delta x}^{c_{2\ell}} - T_{\Delta x}^{c_{2\ell+1}}$, the “difference” on the ℓ^{th} link, for any $\ell \in \llbracket 1, W \rrbracket$. Elementary computations show that

$$V_2 = \begin{pmatrix} \frac{(1-s)D_1}{2\lambda} & \frac{(1-s)(2-s)D_1}{2\lambda} \\ -\frac{(1-s)(A_1-2)}{2\lambda^2} & -\frac{(1-s)(2-s)(A_1-2)}{2\lambda^2} \\ \frac{(1-s)D_2}{2\lambda} & \frac{(1-s)(2-s)D_2}{2\lambda} \\ -\frac{(1-s)(A_2-2)}{2\lambda^2} & -\frac{(1-s)(2-s)(A_2-2)}{2\lambda^2} \\ \vdots & \vdots \\ \frac{(1-s)D_W}{2\lambda} & \frac{(1-s)(2-s)D_W}{2\lambda} \\ -\frac{(1-s)(A_W-2)}{2\lambda^2} & -\frac{(1-s)(2-s)(A_W-2)}{2\lambda^2} \end{pmatrix} \in \mathcal{M}_{(2W) \times 2}(\mathcal{D}_{\Delta x}^d).$$

The equations have the same structure for every 2×2 block: thus we can find a solution by studying each block if it turns out that the solution does not depend on the block indices. Let $\ell \in \llbracket 1, W \rrbracket$. We want to solve for non-trivial ψ_1, ψ_2 such that

$$\begin{cases} \frac{(1-s)D_\ell}{2\lambda} \psi_1 + \frac{(1-s)(2-s)D_\ell}{2\lambda} \psi_2 & = 0, \\ -\frac{(1-s)(A_\ell-2)}{2\lambda^2} \psi_1 - \frac{(1-s)(2-s)(A_\ell-2)}{2\lambda^2} \psi_2 & = 0, \end{cases}$$

thus we clearly see that the solution is $\psi_1 = -(2-s)\psi_2$, but we can pick $\psi_2 = 1$ to have a monic polynomial. Therefore $\psi_1 = -(2-s)$ independently from ℓ . Thus, the polynomial $\nu_{\mathbf{A}} = X^2 - (2-s)X + \psi_0$. Picking $\psi_0 = -\psi_2(\mathbf{A}^2)_{11} - \psi_1(\mathbf{A})_{11} = -1 + (2-s) = 1-s$ yields the polynomial $\tilde{\nu}_{\mathbf{A}}$ as previously seen.

This approach correctly recovers the result from [22] following a different path. However, to our understanding, this new strategy is of moderate interest since it relies on an *ad hoc* and problem-dependent procedure Equation (12) which can be practically exploited only for highly constrained systems, see Example 7 or for schemes of modest size. Moreover, for general schemes, it yields the same result than Proposition 4 using the characteristic polynomial (take Example 1 for instance) but passing from an inefficient approach to the computation of the polynomial instead of using the more performant Algorithm 1.

5.4 Conclusion and future perspectives

Beyond the divisibility property Proposition 8, the fact of not utilizing the characteristic polynomial with its explicit Definition 4 constitutes – due to the previously highlighted lack of generality – an obstruction to show the link with the Taylor expansions [17], as we did in [1]. We therefore stress once more the interest of the general formulations by Proposition 4 and Proposition 6, which shall allow to enlighten the issue of the stability of the schemes, as in the following Section.

6 Stability

Arguably, the *von Neumann* analysis is the most widely used technique to investigate the stability of lattice Boltzmann schemes. Though employed for any number N of conserved moments, we shall consider it only for $N = 1$, to keep mathematical rigour. The *von Neumann* analysis consists in the linearization of the problem around an equilibrium state [37], followed by the rewrite of the scheme using the Fourier transform and the study of the spectrum of the derived matrix. Unsurprisingly, this is also common in the framework of Finite Difference methods, see Chapter 4 in [24] and Chapter 4 in [38]. We observe that the linear L^2 stability, though being widespread, is not the only possible one for lattice Boltzmann schemes: the interested reader can refer to [28, 27] for the L^2 -weighted stability, to [7] for the L^1 stability and finally to [18] for the L^∞ stability. Future efforts shall be dedicated to the investigation of the impact of Proposition 4 and Proposition 6 on these different notions of stability.

6.1 Fourier analysis

We briefly introduce the Fourier analysis on lattices following Chapter 2 of [38]. We define $\mathcal{F} : \ell^2(\mathcal{L}) \cap \ell^1(\mathcal{L}) \rightarrow L^2([-\pi/\Delta x, \pi/\Delta x]^d)$, called Fourier transform, defined as follows. Let $f \in \ell^2(\mathcal{L}) \cap \ell^1(\mathcal{L})$,

then

$$\mathcal{F}[f](\xi) := \frac{1}{(2\pi)^{d/2}} \sum_{x \in \mathcal{L}} e^{-i x \cdot \xi} f(x), \quad \xi \in \left[-\frac{\pi}{\Delta x}, \frac{\pi}{\Delta x}\right]^d.$$

In this Section, the regularity assumptions shall hold for any function. The Fourier transform is extended to less regular entities by density arguments. The interest of the Fourier transform lies in the fact that it is an isometry, thanks to the Parseval's identity [38] and that it allows to represent the action of operators acting *via* the convolution product (also called filters) like the Finite Difference operators $\mathcal{D}_{\Delta x}^d$ as a multiplication on \mathbb{C} . We can therefore represent any shift operator in the Fourier space.

Lemma 11 (Shift operator in the Fourier space). *Let $z \in \mathbb{Z}^d$ and $f \in \ell^2(\mathcal{L}) \cap \ell^1(\mathcal{L})$, then*

$$\mathcal{F}[T_{\Delta x}^z f](\xi) = e^{-i \Delta x z \cdot \xi} \mathcal{F}[f](\xi), \quad \xi \in \left[-\frac{\pi}{\Delta x}, \frac{\pi}{\Delta x}\right]^d.$$

Therefore, the representation of the shift operator $T_{\Delta x}^z$ in the Fourier space is $\hat{T}_{\Delta x}^z := e^{-i \Delta x z \cdot \xi}$ and acts multiplicatively.

