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An analysis of over-relaxation in kinetic approximation $\stackrel{\text{\tiny{free}}}{\to}$

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Abstract

The over-relaxation approach is an alternative to the Jin-Xin relaxation method (Jin and Xin [1]) in order to apply the equilibrium source term in a more precise way (Coulette et al. [2, 3]). This is also a key ingredient of the Lattice-Boltzmann method for achieving second order accuracy (Dellar [4]). 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.

Keywords: kinetic relaxation, equivalent equation, boundary conditions, asymptotic preserving 2010 MSC: 35L04, 76M28

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 $t \ge 0$. 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 conservative variables \mathbf{u} , the jacobian of the flux

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

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is diagonalizable with real eigenvalues.

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

$$\partial_t \mathbf{w}_{\varepsilon} + \partial_x \mathbf{z}_{\varepsilon} = 0, \qquad (4)$$

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

with the initial condition

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

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}_{ε} tends to \mathbf{u} , the entropy solution of (1)-(2), when ε tends to zero (Jin and Xin [1]).

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 source term.

A simple way to solve numerically the Jin-Xin system is to use a timesplitting 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 differential equations (relaxation step)

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

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

Both sub-steps admit a simple explicit solution. Indeed, if we define the functional translation operator $\tau(\Delta t)$ by

$$(\tau(\Delta t)\mathbf{v})(x) = \mathbf{v}(x - \lambda \Delta t),$$

then the solution of the free transport step (7)-(8) is given by

$$\left(\begin{array}{c} \mathbf{w}(\cdot,t+\Delta t)\\ \mathbf{z}(\cdot,t+\Delta t) \end{array}\right) = T(\Delta t) \left(\begin{array}{c} \mathbf{w}(\cdot,t)\\ \mathbf{z}(\cdot,t) \end{array}\right),$$

with

$$T(\Delta t) \coloneqq \frac{1}{2} \begin{pmatrix} \tau(\Delta t) + \tau(-\Delta t) & (\tau(\Delta t) - \tau(-\Delta t))/\lambda \\ \lambda(\tau(\Delta t) - \tau(-\Delta t)) & \tau(\Delta t) + \tau(-\Delta t) \end{pmatrix}.$$
 (11)

This can be easily obtained noting that the characteristic quantities $\mathbf{w}/2\pm\mathbf{z}/2\lambda$ are transported at velocities $\pm\lambda$. The solution of 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

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

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

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

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. 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 in the case $\varepsilon = 0$ (Coulette et al. [2, 3]). 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

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

We would obtain the same formula by applying a Crank-Nicolson scheme for approximating the differential equation (9)-(10). Now, we observe that

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

This operator does not depend on Δt anymore. 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 of (1)-(2). It is defined by

$$S_2(\Delta t) \coloneqq T(\frac{\Delta t}{4}) R_0 T(\frac{\Delta t}{2}) R_0 T(\frac{\Delta t}{4}).$$
(16)

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

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

This property ensures that the over-relaxation scheme is second order in time (Hairer et al. [5], McLachlan and Quispel [6]). 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 **u** is the exact solution of (1)-(2).

3. Equivalent equation

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

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

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, we obtain the following result:

Theorem 1. Let \mathbf{w} and \mathbf{z} be smooth solutions of the time marching algorithm (17). Let us define the flux error \mathbf{y} by

$$\mathbf{y} \coloneqq \mathbf{z} - \mathbf{f}(\mathbf{w}).$$

Then, up to second order terms in Δt , **w** and **y** are solutions of the following (non conservative) hyperbolic system of conservation laws:

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

Remark 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 2. Generally, when the relaxation operator is a projection, the equivalent equation is only available for \mathbf{w} . See for instance [7, 8]

Remark 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. In practice, if λ is too small, the scheme becomes unstable. This indicates that a subcharacteristic condition still has to be satisfied.

