ANNALES DE LA FACULTÉ DES SCIENCES TOULOUSE Mathématiques

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Tome XXIX, nº 4 (2020), p. 927-950.

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Volume XXIX, nº 4, 2020 pp. 927-950

Ghost solutions with centered schemes for one-dimensional transport equations with Neumann boundary conditions ^(*)

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ABSTRACT. — This paper is devoted to the space-centered θ -scheme for the transport equation with constant velocity on an interval, with homogeneous Neumann boundary data on each side. The numerical solution presents a weird behavior, as if the initial datum was periodical over \mathbb{R} , with a period that would be twice or four times (depending on the case) the length of the considered interval. We precisely formulate this statement and prove it. We also study a similar behavior in the case of Dirichlet boundary conditions.

RÉSUMÉ. — Dans cet article, nous nous intéressons au θ -schéma centré en espace pour la résolution approchée de l'équation de transport à vitesse constante dans un segment en dimension 1, avec données de Neumann homogènes aux deux bords du domaine. De manière très surprenante, la solution numérique présente un caractère périodique, comme si la donnée initiale était périodique sur \mathbb{R} avec une période égale à deux fois ou quatre fois, suivant les cas, la longueur du segment. Nous énonçons précisément ce résultat et le démontrons, puis évoquons un comportement similaire dans le cas où les deux conditions de bord sont de type Dirichlet.

^(*) Reçu le 22 octobre 2018, accepté le 18 janvier 2019.

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Research of the second author was supported by ANR project BoND, ANR-13-BS01-0009, and by ANR project NABUCO, ANR-17-CE40-0025.

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Article proposé par David Lannes.

1. Introduction

The transport partial differential equation with constant velocity a in an interval I,

$$\partial_t u(t,x) + a \partial_x u(t,x) = 0, \quad t \in \mathbb{R}_+, x \in I,$$

is essentially trivial from a mathematical point of view and does not a priori merit much academic consideration. Through numerical simulations, however, we came across a rather astonishing and apparently unknown phenomenon involving "ghost" solutions which we are going to describe in the following. To be more specific, consider the transport equation with constant velocity a on the interval (0, 1). As numerical approximation we use a space-centered θ -scheme. The terminology space-centered here means that the space derivative $\partial_x u(x_i)$ is "replaced" with the centered finite difference $(U_{j+1} - U_{j-1})/(2\Delta x)$, with standard notations, and the real number θ is an implicitness parameter (namely, it allows to pass continuously from the explicit Euler time discretization, $\theta = 0$, to the implicit Euler one, $\theta = 1$), see (2.1) in the following. It is known (see [7]) that on the whole real line, the θ -scheme is stable in a strong sense in l^2 for $\theta \ge 1/2$ (it makes the l^2 norm of the solution non-increase at every time step). For $\theta \in [0, 1/2)$, it can lead to a stable (in the sense that the l^2 norm can increase in a bounded way) and convergent scheme, but under a stability condition asking Δt to be of the order of Δx^2 , which makes the scheme less interesting. In the following, we consider $\theta \ge 1/2$.

A first difficulty comes from the fact that the centered scheme requires two numerical boundary conditions (one for each boundary). The study of finite difference schemes for initial boundary value problems has a long story. The transport equation on the half line with Dirichlet boundary conditions has been studied, for *dissipative* schemes, by Kreiss and Lundqvist in [9], but the present scheme is not dissipative in their sense, and we here consider the equation on an interval. The problem of the convergence order of schemes on the half line, under rather stability and consistency condition, has also been studied, for example in [6]. Dirichlet boundary conditions at an outflow boundary often create boundary layers (see [9], and also [2] for their precise study), and a lot of papers have been devoted to avoid these boundary layers, to "let the solution go outside of the domain". Among these methods, let us cite the transparent boundary conditions (see the review paper [1]) and the absorbing boundary conditions (see [4]). A common way to "let the solution go out" is to provide the scheme with artificial (numerical) homogeneous Neumann boundary conditions (which is especially useful when dealing with non-linear systems), and this is the center of the present paper. These conditions are also called extrapolation (of order 0) in the literature.