Proof. Let $f : \mathcal{L} \rightarrow \mathbb{R}$ with $f \in \ell^2(\mathcal{L}) \cap \ell^1(\mathcal{L})$. We have, for every wave number $\xi \in [-\pi/\Delta x, \pi/\Delta x]^d$

$$\begin{aligned} \mathcal{F}[T_{\Delta x}^z f](\xi) &= \frac{1}{(2\pi)^{d/2}} \sum_{x \in \mathcal{L}} e^{-i x \cdot \xi} f(x - z \Delta x), \\ &= \frac{1}{(2\pi)^{d/2}} \sum_{y \in \mathcal{L}} e^{-i (y + z \Delta x) \cdot \xi} f(y) = e^{-i \Delta x z \cdot \xi} \mathcal{F}[f](\xi). \end{aligned}$$

□

The rewrite of $\mathcal{T}_{\Delta x}^d$ and $\mathcal{D}_{\Delta x}^d$ in the Fourier space is done in the straightforward manner, namely

$$\hat{\mathcal{T}}_{\Delta x}^d := \left\{ \hat{T}_{\Delta x}^z = e^{-i \Delta x z \cdot \xi} \text{ with } z \in \mathbb{Z}^d \right\}, \quad \hat{\mathcal{D}}_{\Delta x}^d := \mathbb{R} \hat{\mathcal{T}}_{\Delta x}^d,$$

where the sum and the products are the standard ones on \mathbb{C} . All that has been said for $\mathcal{D}_{\Delta x}^d$ holds for the new representation in the Fourier space $\hat{\mathcal{D}}_{\Delta x}^d$. Indeed, for any $D = \sum_{T \in \mathcal{T}_{\Delta x}^d} \alpha_T T \in \mathcal{D}_{\Delta x}^d$, we indicate $\hat{D} := \sum_{T \in \mathcal{T}_{\Delta x}^d} \alpha_T \hat{T} \in \hat{\mathcal{D}}_{\Delta x}^d$ its representative in the Fourier space. Considering a matrix $C \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$, its Fourier representation $\hat{C} \in \mathcal{M}_q(\hat{\mathcal{D}}_{\Delta x}^d)$ is obtained by taking the entry-wise Fourier transform of C . Moreover, we have that

$$\chi_C = \sum_{k=0}^q \gamma_k X^k, \quad \xleftrightarrow{\mathcal{F}} \quad \chi_{\hat{C}} = \sum_{k=0}^q \hat{\gamma}_k X^k, \quad (15)$$

where $(\gamma_k)_{k=0}^{k=q} \subset \mathcal{D}_{\Delta x}^d$ and $(\hat{\gamma}_k)_{k=0}^{k=q} \subset \hat{\mathcal{D}}_{\Delta x}^d$.

6.2 Correspondence between the stability analysis for Finite Difference and lattice Boltzmann schemes

Considering linear (or linearized) schemes written in the Fourier space is, thanks to the Parseval's identity, the standard setting to perform the L^2 linear stability analysis both for lattice Boltzmann and Finite Difference schemes. Assume to deal only with one conserved variable, thus $N = 1$.

The polynomial associated with a linear Finite Difference scheme – or quite often, its Fourier representation – is called amplification polynomial, see Chapter 4 of [38]. The study of its roots in the Fourier space is the key of the so-called *von Neumann* stability analysis.

Definition 8 (*von Neumann* stability of a Finite Difference scheme). *Consider a multi-step linear Finite Difference scheme for the variable u under the form¹²*

$$\sum_{k=0}^q \varphi_{q-k} u^{n+1-k} = 0, \quad (16)$$

*for $(\varphi_k)_{k=0}^{k=q} \subset \mathcal{D}_{\Delta x}^d$. Consider its amplification polynomial $\Phi := \sum_{k=0}^{k=q} \varphi_k X^k$, with corresponding amplification polynomial in the Fourier space $\hat{\Phi} := \sum_{k=0}^{k=q} \hat{\varphi}_k X^k$. We say that the Finite Difference scheme Equation (16) is stable in the *von Neumann* sense if for every $\hat{g} : [-\pi/\Delta x, \pi/\Delta x]^d \rightarrow \mathbb{C}$ such that $\hat{\Phi}(\hat{g}(\xi)) = \sum_{k=0}^{k=q} \hat{\varphi}_k(\xi) \hat{g}(\xi)^k = 0$, then*

¹²In this formulation, we do not account for the presence of source terms, since they do not play any role in the linear stability analysis.

1. $|\hat{g}(\boldsymbol{\xi})| \leq 1$, for every $\boldsymbol{\xi} \in [-\pi/\Delta x, \pi/\Delta x]^d$.
2. If $|\hat{g}(\boldsymbol{\xi})| = 1$ for some $\boldsymbol{\xi} \in [-\pi/\Delta x, \pi/\Delta x]^d$, then $\hat{g}(\boldsymbol{\xi})$ is a simple root.

The conditions by Definition 8 are necessary and sufficient for stability (Theorem 4.2.1 in [38]) if the scheme is explicitly independent of Δx and Δt .

Consider now the lattice Boltzmann scheme Equation (6) with linear (or linearized) equilibria, that is, there exists $\boldsymbol{\epsilon} \in \mathbb{R}^q$ such that $\mathbf{m}^{eq} = \boldsymbol{\epsilon} m_1 = (\boldsymbol{\epsilon} \otimes \mathbf{e}_1) \mathbf{m}$. Writing the corresponding Finite Difference scheme from Proposition 4, we have

$$m_1^{n+1} + \sum_{k=0}^{q-1} \gamma_k m_1^{n+1-q+k} - \left(\sum_{k=0}^{q-1} \left(\sum_{\ell=0}^k \gamma_{q+\ell-k} \mathbf{A}^\ell \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1 \right)_{11} m_1^{n-k} \right) = 0, \quad (17)$$

where $\chi_{\mathbf{A}} = \sum_{k=0}^{k=q} \gamma_k X^k$. Rearranging gives

$$m_1^{n+1} + \sum_{k=0}^{q-1} \left(\gamma_{q-1-k} - \left(\sum_{\ell=0}^k \gamma_{q+\ell-k} \mathbf{A}^\ell \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1 \right)_{11} \right) m_1^{n-k} = 0, \quad (18)$$

which is a Finite Difference scheme of the form given in Equation (16) (with $u = m_1$) by setting

$$\varphi_k = \begin{cases} 1, & \text{if } k = q, \\ \gamma_k - \left(\sum_{\ell=0}^{q-1-k} \gamma_{k+1+\ell} \mathbf{A}^\ell \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1 \right)_{11}, & \text{if } k \in \llbracket 0, q-1 \rrbracket. \end{cases} \quad (19)$$

Proposition 12. *Let $N = 1$ and consider the lattice Boltzmann scheme Equation (6) with linear equilibria, that is, there exists $\boldsymbol{\epsilon} \in \mathbb{R}^q$ such that $\mathbf{m}^{eq} = \boldsymbol{\epsilon} m_1 = (\boldsymbol{\epsilon} \otimes \mathbf{e}_1) \mathbf{m}$. It thus reads $\mathbf{m}^{n+1} = (\mathbf{A} + \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1) \mathbf{m}^n$, where $\mathbf{A} + \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1 \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$. Then*

$$\Phi \equiv \chi_{\mathbf{A} + \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1},$$

where $\Phi := \sum_{k=0}^q \varphi_k X^k$, with $(\varphi_k)_{k=0}^{k=q}$ given by Equation (19).

This result – proved at the end of the section – states that, under adequate assumptions, the amplification polynomial of the corresponding Finite Difference scheme coincides with the characteristic polynomial associated with the original lattice Boltzmann scheme. Proposition 12 has also confirmed that assuming the linearity of the equilibria and then performing the computation of the corresponding Finite Difference scheme using the polynomial $\chi_{\mathbf{A} + \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1}$ yields the same result than performing the computation with $\chi_{\mathbf{A}}$ on the possibly non-linear scheme and then considering linear equilibria only at the very end. Thus, a similar notion of stability holds for lattice Boltzmann schemes.

