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An analysis of over-relaxation in a kinetic approximation of systems of conservation laws ☆

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A R T I C L E   I N F O

A B S T R A C T

The over-relaxation approach is an alternative to the Jin–Xin relaxation method in order to apply the equilibrium source term in a more precise way. This is also a key ingredient of the lattice Boltzmann method for achieving second-order accuracy. In this work, we provide an analysis of the over-relaxation kinetic scheme. We compute its equivalent equation, which is particularly useful for devising stable boundary conditions for the hidden kinetic variables.

1. Introduction

In this note, we are interested in the numerical resolution of the following system of conservation laws

$$\partial_t \mathbf{u} + \partial_x \mathbf{f}(\mathbf{u}) = 0 \tag{1}$$

where the unknown is the vector of conservative variables $\mathbf{u}(x, t) \in \mathbb{R}^m$, depending on a space variable x and a time variable $t \geq 0$. In the first part of the paper, we consider the case with no boundaries ($x \in \mathbb{R}$). In Section 4.3, we will discuss the case with boundaries ($x \in [0, 1]$). The conservative variables satisfy an initial condition

$$\mathbf{u}(x, 0) = \mathbf{v}(x) \tag{2}$$

The flux $\mathbf{f}$ is a non-linear function of $\mathbf{u}$. The system of conservation laws (1) is assumed to be hyperbolic: for any vector of conserved variables $\mathbf{u}$, the Jacobian of the flux

$$\mathbf{A}(\mathbf{u}) = \mathbf{f}'(\mathbf{u}) \tag{3}$$

is diagonalizable with real eigenvalues.

Jin and Xin [1] have proposed an approximation of (1) of the following form

$$\partial_t \mathbf{w}_\varepsilon + \partial_x \mathbf{z}_\varepsilon = 0 \tag{4}$$

$$\partial_t \mathbf{z}_\varepsilon + \lambda^2 \partial_x \mathbf{w}_\varepsilon = \frac{1}{\varepsilon}(\mathbf{f}(\mathbf{w}_\varepsilon) - \mathbf{z}_\varepsilon) \tag{5}$$

with the initial conditions

$$\mathbf{w}_\varepsilon(x, 0) = \mathbf{v}(x), \quad \mathbf{z}_\varepsilon(x, 0) = \mathbf{f}(\mathbf{v}(x)) \tag{6}$$

In this formulation, ε is a small positive parameter and λ a constant positive velocity. If λ is large enough ("subcharacteristic" condition), it can be proved that $\mathbf{w}_\varepsilon$ tends to $\mathbf{u}$, the entropy solution to (1)–(2), when ε tends to zero (Jin and Xin [1]). Further studies about relaxation systems like (4)–(5) can be found in Chen et al. [2], or in Natalini [3], for instance. We refer also to the retrospective of Mascia [4].

The advantage of the Jin–Xin formulation is that the partial differential equations are now linear with constant coefficients and the non-linearity is concentrated in a simple algebraic source term.

A simple way to solve numerically the Jin–Xin system is to use a time-splitting algorithm. For advancing by one time-step of size Δt, one first solves

$$\partial_t \mathbf{w} + \partial_x \mathbf{z} = 0 \tag{7}$$

$$\partial_t \mathbf{z} + \lambda^2 \partial_x \mathbf{w} = 0 \tag{8}$$

for a duration of Δt (free transport step). Then, for the same duration, one solves the system of ordinary differential equations (relaxation step)

$$\partial_t \mathbf{w} = 0 \tag{9}$$

$$\partial_t \mathbf{z} = \frac{1}{\varepsilon}(\mathbf{f}(\mathbf{w}) - \mathbf{z}) \tag{10}$$

Both sub-steps admit a simple explicit solution. Indeed, if we define the functional shift (or translation) operator $s(\Delta t)$ applying on function f by

$$(s(\Delta t)f)(x) = f(x - \lambda \Delta t)$$

then the solution to the free transport step (7)–(8) is given by

$$\begin{pmatrix} \mathbf{w}(\cdot, t + \Delta t) \\ \mathbf{z}(\cdot, t + \Delta t) \end{pmatrix} = T(\Delta t) \begin{pmatrix} \mathbf{w}(\cdot, t) \\ \mathbf{z}(\cdot, t) \end{pmatrix}$$

with

$$T(\Delta t) := \frac{1}{2} \begin{pmatrix} s(\Delta t) + s(-\Delta t) & (s(\Delta t) - s(-\Delta t))/\lambda \\ \lambda(s(\Delta t) - s(-\Delta t)) & s(\Delta t) + s(-\Delta t) \end{pmatrix} \tag{11}$$