We consider here two ways to provide the scheme with boundary conditions: First, we propose *homogeneous Neumann* conditions on both sides and observe the appearance of "ghost" solutions with a periodic behavior (see Section 2): although at the beginning of the computation the homogeneous Neumann conditions seem to "do the job" (let the solution go out of the domain), a kind of ghost of the initial condition then re-enters the domain, from the other side. On the continuous level the Neumann conditions could be interpreted as a natural discretization of the initial boundary problem

$$\begin{cases} \partial_t u + a \partial_x u = 0, & t \in \mathbb{R}_+, & x \in (0, 1), \\ \partial_x u(t, 0) = 0, & t \in \mathbb{R}_+, \\ \partial_x u(t, 1) = 0, & t \in \mathbb{R}_+, \\ u(0, x) = u^0(x), & x \in (0, 1) \end{cases}$$
(1.1)

(although this analogy could be discussed; in particular, keep in mind that from the numerical point of view, the boundary conditions, especially the outflow one, is *technically* required to "close" the scheme). This problem is known to be ill-posed in L^2 , what is easy to understand: with initial condition $u^0 = 0$, the function u(t, x) = 0 is a solution to the problem. But taking a perturbation of the initial condition of the form $u_{\epsilon}^0(x) = \chi_{(0,\epsilon)}(x)$, for $\epsilon \in (0, 1)$ one observes that $u_{\epsilon}(t, x) = \chi_{(0,\epsilon+at)}(x)$ is a solution for $t < (1 - \epsilon)/a$. Thus $\|u^0 - u_{\epsilon}^0\|_2 = \epsilon^{1/2}$, but $\|u(t, \cdot) - u_{\epsilon}(t, \cdot)\|_2 = (\epsilon + at)^{1/2}$, which implies the lack of continuous dependence in $L^{\infty}(0, (1 - \epsilon)/a, L^2(0, 1))$ (take ϵ small and a > 0). Note that the ill-posedness here comes from the Neumann condition at the *inflow* boundary. In particular, the outflow boundary condition is not needed, but the inflow one is responsible for instability.

Second, we analyze the case of *homogeneous Dirichlet* conditions on both sides and show another strange periodical behavior, also involving ghost solutions.

Our purpose here is not to discuss whether or not Neumann (or Dirichlet) boundary conditions are legitimate: they are *not*, in the strong sense. Nevertheless, they are natural conditions when performing numerical simulations and the "ghost" phenomenon that we describe seems robust and could turn out to be a general phenomenon in similar numerical situations even for more complex nonlinear hyperbolic systems (for which it is a rather usual cheap way to impose numerical homogeneous Neumann conditions, as the correct ones are quite hard to know). Indeed, similar experiments to those in the present paper but performed for the non-linear scalar Burgers' equation, as well as for the Euler system of compressible gas dynamics in dimension 1 exhibit the same strange characteristics. The paper is organized as follows. In Section 2, we present the θ -scheme with Neumann boundary conditions, and the peculiar numerical results that motivated the present study, and we formulate a convergence theorem. In Section 3, we prove the theorem. Then, in section 4, we state a similar result in the case where (homogeneous) Dirichlet boundary conditions are put on both sides. Finally, some numerical results for various situations are reported in Section 5.

2. The θ -scheme for the one-dimensional transport equation with Neumann boundary conditions

For a given (smooth) initial condition u_0 , we consider Problem (1.1) where a is a given real parameter. Let $J \in \mathbb{N} \setminus \{0\}$ be the number of cells in [0, 1], $\Delta x = 1/J$ their length, and $\Delta t > 0$. We define as $x_j = (j-1/2)\Delta x$ the center of the cell number $j, j \in \{1, \ldots, J\}$. Let $\theta \ge 0$. The centered θ -scheme for the above initial boundary value problem is

$$\begin{cases} \frac{U_{j}^{n+1} - U_{j}^{n}}{\Delta t} + a\theta \frac{U_{j+1}^{n+1} - U_{j-1}^{n+1}}{2\Delta x} + a(1-\theta) \frac{U_{j+1}^{n} - U_{j-1}^{n}}{2\Delta x} = 0, & n \ge 0, \\ \frac{U_{1}^{n+1} - U_{1}^{n}}{\Delta t} + a\theta \frac{U_{2}^{n+1} - U_{1}^{n+1}}{2\Delta x} + a(1-\theta) \frac{U_{2}^{n} - U_{1}^{n}}{2\Delta x} = 0, & n \ge 0, \\ \frac{U_{j}^{n+1} - U_{j}^{n}}{\Delta t} + a\theta \frac{U_{j}^{n+1} - U_{j-1}^{n+1}}{2\Delta x} + a(1-\theta) \frac{U_{j}^{n+1} - U_{j-1}^{n+1}}{2\Delta x} = 0, & n \ge 0, \\ U_{j}^{0} = u^{0}(x_{j}), & j \in \{1, ..., J\}. \end{cases}$$
(2.1)

The second and the third equations above can be obtained from the first by defining the fictive boundary values $U_0^n = U_1^n$ and $U_{J+1}^n = U_J^n$ for every n. Note that this is consistent with homogeneous Neumann conditions.