Definition 9 (von Neumann stability of a lattice Boltzmann scheme). *Let $N = 1$ and consider the lattice Boltzmann scheme Equation (6) with linear equilibria. It thus reads*

$$\mathbf{m}^{n+1} = (\mathbf{A} + \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1) \mathbf{m}^n, \quad (20)$$

where $\mathbf{A} + \mathbf{B} \boldsymbol{\epsilon} \otimes \mathbf{e}_1 \in \mathcal{M}_q(\mathcal{D}_{\Delta x}^d)$. We say that the lattice Boltzmann scheme Equation (20) is stable in the von Neumann sense if for every $\boldsymbol{\xi} \in [-\pi/\Delta x, \pi/\Delta x]^d$, then every $\hat{g} \in \sigma(\hat{\mathbf{A}}(\boldsymbol{\xi}) + \hat{\mathbf{B}}(\boldsymbol{\xi}) \boldsymbol{\epsilon} \otimes \mathbf{e}_1)$ is such that

1. $|\hat{g}| \leq 1$.
2. If $|\hat{g}| = 1$, then \hat{g} is a simple eigenvalue of $\hat{\mathbf{A}}(\boldsymbol{\xi}) + \hat{\mathbf{B}}(\boldsymbol{\xi}) \boldsymbol{\epsilon} \otimes \mathbf{e}_1$.

Here, $\sigma(\cdot)$ denotes the spectrum of a matrix.

Item 1 alone, in Definition 9, coincides with the standard definition of stability for lattice Boltzmann schemes, see [37]. With Item 2, we have been more precise on the subtle question of multiple eigenvalues¹³ by bringing this definition closer to Definition 8. Thus, Proposition 12 has the following Corollary.

Corollary 13. *For $N = 1$, the lattice Boltzmann scheme Equation (6), rewritten as Equation (20) under linearity assumption on the equilibria, is stable in the von Neumann sense according to Definition 9 if and only if its corresponding Finite Difference scheme obtained by Proposition 4 is stable in the von Neumann sense according to Definition 8.*

¹³This question is not harmless since for instance the D_1Q_2 scheme rewrites as a leap-frog scheme [11] if the relaxation parameter is equal to two (see Appendices). This very Finite Difference scheme can suffer from linear growth of the solution due to this issue, see Chapter 4 of [38].

This result gives a precise and rigorous framework to the widely employed notion of stability [37] for lattice Boltzmann schemes.

We finish on the proof of Proposition 12. We need the following result concerning the determinant of matrices under rank-one updates, see [14] for the proof.

Lemma 14 (Matrix determinant). *Let \mathcal{R} be a commutative ring, $\mathbf{C} \in \mathcal{M}_r(\mathcal{R})$ for some $r \in \mathbb{N}^*$ and $\mathbf{u}, \mathbf{v} \in \mathcal{R}^r$, then $\det(\mathbf{C} + \mathbf{u} \otimes \mathbf{v}) = \det(\mathbf{C}) + \mathbf{v}^\top \text{adj}(\mathbf{C})\mathbf{u}$, where $\text{adj}(\cdot)$ denotes the adjugate matrix, also known as classical adjoint.*

We are ready to prove Proposition 12.

Proof. Using Lemma 14, one has

$$\begin{aligned}\chi_{\mathbf{A} + \mathbf{B}\epsilon \otimes \mathbf{e}_1} &:= (-1)^q \det(\mathbf{A} + (\mathbf{B}\epsilon \otimes \mathbf{e}_1) - X\mathbf{I}), \\ &= (-1)^q \det(\mathbf{A} - X\mathbf{I}) + (-1)^q \mathbf{e}_1^\top \text{adj}(\mathbf{A} - X\mathbf{I})\mathbf{B}\epsilon, \\ &= \chi_{\mathbf{A}} + (-1)^q \mathbf{e}_1^\top \text{adj}(\mathbf{A} - X\mathbf{I})\mathbf{B}\epsilon.\end{aligned}$$

By the definition of adjugate and by the Cayley-Hamilton Theorem 3, we have

$$\begin{aligned}(-1)^q (\mathbf{A} - X\mathbf{I}) \text{adj}(\mathbf{A} - X\mathbf{I}) &= (-1)^q \det(\mathbf{A} - X\mathbf{I}) \mathbf{I} = (-1)^q \det(\mathbf{A} - X\mathbf{I}) \mathbf{I} - \chi_{\mathbf{A}}(\mathbf{A}) \\ &= -\sum_{k=0}^q \gamma_k (\mathbf{A}^k - X^k \mathbf{I}) = -\sum_{k=1}^q \gamma_k (\mathbf{A}^k - (X\mathbf{I})^k), \\ &= -(\mathbf{A} - X\mathbf{I}) \sum_{k=1}^q \gamma_k \sum_{\ell=0}^{k-1} \mathbf{A}^\ell (X\mathbf{I})^{k-1-\ell}, \\ &= -(\mathbf{A} - X\mathbf{I}) \sum_{k=1}^q \gamma_k \sum_{\ell=0}^{k-1} \mathbf{A}^\ell X^{k-1-\ell},\end{aligned}$$

where we have used that if $\mathbf{C}, \mathbf{D} \in \mathcal{M}_q(\mathcal{R})$ on a commutative ring, then $\mathbf{C}^k - \mathbf{D}^k = (\mathbf{C} - \mathbf{D})(\mathbf{C}^{k-1} + \mathbf{C}^{k-2}\mathbf{D} + \dots + \mathbf{C}\mathbf{D}^{k-2} + \mathbf{D}^{k-1})$. We deduce that

$$\text{adj}(\mathbf{A} - X\mathbf{I}) = -(-1)^q \sum_{k=1}^q \gamma_k \sum_{\ell=0}^{k-1} \mathbf{A}^\ell X^{k-1-\ell}. \quad (21)$$

This yields

$$\chi_{\mathbf{A} + \mathbf{B}\epsilon \otimes \mathbf{e}_1}(X) = X^q + \sum_{k=0}^{q-1} \gamma_k X^k - \mathbf{e}_1^\top \sum_{k=1}^q \gamma_k \sum_{\ell=0}^{k-1} \mathbf{A}^\ell X^{k-1-\ell} \mathbf{B}\epsilon.$$

Performing the following change of variable $t = k - 1 - \ell \in \llbracket 0, q - 1 \rrbracket$ with $\ell \in \llbracket 0, q - 1 - t \rrbracket$, thus $k = t + 1 + \ell$, gives

$$\begin{aligned}\chi_{\mathbf{A} + \mathbf{B}\epsilon \otimes \mathbf{e}_1}(X) &= X^q + \sum_{k=0}^{q-1} \left(\gamma_k - \mathbf{e}_1^\top \sum_{\ell=0}^{q-1-k} \mathbf{A}^\ell \mathbf{B}\epsilon \gamma_{k+1+\ell} \right) X^k, \\ &= X^q + \sum_{k=0}^{q-1} \left(\gamma_k - \left(\sum_{\ell=0}^{q-1-k} \gamma_{k+1+\ell} \mathbf{A}^\ell \mathbf{B}\epsilon \otimes \mathbf{e}_1 \right)_{11} \right) X^k.\end{aligned}$$