This can be easily obtained noting that the Riemann invariants $\mathbf{w} \pm \mathbf{z}/\lambda$ are transported at velocities $\pm\lambda$. The operator T is a morphism of group, meaning that $T(2\Delta t) = T(\Delta t)T(\Delta t)$. We will use this property in our concrete applications. The solution to the relaxation step is given by

$$\begin{pmatrix} \mathbf{w}(\cdot, t + \Delta t) \\ \mathbf{z}(\cdot, t + \Delta t) \end{pmatrix} = P_\varepsilon(\Delta t) \begin{pmatrix} \mathbf{w}(\cdot, t) \\ \mathbf{z}(\cdot, t) \end{pmatrix}$$

with

$$P_\varepsilon(\Delta t) \begin{pmatrix} \mathbf{w} \\ \mathbf{z} \end{pmatrix} := \begin{pmatrix} \mathbf{w} \\ \mathbf{f}(\mathbf{w}) \end{pmatrix} + \exp(-\Delta t/\varepsilon) \begin{pmatrix} 0 \\ \mathbf{z} - \mathbf{f}(\mathbf{w}) \end{pmatrix} \tag{12}$$

These operators being defined, we obtain a first-order-in-time approximation of the solution to (4)–(5)–(6):

$$\begin{pmatrix} \mathbf{w}_\varepsilon(\cdot, t + \Delta t) \\ \mathbf{z}_\varepsilon(\cdot, t + \Delta t) \end{pmatrix} = S_1(\Delta t) \begin{pmatrix} \mathbf{w}_\varepsilon(\cdot, t) \\ \mathbf{f}(\mathbf{w}_\varepsilon)(\cdot, t) \end{pmatrix} + O(\Delta t^2)$$

with

$$S_1(\Delta t) = P_\varepsilon(\Delta t)T(\Delta t) \tag{13}$$

The splitting error is of order $O(\Delta t^2)$, but when this approximation is accumulated on $t/\Delta t$ time steps, S_1 is indeed a first-order scheme. The Jin–Xin scheme is very robust and can handle shock solutions. However, for smooth solutions, its accuracy is not sufficient.

For achieving second-order accuracy for smooth solutions, a simple idea would be to replace the splitting (13) by a Strang procedure (Dellar [5]). We observe that $T(0) = I$, where I is the identity operator. For $\varepsilon > 0$ fixed, we also have $P_\varepsilon(0) = I$. However, when ε tends to zero, the relaxation step becomes

$$P_0(\Delta t) \begin{pmatrix} \mathbf{w} \\ \mathbf{z} \end{pmatrix} = \begin{pmatrix} \mathbf{w} \\ \mathbf{f}(\mathbf{w}) \end{pmatrix}$$

and we observe that the limit relaxation operator does not satisfy $P_0(0) = I$ anymore. It has become a projection operator

$$P_0(0) P_0(0) = P_0(0)$$

The fact that $P_0(0) \neq I$ is the main reason why a Strang splitting procedure like

$$S(\Delta t) = T(\frac{\Delta t}{2}) P_\varepsilon(\Delta t) T(\frac{\Delta t}{2})$$

would not lead to a second-order scheme for the original system (1) in the case $\varepsilon = 0$ (Coulette et al. [6,7]). Other analyses about the splitting error in the Strang procedure in the cases of equations with stiff source terms can be found in the context of the Schrödinger equations in Jahnke and Lubich [8] or Descombes and Thalhammer [9].

The objectives of this paper are:

1) recall how to construct a splitting that remains second order when $\varepsilon = 0$;
2) compute the formal equivalent equation of the resulting scheme;
3) from this equivalent system of partial differential equations, construct compatible boundary conditions ensuring stability and high order;
4) test the whole approach for a simple hyperbolic problem solved with a lattice Boltzmann Method.

2. Over-relaxation scheme

For constructing a second-order-in-time over-relaxation scheme, a possibility is to perform a Padé approximation when $\Delta t \simeq 0$ of the exponential operator

$$\exp(-\frac{\Delta t}{\varepsilon}) \simeq \frac{1 - \frac{\Delta t}{2\varepsilon}}{1 + \frac{\Delta t}{2\varepsilon}} = \frac{2\varepsilon - \Delta t}{2\varepsilon + \Delta t}$$

and to replace the exact relaxation (12) step by

$$R_\varepsilon(\Delta t) \begin{pmatrix} \mathbf{w} \\ \mathbf{z} \end{pmatrix} := \begin{pmatrix} \mathbf{w} \\ \mathbf{f}(\mathbf{w}) \end{pmatrix} + \frac{2\varepsilon - \Delta t}{2\varepsilon + \Delta t} \begin{pmatrix} 0 \\ \mathbf{z} - \mathbf{f}(\mathbf{w}) \end{pmatrix} \tag{14}$$

We would obtain the same formula by applying a Crank–Nicolson scheme for approximating the differential equation (9)–(10). This over-relaxation approach is commonly used in lattice Boltzmann schemes with BGK collision operator. For instance, in Brownlee et al. [10], the authors show its second-order accuracy and they study its stability in the regime $\varepsilon \ll \Delta t$. Now, for $\varepsilon = 0$, we observe that

$$R_0(\Delta t) \begin{pmatrix} \mathbf{w} \\ \mathbf{z} \end{pmatrix} = \begin{pmatrix} \mathbf{w} \\ 2\mathbf{f}(\mathbf{w}) - \mathbf{z} \end{pmatrix} \tag{15}$$