4. Numerical method

4.1. Transport model

In this section, we describe a numerical discretization of S_2 in 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

$$\partial_t u + c \,\partial_x u = 0.$$

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 of 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

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

Like in the Lattice Boltzmann Method (Chen and Doolen [9]) 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

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

Thus, the transport step reads:

$$w_i^{n+1/4} = \frac{w_{i-1}^n + w_{i+1}^n}{2} + \frac{z_{i-1}^n - z_{i+1}^n}{2\lambda},$$

$$z_i^{n+1/4} = \frac{z_{i-1}^n + z_{i+1}^n}{2} + \lambda \frac{w_{i-1}^n - w_{i+1}^n}{2}.$$
(19)

Note that, these discrete equations are equivalent to:

$$z_i^{n+1/4} - \lambda w_i^{n+1/4} = z_{i+1}^n - \lambda w_{i+1}^n, \tag{20}$$

$$z_i^{n+1/4} + \lambda w_i^{n+1/4} = z_{i-1}^n + \lambda w_{i-1}^n.$$
(21)

In practice, we also use the fact that $T(\Delta t/2) = T(\Delta t/4)T(\Delta t/4)$.

4.3. Boundary conditions, relaxation

4.3.1. 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 $i = 0 \dots N + 1$. The transport operator $T(\Delta t/4)$ can be applied to internal grid points x_i , corresponding to indices $i = 1 \dots N$. Thus, using (19), it is possible to compute $w_i^{n+1/4}$, $z_i^{n+1/4}$ for $i = 1 \dots N$. At the left boundary i = 0, one 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 the boundary condition on w (because it is an inflow boundary) at the middle of the time step (in order to respect the time-symmetry):

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

It is discretized by

$$\frac{w_0^n + w_0^{n+1/4}}{2} = v(-c(t_n + \frac{\Delta t}{8})), \tag{22}$$

which provides the missing relation and enables to compute $w_0^{n+1/4}$. Then, from (20), the value of $z_0^{n+1/4}$ can be computed:

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

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

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 complex equations and solutions. In addition, we expect it to generate oscillations, because the boundary condition is not compatible with an outflow boundary. As for the left boundary, we write

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

4.4 Numerical results

Dirichlet strategy on y. In this method, we simply apply the condition y = 0 at the middle of the time step. This gives

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

which provides the missing relation. For instance, using this relation and expression (21), one obtains

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

Neumann strategy on y. The last method consists in imposing the condition $\partial_x y(L,t) = 0$ at the right boundary. Formally, up to second order, this is equivalent to impose $\partial_t y(L,t) = 0$ or y(L,t) = y(L,0) = 0. The missing relation is obtained from

$$z_{N+1}^{n+1/4} - cw_{N+1}^{n+1/4} = z_N^{n+1/4} - cw_N^{n+1/4}.$$

Once again, using this relation and expression (20), one now has the following relation for $w_{N+1}^{n+1/4}$

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

4.3.2. 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.

4.4. Numerical results

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

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

We test the three boundary approaches proposed in Section 4.3.1. We check the stability and order of the scheme. The error is measured by the discrete L^2 norm

$$e_{\Delta x}^{n} = \sqrt{\Delta x \sum_{i=0}^{N+1} \left(w_{i}^{n} - u(x_{i} - cn\Delta t) \right)^{2} + \left(z_{i}^{n} - cu(x_{i} - cn\Delta t) \right)^{2}}.$$



Figure 1: Transport of the w (dashed lines) and y = z - f(w) (plain lines) quantities.



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



Figure 3: Convergence study for the transport equation with Gaussian initial profile. Comparison of Exact, Dirichlet and Neumann strategies.

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

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

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).

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

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

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 Figure 3. One can see that the *Exact* strategy and the *Dirichlet* strategy are first order accurate, while the *Neumann* strategy is second order accurate. The best choice for ensuring stability and second order accuracy seems to be the *Neumann* strategy.

Remark 4. With the Dirichlet strategy, we impose that y = z - cw = 0 at the boundary, while this equality may not be satisfied exactly inside the domain. This creates small discontinuities that may explain the loss of accuracy.

5. Conclusion

In this short note, we have derived the equivalent equation of the overrelaxation 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. In a forthcoming work, we will extend the approach to more complex non-linear systems and to higher dimensions. It also important to incorporate in the overrelaxation method a dissipative mechanism in order to compute discontinuous solutions without oscillations.

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