Thus we have that $\Phi := \sum_{k=0}^{k=q} \varphi_k X^k = \chi_{\mathbf{A} + \mathbf{B}\epsilon \otimes \mathbf{e}_1}$. \square

7 Convergence of lattice Boltzmann schemes on an example

In this Section, we show on Example 1 (taking $p = 1$ to simplify the stability analysis, see Example 6) that the theory available for multi-step Finite Difference schemes can be used to study the underlying lattice Boltzmann scheme. The target conservation law is the Cauchy problem

$$\begin{cases} \partial_t u(t, x) + \lambda \mathcal{C} \partial_x u(t, x) = 0, & (t, x) \in [0, T] \times \mathbb{R}, \\ u(t = 0, x) = u_0(x), & x \in \mathbb{R}. \end{cases} \quad (22)$$

The equilibria are considered to be linear as in Section 6: $m_2^{\text{eq}} = \lambda \mathbf{C} m_1$ where \mathbf{C} is the Courant number and $m_3^{\text{eq}} = 2\lambda^2 \mathbf{D} m_1$ with \mathbf{D} the Fourier number. The corresponding Finite Difference scheme from Example 1 and Example 6 is consistent with

$$\partial_t m_1 + \lambda \mathbf{C} \partial_x m_1 - \lambda \Delta x \left(\frac{1}{s} - \frac{1}{2} \right) \left(\frac{2}{3} (1 + \mathbf{D}) - \mathbf{C}^2 \right) \partial_{xx} m_1 = \mathcal{O}(\Delta x^2). \quad (23)$$

In what follows, we shall fix $\mathbf{C} = 1/2$. One can make the residual diffusion in this equation vanish if $s = 2$, which is a staple of lattice Boltzmann schemes [15, 26, 23, 36], or by having $\mathbf{D} = 3\mathbf{C}^2/2 - 1$. We shall analyze both the case $\mathbf{D} > 3\mathbf{C}^2/2 - 1$, where we expect only linear consistency with Equation (22) or – using the notations from [38] – where the scheme is accurate of order $[r, \rho] = [1, 2]$ and the case $\mathbf{D} = 3\mathbf{C}^2/2 - 1$, the scheme is second-order consistent with Equation (22) or $[r, \rho] = [2, 3]$ accurate.

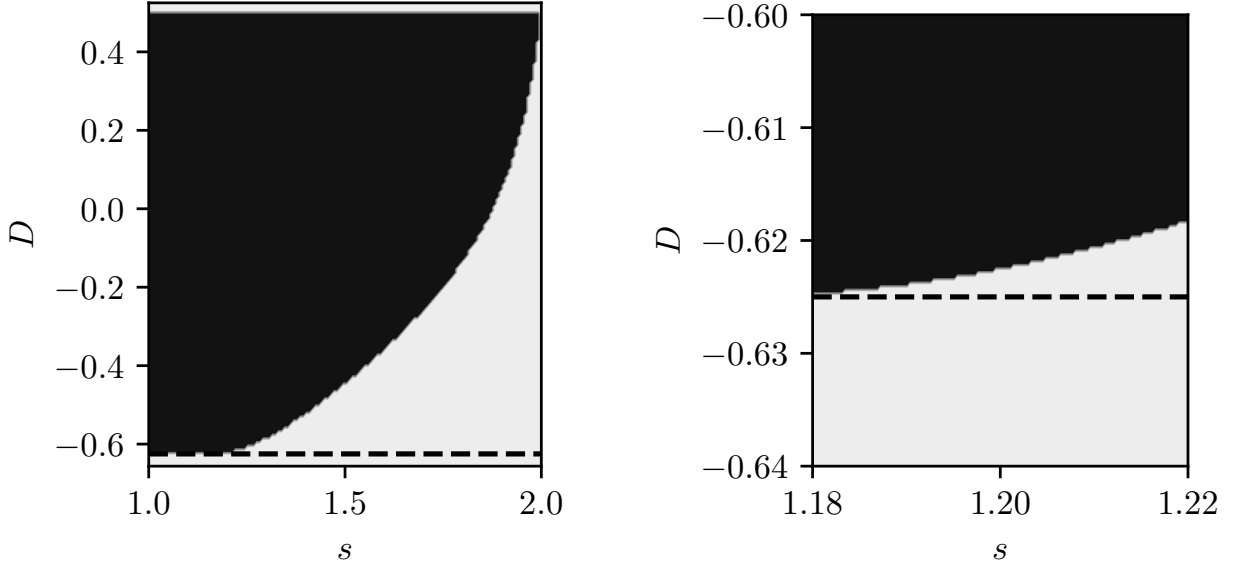


Figure 2: Stability region (in black), obtained numerically, as function of s and \mathbf{D} for the $\mathbf{D}_1\mathbf{Q}_3$ of Example 1, considering $\mathbf{C} = 1/2$. The black dashed line corresponds to $\mathbf{D} = 3\mathbf{C}^2/2 - 1 = -0.625$, for which the residual diffusivity vanishes, see Equation (23). The right image is a magnification of the left one close to $s = 1.2$.

The numerical *von Neumann* stability analysis has been done and the result is shown in Figure 2. One sees that enforcing positive residual diffusivity is necessary but not sufficient to obtain stability. Using the method from [31] to locate the zeros of the amplification polynomial, we show the following.

Proposition 15. *The amplification polynomial of the Finite Difference scheme corresponding to the $\mathbf{D}_1\mathbf{Q}_3$ scheme from Example 6 considered in this Section is a simple von Neumann polynomial, namely fulfills Definition 8, if the following constraints hold.*

$$\frac{3}{2}\mathbf{C}^2 - 1 \leq \mathbf{D} \leq \frac{1}{2}, \quad \text{and} \quad \max_{\gamma \in [-1, 1]} \left\{ s^2 \mathbf{C}^2 (1 + \gamma) (1 + \Omega)^2 + \frac{4}{9} (2 - s)(\mathbf{D} + 1)(1 - \Omega) \left((2 - s)(\mathbf{D} + 1)(1 - \gamma)(1 - \Omega) + 3(\Omega^2 - 1) \right) \right\} \leq 0,$$

where $\Omega = \Omega(\gamma; \mathbf{D}, s) := (1 - s)(\gamma + 2 + 2\mathbf{D}(1 - \gamma))/3$.

The first inequality from this Proposition gives only a necessary condition selecting a rectangle in the (s, \mathbf{D}) plane. The second one provides a sufficient condition yielding the non-straightforward profile visible on Figure 2. This comes from the fact that the maximum can be reached either on the boundary of $[-1, 1]$ (for $s \leq 1.18$ approximately) yielding the flat profile close to $s = 1$, or inside this compact (for $s > 1.18$), giving the tightening shape as s increases towards $s = 2$.

Using the generalization of Theorem 10.1.4 from [38] to multi-step schemes for regular data and that of Corollary 10.3.2 for non-smooth data, one obtains the following convergence result for the lattice Boltzmann scheme.