This operator does not depend on Δt any longer. We also observe that, as for the usual Strang splitting procedure, $R_0(0) \neq I$. In addition, R_0 is no more a projection, but an involutory operator

$$R_0 R_0 = I$$

With this observation in mind, we propose the following over-relaxation scheme $S_2(\Delta t)$ for approximating the solution to (1)–(2). It is defined by

$$S_2(\Delta t) := T(\frac{\Delta t}{4}) R_0 T(\frac{\Delta t}{2}) R_0 T(\frac{\Delta t}{4}) \tag{16}$$

With this definition, we can check that the over-relaxation scheme is time-symmetric:

$$S_2(-\Delta t) = S_2(\Delta t)^{-1}, \quad S_2(0) = I$$

For now, let us also assume that the scheme is consistent at least at first order with equation (1). This point will be made more rigorous in Theorem 3.1. Time-symmetry and consistency ensure that the over-relaxation scheme is second order in time (Hairer et al. [11], McLachlan and Quispel [12]). For one single time step, we thus have

$$\begin{pmatrix} \mathbf{u}(\cdot, \Delta t) \\ \mathbf{f}(\mathbf{u}(\cdot, \Delta t)) \end{pmatrix} = S_2(\Delta t) \begin{pmatrix} \mathbf{v} \\ \mathbf{f}(\mathbf{v}) \end{pmatrix} + O(\Delta t^3)$$

where $\mathbf{u}$ is the exact solution to (1)–(2).

3. Equivalent equation

3.1. General case

In this section, we will compute the equivalent equation of the over-relaxation scheme. The objective is to derive a system of partial differential equations satisfied by the approximations of $\mathbf{w}$ and $\mathbf{z}$ when Δt tends to zero. Of course, if $\mathbf{z} = \mathbf{f}(\mathbf{w})$ at the initial time, we expect $\mathbf{w}$ and $\mathbf{z}$ to satisfy

$$\partial_t \mathbf{w} + \partial_x \mathbf{f}(\mathbf{w}) = O(\Delta t^2), \quad \mathbf{z} - \mathbf{f}(\mathbf{w}) = O(\Delta t^2)$$

A more interesting question is to find a partial differential equation satisfied by the approximation of the flux $\mathbf{z}$. This is important in practice in order to construct stable boundary conditions to be applied to $\mathbf{z}$, or for designing schemes that remain second order at the boundaries.

Let $\mathbf{w}$ and $\mathbf{z}$ denote now the numerical solution given by the second-order scheme (16). We have

$$\frac{1}{\Delta t} \begin{pmatrix} \mathbf{w}(\cdot, t + \frac{\Delta t}{2}) - \mathbf{w}(\cdot, t - \frac{\Delta t}{2}) \\ \mathbf{z}(\cdot, t + \frac{\Delta t}{2})) - \mathbf{z}(\cdot, t - \frac{\Delta t}{2})) \end{pmatrix} =$$
$$\frac{1}{\Delta t}(S_2(\frac{\Delta t}{2}) - S_2(-\frac{\Delta t}{2})) \begin{pmatrix} \mathbf{w}(\cdot, t) \\ \mathbf{z}(\cdot, t) \end{pmatrix} \tag{17}$$

where the over-relaxation scheme S_2 has an explicit form given by (11), (15), and (16). We can perform a Taylor expansion of both sides of (17) when Δt tends to zero. By symmetry considerations, the first-order terms vanish. An essential point is that $S_2(0) = I$. After simple but long calculations,[1] we obtain the following result.

Theorem 3.1. *Let $\mathbf{w}$ and $\mathbf{z}$ be smooth solutions to the time marching algorithm (17). Let us define the* **flux error** $\mathbf{y}$ *by*

$$\mathbf{y} := \mathbf{z} - \mathbf{f}(\mathbf{w})$$

Then, up to second-order terms in Δt, $\mathbf{w}$ and $\mathbf{y}$ are solutions to the following (non conservative) hyperbolic system of conservation laws:

$$\partial_t \begin{pmatrix} \mathbf{w} \\ \mathbf{y} \end{pmatrix} + \begin{pmatrix} \mathbf{f}'(\mathbf{w}) & 0 \\ 0 & -\mathbf{f}'(\mathbf{w}) \end{pmatrix} \partial_x \begin{pmatrix} \mathbf{w} \\ \mathbf{y} \end{pmatrix} = 0 \tag{18}$$

Remark 3.1. The equivalent equation (18) shows that the over-relaxation scheme tends to propagate the conservative variables $\mathbf{w}$ and the flux error $\mathbf{y}$ with opposite wave velocities. This gives hints to build stable boundary conditions on $\mathbf{z}$. Roughly speaking, at an inflow boundary for $\mathbf{w}$, one should impose $\mathbf{w}$ and not $\mathbf{y}$, while at an outflow boundary for $\mathbf{w}$ one should impose $\mathbf{y}$ and not $\mathbf{w}$. Numerical experiments that confirm this heuristic are given in the next section.