In the sequel we will often make use of two versions of J by J "difference matrices". The first corresponds to Neumann boundary conditions, the second to periodic boundary conditions:

$$D_{J} = \begin{pmatrix} -1 & 1 & 0 & \cdots & \cdots & 0 \\ -1 & 0 & 1 & & \vdots \\ \vdots & & \ddots & \ddots & & \vdots \\ \vdots & & -1 & 0 & 1 \\ 0 & \cdots & \cdots & 0 & -1 & 1 \end{pmatrix} \text{ and } T_{J} = \begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & -1 \\ -1 & 0 & 1 & & \vdots \\ \vdots & & \ddots & \ddots & & \vdots \\ \vdots & & \cdots & -1 & 0 & 1 \\ 1 & \cdots & \cdots & 0 & -1 & 0 \end{pmatrix},$$
(2.2)

both matrices belonging to $\mathcal{M}_J(\mathbb{R})$. We shall often omit the subscript J in order to ease notation. Set $U^n = (U_j^n)_{j=1}^J \in \mathbb{R}^J$ and denote by $c = a\Delta t/\Delta x$

the Courant number, The matrix form of the scheme (2.1) is then given by:

$$AU^{n+1} + BU^n = 0, (2.3)$$

where $A = I + \frac{\theta c}{2}D$, $B = -I + \frac{(1-\theta)c}{2}D$ and I is the $J \times J$ identity matrix.

To see that this scheme always has a solution it suffices to show that $d_J(z) = \det(1 - sD_J)$ has no real roots. Developing e.g. from the top left one shows that $d_{J+2}(z) = d_{J+1}(z) + z^2 d_J(z)$, $J \ge 2$. As $d_2(z) = 1$ and $d_3(z) = 1 + z^2$ it follows that every $d_J(z)$, $J \ge 2$ is a polynomial in z^2 with only positive coefficients so indeed there can be no real roots.

Figures 2.1 and 2.2 shows some results obtained with a = 1, $\theta = 1$ (the implicit scheme), and c = 1, for the C^{∞} initial condition

$$u^{0}(x) = \begin{cases} \frac{1}{\exp(-9)} \exp\left(\frac{1}{\left(x - 1/2\right)^{2} - \frac{1}{9}}\right) & \text{if } \left|x - \frac{1}{2}\right| < \frac{1}{3}, \\ 0 & \text{if } x \in (0, 1) \setminus (1/6, 5/6) \end{cases}$$

with a number of cells that is even or odd.

Let us comment upon the observed numerical solutions. At the beginning of the computation (until time 1), the results are as "expected": the profile translates to the right, and the numerical Neumann boundary conditions behave "normally" and resembles a transparency condition, i.e. the profile seems to go out of (0, 1). This is, however, not really the case. Looking closely at the graphs the reader should notice at time 1 the presence of some very small "noise". The noise is in fact a wave-packet that, although small in the uniform norm (so visually appearing small), has a very high derivative and travels to the left, with velocity -a, see the last section of the paper. When it reaches the left boundary it will reconstitute to a smooth solution once again travelling to the right, thus visually making the appearence of a ghost solution suddenly reentering from the left. This will be made clearer in the following, in the proof of the convergence theorem, and at the end of the paper, with other numerical illustrations. Oddly enough, with 1000 cells, the initial condition re-enters the domain from the left boundary, whereas, with 1001 cells, the opposite of the initial condition re-enters. At time 2, the solution with 1000 cells coincides (almost exactly) with the initial condition. In fact, one observes numerically that the solution at time 2 converges towards the initial condition as the number of cells, J, tends to ∞ taking even values only. On the other hand, the solution with 1001 cells coincides (almost exactly) with the opposite of the initial condition. The ongoing process continues periodically, so that at time T = 4 one recovers in both cases the (almost exact) initial condition. The period is T = 4/a for a general velocity a. See Section 5 for a more precise observation of numerical results.

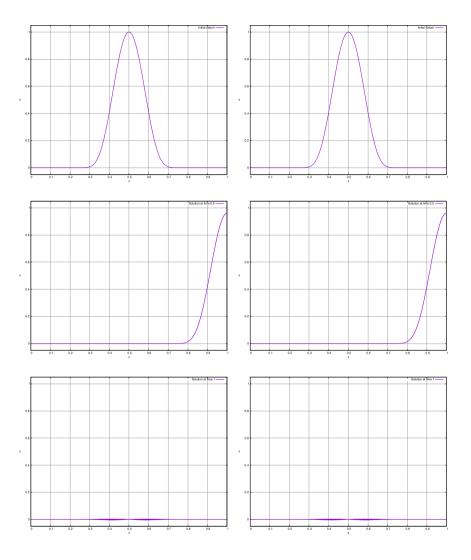


Figure 2.1. Numerical results: with 1000 cells on the left, 1001 cells on the right. From top to bottom: time 0, 0.5, 1.