Proposition 16 (Convergence of the D_1Q_3 scheme). *Consider the D_1Q_3 linear scheme of Example 1 presented in this Section with a choice of $(\mathcal{C}, \mathcal{D}, s)$ rendering a stable scheme according to Definition 9, as discussed in Proposition 15. The scheme is initialized with the point values of u_0 and at equilibrium. Then*

- For $\mathcal{D} > 3\mathcal{C}^2/2 - 1$, namely the corresponding Finite Difference scheme is accurate of order $[r, \rho] = [1, 2]$.
 - If $u_0 \in H^2$, the convergence of the lattice Boltzmann scheme is linear:

$$\|\mathcal{E}u(t^n, \cdot) - m_1^n\|_{\ell^2, \Delta x} \leq C\Delta x \|u_0\|_{H^2}, \quad n \in \llbracket 0, [T/\Delta t] \rrbracket,$$

where \mathcal{E} is the evaluation operator such that $\mathcal{E}u : \mathcal{L} \rightarrow \mathbb{R}$ with $(\mathcal{E}u)(x) = u(x)$ for every $x \in \mathcal{L}$.

- If $u_0 \in H^\sigma$ for any $\sigma < \sigma_0 < 2$ and there exists a constant $C(u_0)$ such that $\|u_0\|_{H^\sigma} \leq C(u_0)/\sqrt{\sigma - \sigma_0}$, then

$$\|\mathcal{E}u(t^n, \cdot) - m_1^n\|_{\ell^2, \Delta x} \leq C\Delta x^{\sigma_0/2} \sqrt{|\ln(\Delta x)|} C(u_0), \quad n \in \llbracket 0, [T/\Delta t] \rrbracket.^{14}$$

- For $\mathcal{D} = 3\mathcal{C}^2/2 - 1$, namely the corresponding Finite Difference scheme is accurate of order $[r, \rho] = [2, 3]$.
 - If $u_0 \in H^3$, the convergence of the lattice Boltzmann scheme is quadratic:

$$\|\mathcal{E}u(t^n, \cdot) - m_1^n\|_{\ell^2, \Delta x} \leq C\Delta x^2 \|u_0\|_{H^3}, \quad n \in \llbracket 0, [T/\Delta t] \rrbracket.$$

- If $u_0 \in H^\sigma$ for any $\sigma < \sigma_0 < 3$ and there exists a constant $C(u_0)$ such that $\|u_0\|_{H^\sigma} \leq C(u_0)/\sqrt{\sigma - \sigma_0}$, then

$$\|\mathcal{E}u(t^n, \cdot) - m_1^n\|_{\ell^2, \Delta x} \leq C\Delta x^{2\sigma_0/3} \sqrt{|\ln(\Delta x)|} C(u_0), \quad n \in \llbracket 0, [T/\Delta t] \rrbracket.$$

The constants C have the following dependencies: $C = C(T, \mathcal{C}, \mathcal{D}, s)$.

We now corroborate these results with numerical simulations, which are carried, for the sake of the numerical implementation, on the bounded domain $[-1, 1]$ enforcing periodic boundary conditions. The final simulation time is $T = 1/2$ and $\lambda = 1$. We stress the fact that we employ the lattice Boltzmann scheme and not its corresponding Finite Difference scheme. Guided by the considerations from Proposition 16 in terms of regularity, we take different initial functions with various smoothness, inspired by [38].

- (a) $u_0(x) = \chi_{|x| \leq 1/2}(x) \in H^\sigma$, for any $\sigma < \sigma_0 = 1/2$.
- (b) $u_0(x) = (1 - 2|x|)\chi_{|x| \leq 1/2}(x) \in H^\sigma$, for any $\sigma < \sigma_0 = 3/2$.
- (c) $u_0(x) = \cos^2(\pi x)\chi_{|x| \leq 1/2}(x) \in H^\sigma$, for any $\sigma < \sigma_0 = 5/2$.
- (d) $u_0(x) = \exp(-1/(1 - |2x|^2))\chi_{|x| \leq 1/2}(x) \in C_c^\infty$.

The numerical convergence for the case $\mathcal{D} = 0.4$ is given on Figure 3. According to Figure 2 and Proposition 15, we expect stability for every choice of s . Thus, the empirical convergence rates are in excellent agreement with Proposition 16. The error constant is smaller for larger s , since for this choice, less numerical diffusion is present.

Concerning the case $\mathcal{D} = -0.625$ presented on Figure 4, we had to utilize relaxation parameters s close to one in order to remain in the stability region as prescribed by Figure 2 and Proposition 15. As far as the scheme stays stable, for $s \leq 1.15$, we observe the expected convergence rates according to Proposition 16. Nevertheless, looking at the right image in Figure 2, we see that $s = 1.2$ is not in the stability region. This is why we observe, in (a) from Figure 4, thus for the less smooth solution, that the scheme is not convergent. The instability originates from high-frequency modes which are abundant in the test case (a). This is the empirical evidence that the Lax-Richtmyer theorem [29] holds for lattice Boltzmann schemes: an unstable scheme cannot be convergent.

8 Conclusions

In this paper, we proved that any lattice Boltzmann scheme corresponds to a multi-step Finite Difference scheme on the conserved moments, using a simple yet crucial result of linear algebra.

¹⁴The logarithmic term is rarely observed in simulations.