Remark 3.2. Generally, when the relaxation operator is a projection, the equivalent equation is only available for $\mathbf{w}$. See, for instance, [13,14].

Remark 3.3. The kinetic speed λ does not appear in the equivalent equation (18). It appears in the $O(\Delta t^2)$ terms, which are complicated. We do not know yet how to perform the stability analysis of these terms for an arbitrary system of equations. However, for the scalar transport equation, we show below that the standard subcharacteristic condition ensures L^2 stability.

3.2. Scalar transport equation

Let us study the simple case where $m = 1$, $\mathbf{u} = u \in \mathbb{R}$ and $\mathbf{f}(\mathbf{u}) = f(u) = cu$, $c > 0$. We thus solve a simple transport equation at velocity $c > 0$

$$\partial_t u + c \, \partial_x u = 0 \tag{19}$$

With the same notations as in the general case, simple but long calculations show that, up to third-order terms in Δt, the functions w and y satisfy the equations

$$\partial_t w + c \partial_x w + \frac{c}{24} \Delta t^2 \left((\lambda^2 + 3c^2) \partial_{xxx} w + 3c \partial_{xxx} y \right) + \frac{1}{6} \Delta t^2 \partial_{ttt} w = 0$$
$$\partial_t y - c \partial_x y + \frac{c}{24} \Delta t^2 \left(3c(\lambda^2 - c^2) \partial_{xxx} w - (\lambda^2 + 3c^2) \partial_{xxx} y \right) + \frac{1}{6} \Delta t^2 \partial_{ttt} y = 0$$

---

[1] The calculations can be made with a computer algebra system, such as Maple or Mathematica.

Then, observing that $\partial_{ttt} w = -c^3 \partial_{xxx} w + O(\Delta t^2)$ and $\partial_{ttt} y = c^3 \partial_{xxx} y + O(\Delta t^2)$, one obtains the equivalent equation of the scheme at third order:

$$\partial_t \begin{pmatrix} w \\ y \end{pmatrix} + \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} \partial_x \begin{pmatrix} w \\ y \end{pmatrix} + A\Delta t^2 \partial_{xxx} \begin{pmatrix} w \\ y \end{pmatrix} = O(\Delta t^3) \tag{20}$$

with

$$A = \begin{pmatrix} (\lambda^2 - c^2) & 3c \\ 3c(\lambda^2 - c^2) & -(\lambda^2 - c^2) \end{pmatrix}$$

Theorem 3.2 (L^2 stability). *On a periodic domain $x \in \Omega$, the third-order equivalent equation* (20) *of the numerical scheme* (17) *preserves the following energy*

$$E(t) = \int_\Omega \left((\lambda^2 - c^2) \frac{w^2}{2} + \frac{y^2}{2} \right)$$

Under the subcharacteristic condition $\lambda > c$ the energy is strictly convex and consequently the model is stable.

To prove the theorem, we can rewrite the energy in the form

$$E(t) = \int_\Omega \left(D \begin{pmatrix} w \\ y \end{pmatrix}, \begin{pmatrix} w \\ y \end{pmatrix} \right)$$

with D a diagonal 2×2 matrix with coefficients $\lambda^2 - c^2$ and 1 and $(,)$ the usual scalar product. The energy satisfies

$$\partial_t E(t) + \int_\Omega \left(D \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix} \partial_x \begin{pmatrix} w \\ y \end{pmatrix}, \begin{pmatrix} w \\ y \end{pmatrix} \right)$$

$$+ \int_\Omega \left(DA\partial_{xxx} \begin{pmatrix} w \\ y \end{pmatrix}, \begin{pmatrix} w \\ y \end{pmatrix} \right) = 0 \tag{21}$$

This choice for D ensures that the matrix DA is symmetric. Then, the second and third terms of (21) vanish after applying integration by parts. Finally, we find that

$$\partial_t E(t) = 0$$

4. Numerical method

4.1. Transport model

In this section, we describe a numerical discretization of S_2 for the transport equation (19). We assume that $x \in [0, 1]$. We also provide an initial condition and a boundary condition at the left point

$$u(x, 0) = v(x), \quad u(0, t) = v(-ct)$$

where $v : \mathbb{R} \to \mathbb{R}$ is a given function. It can be checked that the exact solution to this initial boundary value problem is

$$u(x, t) = v(x - ct)$$

With this transport equation, we can associate its over-relaxation system with the approximated conservative data $\mathbf{w} = w \in \mathbb{R}$ and the approximated flux $\mathbf{z} = z \in \mathbb{R}$.