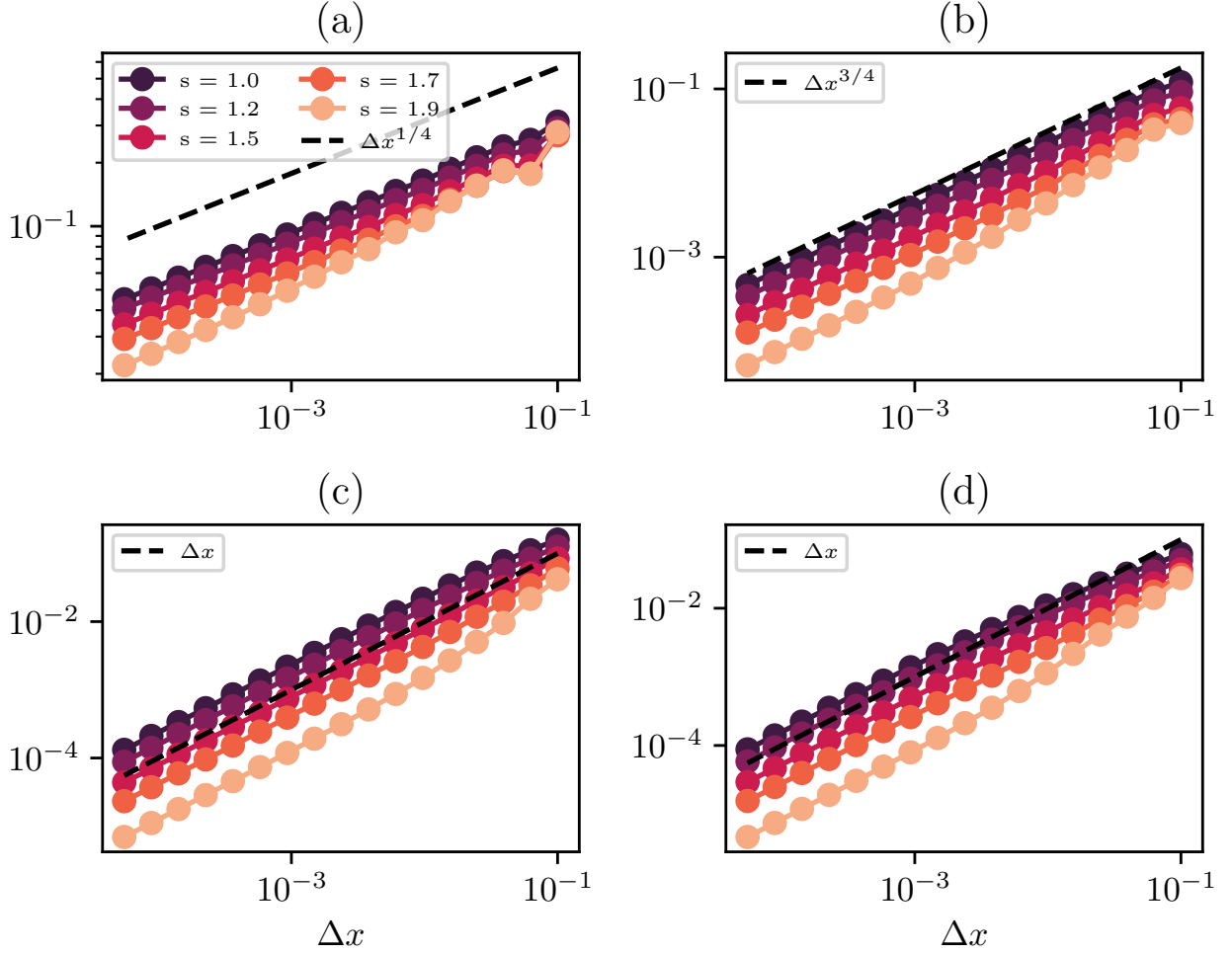


Figure 3: $D = 0.4$. ℓ^2 error at final time T between the solution (conserved moment) of lattice Boltzmann scheme and the exact solution, for different initial data (a), (b), (c) and (d) and different relaxation parameters s .

This showed that lattice Boltzmann schemes, in all their richness, fall in the framework of this latter category of well-known numerical schemes. Moreover, for linear problems and one conserved moment, we proved that the usual notion of stability employed for lattice Boltzmann schemes is relevant, since it corresponds to the *von Neumann* stability analysis for the Finite Difference schemes. Therefore, the Lax-Richtmyer theorem [29, 38], stipulating that consistency and stability are the necessary and sufficient conditions for the convergence of linear Finite Difference schemes, also holds for the lattice Boltzmann schemes.

A question left unanswered in this work, being the object of current investigations, concerns the link between the consistency for the corresponding Finite Difference scheme and the theory of equivalent equations by [15, 17]. In a complementary work [1], we have proved that the two notions are equivalent up to second-order. The conjecture is that this holds for higher orders. The difficulty lies in the fact that performing *a priori* Taylor expansions on the coefficients of the characteristic polynomial of \mathbf{A} is generally a hard task, due to their intrinsic non-linear dependence on \mathbf{A} . Furthermore, the multi-step nature of the corresponding Finite Difference scheme is an additional toil.

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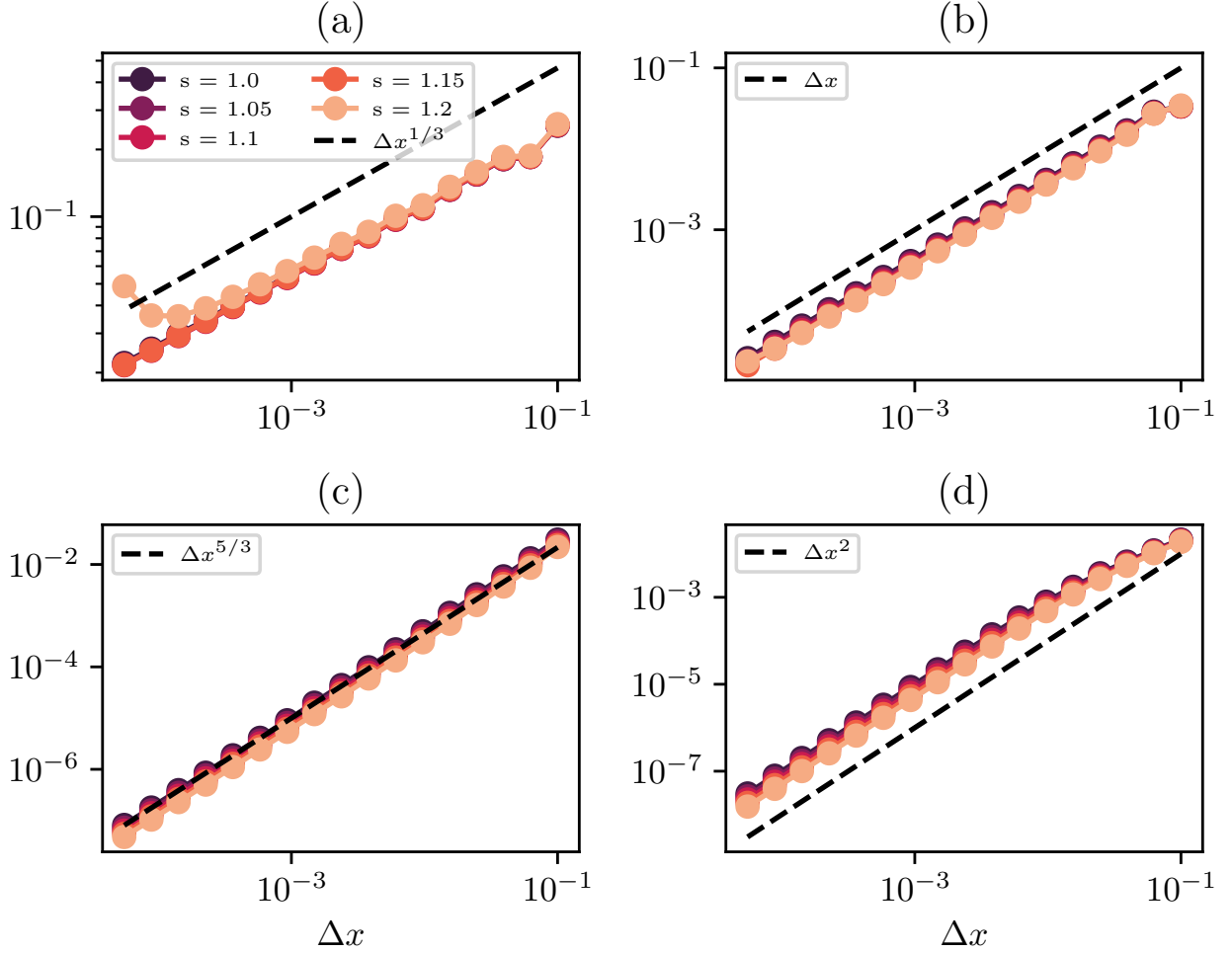


Figure 4: $D = -0.625$. ℓ^2 error at final time T between the solution (conserved moment) of lattice Boltzmann scheme and the exact solution, for different initial data (a), (b), (c) and (d) and different relaxation parameters s .

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Appendices

Proof of Proposition 8

Proof. By the choice of polynomial, we have that

$$\left(\sum_{k=0}^{\deg(\nu_{\mathbf{A}})} \psi_k \mathbf{A}^k \right)_1 = \left(\psi_0 + \sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k (\mathbf{A}^k)_{11}, 0, \dots, 0 \right).$$

Restarting from the proof of Proposition 4, we have

$$\begin{aligned} \sum_{k=0}^{\deg(\nu_{\mathbf{A}})} \psi_k m_1^{\tilde{n}+k} &= m_1^{\tilde{n}+\deg(\nu_{\mathbf{A}})} + \sum_{k=1}^{\deg(\nu_{\mathbf{A}})-1} \psi_k m_1^{\tilde{n}+k} + \psi_0 m_1^{\tilde{n}}, \\ &= \left(\left(\sum_{k=0}^{\deg(\nu_{\mathbf{A}})} \psi_k \mathbf{A}^k \right) \mathbf{m}^{\tilde{n}} \right)_1 + \sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k \left(\sum_{\ell=0}^{k-1} \mathbf{A}^{\ell} \mathbf{B} \mathbf{m}^{\text{eq}|\tilde{n}+k-1-\ell} \right)_1, \\ &= \psi_0 m_1^{\tilde{n}} + \left(\sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k (\mathbf{A}^k)_{11} \right) m_1^{\tilde{n}} \\ &\quad + \sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k \left(\sum_{\ell=0}^{k-1} \mathbf{A}^{\ell} \mathbf{B} \mathbf{m}^{\text{eq}|\tilde{n}+k-1-\ell} \right)_1, \end{aligned}$$

therefore

$$\begin{aligned} m_1^{\tilde{n}+\deg(\nu_{\mathbf{A}})} &= - \sum_{k=1}^{\deg(\nu_{\mathbf{A}})-1} \psi_k m_1^{\tilde{n}+k} + \left(\sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k (\mathbf{A}^k)_{11} \right) m_1^{\tilde{n}} \\ &\quad + \sum_{k=1}^{\deg(\nu_{\mathbf{A}})} \psi_k \left(\sum_{\ell=0}^{k-1} \mathbf{A}^{\ell} \mathbf{B} \mathbf{m}^{\text{eq}|\tilde{n}+k-1-\ell} \right)_1. \end{aligned} \tag{24}$$

Performing the usual change of variable yields the result. \square

Proof of Lemma 10

Proof. The proof goes like the standard one of Lemma 7. Consider $\mu_{\mathbf{A}} = X^{\deg(\mu_{\mathbf{A}})} + \omega_{\deg(\mu_{\mathbf{A}})-1} X^{\deg(\mu_{\mathbf{A}})-1} + \dots + \omega_1 X + \omega_0$. Consider the Euclidian division between $\mu_{\mathbf{A}}$ and $\tilde{\nu}_{\mathbf{A}}$: there exist $Q, R \in \mathcal{D}_{\Delta x}^d[X]$ such that

$$\mu_{\mathbf{A}} = \tilde{\nu}_{\mathbf{A}} Q + R,$$

with either $0 < \deg(R) < \deg(\tilde{\nu}_{\mathbf{A}})$ or $\deg(R) = 0$ (constant reminder polynomial). Let us indeed write

$$\begin{aligned} Q &= q_{\deg(\mu_{\mathbf{A}}) - \deg(\tilde{\nu}_{\mathbf{A}})} X^{\deg(\mu_{\mathbf{A}}) - \deg(\tilde{\nu}_{\mathbf{A}})} + \dots + q_1 X + q_0, \\ R &= r_{\deg(R)} X^{\deg(R)} + \dots + r_1 X + r_0, \end{aligned}$$

Suppose that $R \neq 0$, then we have for every $j \in \llbracket 1, q \rrbracket$

$$\begin{aligned} & \overbrace{(\mathbf{A}^{\deg(\mu_{\mathbf{A}})})_{1j} + \omega_{\deg(\mu_{\mathbf{A}})-1}(\mathbf{A}^{\deg(\mu_{\mathbf{A}})-1})_{1j} + \dots + \omega_1(\mathbf{A})_{1j} + \omega_0 \delta_{1j}}^{=0} \\ &= r_{\deg(R)}(\mathbf{A}^{\deg(R)})_{1j} + \dots + r_1(\mathbf{A})_{1j} + r_0 \delta_{1j} + \\ & \underbrace{\left((\mathbf{A}^{\deg(\tilde{\nu}_{\mathbf{A}})})_{1j} + \psi_{\deg(\tilde{\nu}_{\mathbf{A}})-1}(\mathbf{A}^{\deg(\tilde{\nu}_{\mathbf{A}})-1})_{1j} + \dots + \psi_1(\mathbf{A})_{1j} + \psi_0 \delta_{1j} \right)}_{=0} \\ & \times \left(q_{\deg(\mu_{\mathbf{A}}) - \deg(\nu_{\mathbf{A}})}(\mathbf{A}^{\deg(\mu_{\mathbf{A}}) - \deg(\nu_{\mathbf{A}})})_{1j} + \dots + q_1(\mathbf{A})_{1j} + q_0 \delta_{1j} \right), \end{aligned}$$

thus

$$r_{\deg(R)}(\mathbf{A}^{\deg(R)})_{1j} + \dots + r_1(\mathbf{A})_{1j} + r_0 \delta_{1j} = 0, \quad j \in \llbracket 1, q \rrbracket,$$

with $0 < \deg(R) < \deg(\tilde{\nu}_{\mathbf{A}})$, which contradicts the minimality of $\tilde{\nu}_{\mathbf{A}}$. Thus necessarily $\deg(R) = 0$ so the polynomial is constant, but to have the previous property, the constant must be zero, thus $R \equiv 0$. \square

Additional examples

In this section, we gather more examples concerning the application of our theory to lattice Boltzmann schemes which can be found in the literature.

$\mathbf{D}_1\mathbf{Q}_2$ with one conservation law

Consider the scheme by [11, 23] taking $d = 1$ and $q = 2$ with $c_1 = 1$ and $c_2 = -1$ and

$$\mathbf{M} = \begin{pmatrix} 1 & 1 \\ \lambda & -\lambda \end{pmatrix}, \quad \mathbf{S} = \text{diag}(0, s), \quad \text{with } s \neq 1. \quad (25)$$

The scheme can be used to simulate a non-linear scalar conservation law (advection, Burgers, *etc.*) using an acoustic scaling and a non-linear diffusion equation with a parabolic scaling. However, the scheme is not rich enough to simulate more complex equations. As already pointed out in the introduction, the Finite Difference equivalent of this scheme has already been studied by [11] in the case where the equilibria are linear functions.