4.2. Numerical discretization

For the numerical discretization, we consider a positive integer N and define the space step and grid points by

$$\Delta x = \frac{1}{N+1}, \quad x_i = i\Delta x, \quad i = 0 \dots N+1$$

The grid points $i = 0$ and $i = N+1$ are the border points of the interval $[0, 1]$, where the boundary conditions are applied. We consider an approximation of w and z at the grid points x_i and times $t_n = n\Delta t$

$$w_i^n \simeq w(x_i, t_n), \quad z_i^n \simeq z(x_i, t_n)$$

The initial data are exactly sampled at the grid points

$$w_i^0 = v(x_i), \quad z_i^0 = cv(x_i) + y(x_i)$$

In most cases, we assume initial equilibrium and set $y(x_i) = 0$. But for the numerical experiments presented below, we specifically study the evolution of an initial non-equilibrium solution. Like in the lattice Boltzmann Method (Chen and Doolen [15]), we choose a special time step

$$\Delta t = \frac{4\Delta x}{\lambda}$$

This choice ensures that the transport operator $T(\Delta t/4)$ only involves exact shift operators. For instance, the translation operator is approximated here by

$$(s(\Delta t/4)w)(x_i, t_n) \simeq w_{i-1}^n$$

Thus, the transport step reads:

$$
\begin{aligned}
w_i^{n+1/4} &= \frac{w_{i-1}^n + w_{i+1}^n}{2} + \frac{z_{i-1}^n - z_{i+1}^n}{2\lambda} \\
z_i^{n+1/4} &= \frac{z_{i-1}^n + z_{i+1}^n}{2} + \lambda \frac{w_{i-1}^n - w_{i+1}^n}{2}
\end{aligned}
\tag{22}
$$

Note that, these discrete equations are equivalent to shifting the Riemann invariants $w \pm z/\lambda$:

$$z_i^{n+1/4} - \lambda w_i^{n+1/4} = z_{i+1}^n - \lambda w_{i+1}^n \tag{23}$$

$$z_i^{n+1/4} + \lambda w_i^{n+1/4} = z_{i-1}^n + \lambda w_{i-1}^n \tag{24}$$

In our practical implementation, we also use the fact that

$$T(\Delta t/2) = T(\Delta t/4)T(\Delta t/4)$$

4.3. Boundary conditions

Let us assume that, at the beginning of a time step, for instance at time t_n, we know w_i^n and z_i^n for $i = 0 \ldots N + 1$. The transport operator $T(\Delta t/4)$ can be applied to internal grid points x_i, corresponding to indices $i = 1 \ldots N$. Thus, using (22), it is possible to compute $w_i^{n+1/4}$, $z_i^{n+1/4}$ for $i = 1 \ldots N$. At the left boundary $i = 0$, one piece of information is missing for computing $w_0^{n+1/4}$ and $z_0^{n+1/4}$. According to the previous analysis, it is natural to impose a boundary condition on w (because it is an inflow boundary) at the middle of the time step (in order to respect the time-symmetry):

$$w(0, t_n + \frac{\Delta t}{8}) = v(-c(t_n + \frac{\Delta t}{8})) \tag{25}$$

Other choices are possible. For instance, we have also tested the relation

$$w(0, t_n + \frac{\Delta t}{4}) = v(-c(t_n + \frac{\Delta t}{4})) \tag{26}$$

which would give the same accuracy. Boundary condition (25) is discretized by

$$\frac{w_0^n + w_0^{n+1/4}}{2} = v(-c(t_n + \frac{\Delta t}{8})) \tag{27}$$

which provides the missing relation and enables us to compute $w_0^{n+1/4}$. Then, from (23), we can compute the value of $z_0^{n+1/4}$:

$$z_0^{n+1/4} - \lambda w_0^{n+1/4} = z_1^n - \lambda w_1^n$$

At the right boundary, we will test several approaches: an "exact" strategy, a "Dirichlet" strategy on $y = z - cw$, or a "Neumann" strategy.

4.3.1. Exact strategy

Since we know the analytical solution, we can impose the values of w_{N+1} given by the exact solution. Of course, this method cannot be generalized to more complicated equations and solutions. In addition, we expect it to generate oscillations, because the boundary condition is not compatible with an outflow boundary. Following (27) for the left boundary, we write

$$\frac{w_{N+1}^n + w_{N+1}^{n+1/4}}{2} = v\,(1 - c\,(t_n + \frac{\Delta t}{8}))$$

4.3.2. Dirichlet strategy

In this method, we simply apply the condition $y = 0$ at the middle of the time step. We obtain

$$\frac{z_{N+1}^n + z_{N+1}^{n+1/4}}{2} - c\,\frac{w_{N+1}^n + w_{N+1}^{n+1/4}}{2} = 0$$

which provides the missing relation. For instance, using this relation and expression (24), one obtains

$$w_{N+1}^{n+1/4} = \frac{1}{\lambda + c}\,\left(\lambda\,w_N^n - c\,w_{N+1}^n\right) + \frac{1}{\lambda + c}\,\left(z_N^n + z_{N+1}^n\right)$$

4.3.3. Neumann strategy

The last method imposes the condition $\partial_x y(L, t) = 0$ at the right boundary. The missing relation is obtained from

$$z_{N+1}^{n+1/4} - c w_{N+1}^{n+1/4} = z_N^{n+1/4} - c w_N^{n+1/4}$$

Once again, using this relation and expression (23), one now has the following relation for $w_{N+1}^{n+1/4}$

$$w_{N+1}^{n+1/4} = \frac{1}{2(\lambda + c)}\,\Big[\left(2\,\lambda\,w_N^n + (\lambda + c)\,w_{N+1}^n - (\lambda - c)\,w_{N-1}^n\right) +$$
$$\left(2\,z_N^n - \frac{\lambda + c}{\lambda}z_{N+1}^n - \frac{\lambda - c}{\lambda}z_{N-1}^n\right)\Big]$$

4.4. Relaxation

The relaxation operation, as stated above, consists in replacing in each cell $(\mathbf{w}, \mathbf{z})$ by $(\mathbf{w}, 2\mathbf{f}(\mathbf{w}) - \mathbf{z})$. We emphasize that the relaxation is also performed in the boundary cells $i = 0$ and $i = N + 1$.

4.5. Numerical results for the transport equation

We test the above scheme and boundary conditions with $x \in [0, 1]$, $t \in [0, t_{\max}]$ and the following exact solution

$$u(x, t) = \exp(A(x - \alpha - ct)^2)$$

We may also impose a (non-physical) flux disequilibrium $y = z - f(w) \neq 0$ at the initial time. The initial value of y is given at time $t = 0$ by

$$y(x, t) = B\exp(A\,(x - \beta + ct)^2)$$

We test the three boundary approaches proposed in Section 4.3. We check the stability and order of the scheme. The error is measured by the discrete L^2 norm

$$e_{\Delta x}^n = \sqrt{\Delta x \sum_{i=0}^{N+1} \left(q_i^n - q_{\text{ref},i}^n\right)^2}$$

where q_i^n may be w_i^n or z_i^n. The reference value $v_{\text{ref},i}^n$ is then $u\,(x_i - c n \,\Delta t)$ or $c\,u\,(x_i - c n \,\Delta t)$ respectively.

In Fig. 1, we first show an illustration of the propagation of the quantity $y = z - f(w)$ with the following numerical parameters:

$$c = 1, \quad \lambda = 2, \quad t_{\max} = 0.33, \quad \alpha = 0.25, \quad \beta = 0.75 \quad A = -80, \quad B = 1/2$$

With this choice and sufficiently small final time, the boundary condition has no influence. One checks numerically that w propagates with velocity u, while y propagates with velocity $-u$, which agrees with the equivalent equation (18).
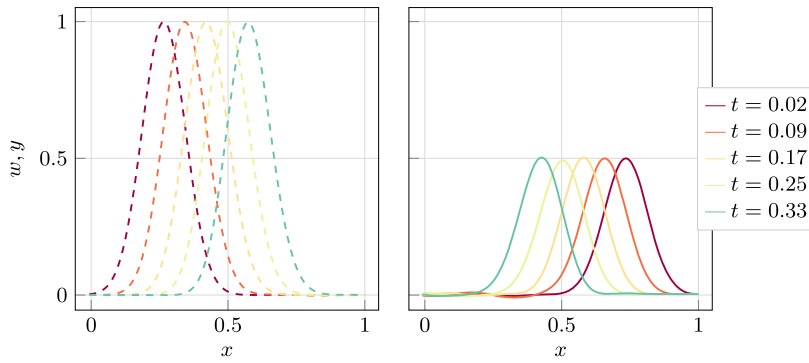
Fig. 1. Transport of the w (dashed lines) and $y = z - f(w)$ (plain lines) quantities.
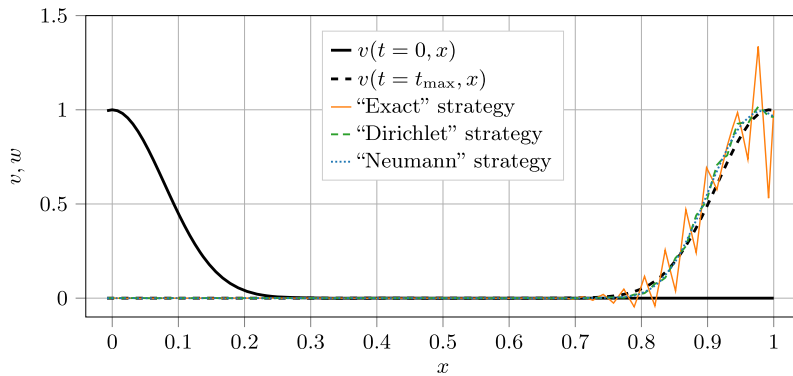