It can be easily seen, even by hand since dealing with a 2×2 matrix, that

$$\chi_{\mathbf{A}} = X^2 - \frac{1}{2}(2-s)(x+\bar{x})X + (1-s).$$

The minimal polynomial coincides with the characteristic polynomial. This can be seen, as usual, by trying to consider α_0 and α_1 such that

$$\alpha_0 \mathbf{I} + \alpha_1 \mathbf{A} = \begin{pmatrix} \alpha_0 + \frac{(x+\bar{x})}{2} \alpha_1 & \frac{(1-s)(x-\bar{x})}{2\lambda} \alpha_1 \\ \frac{\lambda(x-\bar{x})}{2} \alpha_1 & \alpha_0 + \frac{(1-s)(x+\bar{x})}{2} \alpha_1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

The only way of annihilating the first entry is to take $\alpha_0 = 0$, which is trivial. Thus the minimal polynomial is of degree 2 and then coincides with the characteristic polynomial. The equivalent Finite Difference scheme is

$$m_1^{n+1} = \frac{1}{2}(2-s)(x+\bar{x})m_1^n - (1-s)m_1^{n-1} + \frac{s(x-\bar{x})}{2\lambda}m_2^{\text{eq}|n}.$$

The scheme is a θ -scheme between a Lax-Friedrichs scheme (for $s = 1$) and a leap-frog scheme (for $s = 2$).

D₁Q₃ SRT for one conservation law

Consider the D₁Q₃ SRT scheme by [21], also corresponding to that of [39] which reads with our notations $d = 1$, $q = 3$ and $c_1 = 0$, $c_2 = 1$ and $c_3 = -1$ and

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \lambda & -\lambda \\ 0 & \lambda^2 & \lambda^2 \end{pmatrix}, \quad \mathbf{S} = \text{diag}(0, \omega, \omega), \quad \text{with } \omega \neq 1,$$

The characteristic polynomial, corresponding to the minimal polynomial is

$$\chi_{\mathbf{A}} = X^3 + (\omega(x + \bar{x}) - (x + 1 + \bar{x}))X^2 + (1 - \omega)((x + \bar{x}) + (1 - \omega))X - (1 - \omega)^2.$$

Hence the equivalent Finite Difference scheme is

$$\begin{aligned} m_1^{n+1} &= (1 - \omega)(x + \bar{x})m_1^n + m_1^n - (1 - \omega)(x + \bar{x})m_1^{n-1} - (1 - \omega)^2 m_1^{n-1} \\ &\quad + (1 - \omega)^2 m_1^{n-2} + \frac{\omega(x - \bar{x})}{2\lambda} m_2^{\text{eq}|n} - \frac{\omega(1 - \omega)(x - \bar{x})}{2\lambda} m_2^{\text{eq}|n-1} \\ &\quad + \frac{\omega(x - 2 + \bar{x})}{2\lambda^2} m_3^{\text{eq}|n} + \frac{\omega(1 - \omega)(x - 2 + \bar{x})}{2\lambda^2} m_3^{\text{eq}|n-1}, \end{aligned}$$

coinciding with the one found by [21].

D₁Q₃ MRT for one conservation law

Consider the D₁Q₃ MRT scheme by [21], which is constructed in the same way than the previous one except for $\mathbf{S} = \text{diag}(0, \omega_2, \omega_3)$ with $\omega_2, \omega_3 \neq 1$. The characteristic and minimal polynomial coincide and are given by

$$\begin{aligned} \chi_{\mathbf{A}} &= X^3 + (-1 + (x + \bar{x})(\omega_2/2 + \omega_3/2 - 1))X^2 \\ &\quad + (1 + \omega_2\omega_3 - \omega_2 - \omega_3 + (1 - \omega_2/2 - \omega_3/2)(x + \bar{x}))X \\ &\quad - (1 - \omega_2)(1 - \omega_3). \end{aligned}$$

Then the equivalent Finite Difference scheme is

$$\begin{aligned} m_1^{n+1} &= (1 - \omega_2/2 - \omega_3/2)(x + \bar{x})m_1^n + m_1^n - (1 - \omega_2/2 - \omega_3/2)(x + \bar{x})m_1^{n-1} \\ &\quad - (1 - \omega_2 - \omega_3 + \omega_2\omega_3)m_1^{n-1} + (1 - \omega_2)(1 - \omega_3)m_1^{n-2} \\ &\quad + \frac{\omega_2(x - \bar{x})}{2\lambda} m_2^{\text{eq}|n} - \frac{\omega_2(1 - \omega_3)(x - \bar{x})}{2\lambda} m_2^{\text{eq}|n-1} \\ &\quad + \frac{\omega_3(x - 2 + \bar{x})}{2\lambda^2} m_3^{\text{eq}|n} + \frac{\omega_3(1 - \omega_2)(x - 2 + \bar{x})}{2\lambda^2} m_3^{\text{eq}|n-1}, \end{aligned}$$

corresponding to the one found by [21].

D₂Q₄ for one conservation law

Consider $d = 2$ and $q = 4$ with $\mathbf{c}_1 = (1, 0)^\top$, $\mathbf{c}_2 = (0, 1)^\top$, $\mathbf{c}_3 = (-1, 0)^\top$ and $\mathbf{c}_4 = (0, -1)^\top$ and

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \lambda & 0 & -\lambda & 0 \\ 0 & \lambda & 0 & -\lambda \\ \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \end{pmatrix}, \quad \mathbf{S} = \text{diag}(0, s, s, 1), \quad \text{with } s \neq 1. \quad (26)$$

Therefore $N = 1$ and $Q = 2$. This can be used, for example, coupled with other schemes of the same nature (building what we call a “vectorial scheme” [16]) to easily simulate systems of non-linear conservation laws for $d = 2$, see [2]. After some computation, the characteristic polynomial of \mathbf{A} reads

$$\begin{aligned} \chi_{\mathbf{A}} &= X^3 + (2s - 3) \frac{(x + \bar{x} + y + \bar{y})}{4} X^2 + (1 - s) \left((2 - s) \frac{(xy + \bar{x}y + x\bar{y} + \bar{x}\bar{y})}{4} + 1 \right) X \\ &\quad - (1 - s)^2 \frac{(x + \bar{x} + y + \bar{y})}{4}. \end{aligned}$$

One can check as usual that it coincides with the minimal polynomial. The equivalent Finite Difference scheme taking $m_4^{\text{eq}} \equiv 0$ for simplicity is

$$\begin{aligned}
m_1^{n+1} = & - (2s - 3)A_a m_1^n - (1 - s)m_1^{n-1} - (1 - s)(2 - s)A_d m_1^{n-1} + (1 - s)^2 A_a m_1^{n-2} \\
& + \frac{s}{2\lambda}(x - \bar{x})m_2^{\text{eq}}|^n + \frac{s}{2\lambda}(y - \bar{y})m_3^{\text{eq}}|^n \\
& - \frac{s(1 - s)}{\lambda} \frac{1}{2} \left(y \frac{(x - \bar{x})}{2} + \bar{y} \frac{(x - \bar{x})}{2} \right) m_2^{\text{eq}}|^{n-1} \\
& - \frac{s(1 - s)}{\lambda} \frac{1}{2} \left(x \frac{(y - \bar{y})}{2} + \bar{x} \frac{(y - \bar{y})}{2} \right) m_3^{\text{eq}}|^{n-1},
\end{aligned}$$

where we have introduced the short-hands $A_a := (x + \bar{x} + y + \bar{y})/4 \in \mathcal{D}_{\Delta x}^d$ and $A_d := (xy + x\bar{y} + \bar{x}y + \bar{x}\bar{y})/4 \in \mathcal{D}_{\Delta x}^d$, yielding respectively the average between neighbors along the axis and along the diagonals.