Fig. 2. Initial state and comparison of the final states for the transport equation with the Gaussian initial profile, $\Delta x = 2^{-7}$.
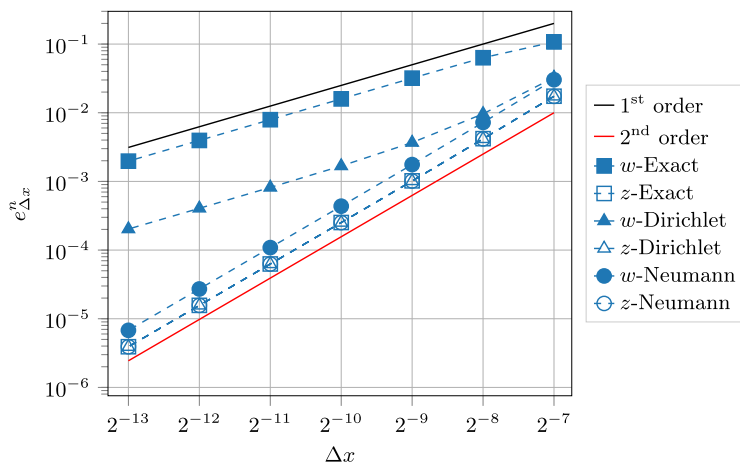

Fig. 3. Convergence study for the transport equation with the Gaussian initial profile. Comparison of exact, Dirichlet and Neumann strategies for the variables w and z.

An illustration of the numerical results using the three strategies for boundary conditions is given in Fig. 2. For this test, we have imposed the following numerical parameters:

$$c = 1, \quad \lambda = 2, \quad t_{max} = 1, \quad \alpha = 0, \quad \beta = 0 \quad A = -80, \quad \text{and} \quad B = 0$$

Therefore, because $B = 0$, in this test there is no flux disequilibrium and the exact solution is such that $y = 0$. One can see that the *exact* strategy generates oscillations at the right boundary. The *Dirichlet* strategy generates weaker oscillations that are not amplified with time. The *Neumann* strategy does not generate any oscillation.

The convergence results are shown in Fig. 3. One can see that the *exact* strategy and the *Dirichlet* strategy are first order
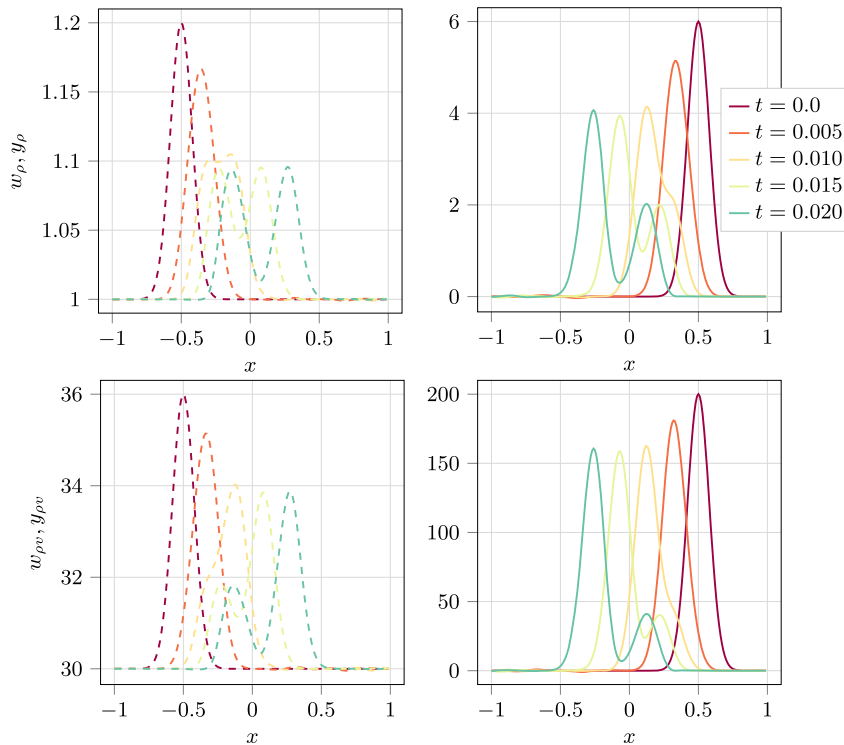
Fig. 4. Wave propagation for the Euler system solved with the over-relaxation kinetic scheme.

accurate for the variable w, while the *Neumann* strategy is second order accurate. The results are superimposed for the variable z. The best choice for ensuring stability and second-order accuracy seems to be the *Neumann* strategy.

Remark 4.1. With the *Dirichlet* strategy, we impose that $y = z - c\,w = 0$ at the boundary, while this equality may not be satisfied exactly inside the domain. The over relaxation approach is based on the Crank–Nicolson scheme. In the stiff limit, the Crank–Nicolson scheme is known to remain stable, but with bounded oscillations. In our case, during the relaxation steps of the splitting procedure, the quantity y is changed into $-y$ on the internal cells. This generates small fluctuations, which are necessary to achieve second order. Imposing directly $y = 0$ on the boundary cell seems to disturb those advantageous fluctuations. On the other hand, the Neumann conditions $\partial_x y = 0$ is compatible with changing y into $-y$. This may explain why the scheme remains second order with the *Neumann* strategy.

4.6. Numerical results for barotropic Euler equations

In this second paragraph about numerical results, we show that our theory and the strategies for the boundary conditions apply for non-linear systems of equations too. We choose to study the barotropic Euler equations in one dimension, for which

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho v \end{pmatrix}, \quad \mathbf{f}(\mathbf{u}) = \begin{pmatrix} \rho v \\ (\rho v)^2/\rho + c^2\rho \end{pmatrix}, \quad \rho > 0, \quad c = 10$$

The initial condition is given by

$$\rho(x, 0) = \rho_0 + C \exp(D(x - x_0)), \quad (\rho v)(x, 0) = \rho(x, 0)v_0, \quad \rho_0 = 1.0, \quad v_0 = 3c$$

We choose a supersonic configuration ($v_0 > c$), so that all the waves associated with the Euler system propagate rightwards. Moreover, the subcharacteristic condition is satisfied by using $\lambda = 5c$.

Let us note w_ρ, $w_{\rho v}$, y_ρ and $y_{\rho v}$ the variables of the over-relaxation kinetic scheme applied to the Euler equations. In Fig. 4, we show an illustration of the propagation of these different variables for the following parameters

$$C = 0.2, \quad D = -80, \quad x_0 = -0.5$$

and for the following initialization

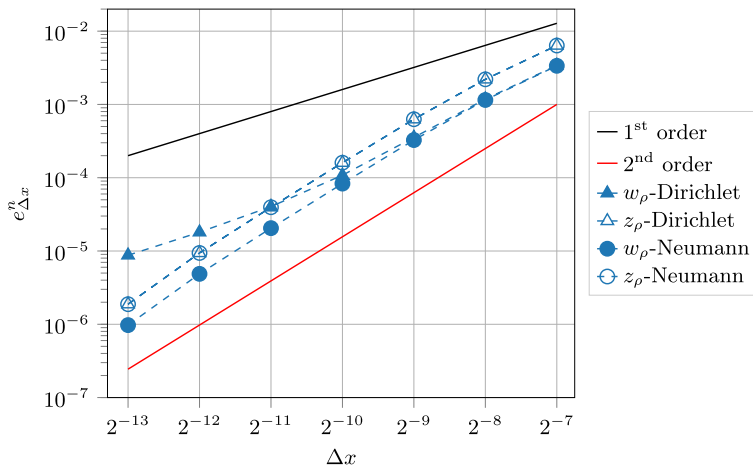$$w_\rho(x, 0) = \rho(x, 0), \quad y_\rho(x, 0) = 6\exp(-80(x - 0.5)) - (\rho v)(x, 0)$$

Fig. 5. Convergence study for the Euler equations with Gaussian initial profile. Comparison of Dirichlet and Neumann strategies for the variables w_ρ and z_ρ.

$$w_{\rho v}(x,0) = (\rho v)(x,0), \quad y_{\rho v}(x,0) = 200\exp(-80(x-0.5)) - \frac{(\rho v)^2}{\rho}(x,0) - c^2\rho(x,0)$$

We choose here large non-equilibrium profiles for variables y_ρ and $y_{\rho v}$, so that we can clearly observe their evolution, since the numerical scheme also generates deviations from the equilibrium. One can see that the waves associated with the variables w_ρ and $w_{\rho v}$ propagate at velocities $u - c = 2c$ and $u + c = 4c$, while the waves associated with the variables y_ρ and $y_{\rho v}$ propagate at velocities $-2c$ and $-4c$, which is in agreement with Theorem 3.1.

The convergence results for the boundary strategies applied to the Euler equations are given in Fig. 5. There, the initial conditions are

$$w_\rho(x,0) = \rho(x,0), \quad w_{\rho v}(x,0) = (\rho v)(x,0), \quad y_\rho(x,0), y_{\rho v}(x,0) = 0$$

and the final simulation time is $t_{\max} = 0.8$. We only display the error computations related to ρ, since the same results are obtained for ρv. The numerical errors are computed using a reference solution, which is the numerical solution provided by the finest grid. Similarly to the results of the transport equation, one can note that the Dirichlet strategy is first order for the variable w_ρ, while the Neumann strategy is second order. Again, the results for the variable z_ρ are superimposed.

5. Conclusion

In this note, we have derived the equivalent equation of the over-relaxation kinetic scheme. The equivalent equation reveals that the conservative variable and the flux error propagate in opposite directions. This allows us to determine natural boundary conditions for the over-relaxation scheme. Numerical experiments confirm the stability and accuracy of these boundary conditions, both for a linear scalar equation and a nonlinear system of equations. In a forthcoming work, we will extend the approach to higher dimensions. Another work in progress aims at incorporating a dissipative mechanism in the over-relaxation method in order to compute discontinuous solutions without oscillations.

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