The above observations have led us to formulate a theorem as follows: We extend the initial condition to all of \mathbb{R} depending on the parity of the number of cells, i.e. we define the functions $u^{0,e}$ (e for even) and

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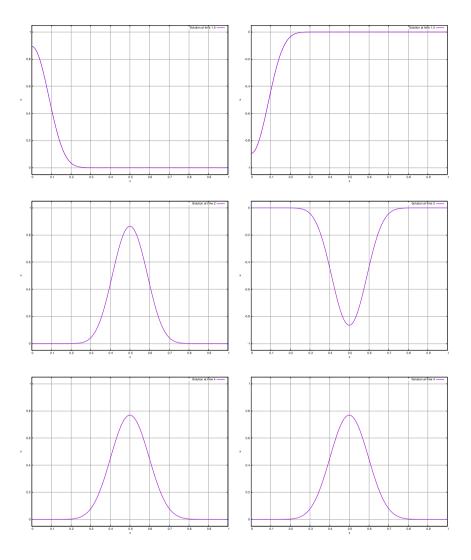


Figure 2.2. Numerical results: with 1000 cells on the left, 1001 cells on the right. From top to bottom: time 1.5, 2, 4.

 $u^{0,o}$ (o for odd) on \mathbb{R} by :

$$u^{0,e}(x) = \begin{cases} 0, & x \in [-1,0), \\ u^{0}(x), & x \in [0,1), \end{cases} \quad u^{0,o}(x) = \begin{cases} -u^{0}(x+2), & x \in [-2,-1), \\ 0, & x \in [-1,0), \\ u^{0}(x), & x \in [0,1), \\ 0, & x \in [1,2) \end{cases}$$
(2.4)

and we require $u^{0,e}$ to be 2-periodic and $u^{0,o}$ to be 4-periodic. Let u^* be the unique (a fortiori 2- or 4-periodical) solution to the transport problem on the full real line:

$$\begin{cases} \partial_t u + a \partial_x u = 0, \quad t \in \mathbb{R}_+, \quad x \in \mathbb{R} \\ u(0, x) = u^{0,*}(x) \end{cases}$$
(2.5)

with $u^{0,*} = u^{0,e}$ or $u^{0,o}$. Also define $e_j^{*,n} = u_j^n - u^*(t^n, x_j)$ for $j \in \{1, \ldots J\}$, $n \in \mathbb{N}$ (defining $t^n = n\Delta t$). Finally, for $u = (u_j)_{j=1}^J$, write

$$|u|_2 = \left(\sum_{j=1}^J \Delta x \ u_j^2\right)^{1/2}$$

for the discrete $l^2(0,1)$ norm. Although it depends on J, we drop this dependence in the notation.

THEOREM 2.1. — Assume $u^0 \in C_c^2(0,1)$ and $u^0(x_1) = u^0(x_J) = 0$. Then, there exists a constant C such that, for any Courant number c and any parameter $\theta \ge 1/2$, for all N > 0, one has for Δx small enough,

$$\sup_{n \leq N} (|e^n|_2) \leq C(1 + N\Delta t)(\Delta t + \Delta x^{1/2}).$$

Remark. — As u^0 is assumed to have compact support the condition $u^0(x_1) = u^0(x_J)$ is satisfied whenever Δx is sufficiently small.

The idea of the proof is:

- First, we create a numerical (discrete) initial condition \widetilde{U}^0 defined on $\{-J+1,\ldots,J\}$ if J is even and on $\{-2J+1,\ldots,2J\}$ if J is odd, in such a manner that the numerical solution U^n is equal to the restriction on $\{1,\ldots,J\}$ of the numerical solution (\widetilde{U}^n) given by the scheme with periodical boundary condition,
- Second, we prove that the numerical solution with periodical boundary conditions converges (towards the restriction of u^* on a period, (-1, 1) or (-2, 2)). This part of the proof is classical and is a straight-forward application of the Lax–Richtmyer theorem: the scheme with these conditions will be shown to be stable and consistent.

3. Proof of Theorem 2.1

3.1. Step 1: construction of a numerical (discrete) initial condition on a larger interval

Ideally, we would like to analyze the scheme on the whole line \mathbb{R} , i.e. \mathbb{Z} on the numerical level, by means of stability and consistency. We may indeed define an initial condition on \mathbb{Z} such that the restriction to $\{1, \ldots, J\}$ of the numerical solution over \mathbb{Z} equals the solution of the scheme on $\{1, \ldots, J\}$ with the homogeneous Neumann boundary conditions. When looking at the numerical results, however, such a reconstructed initial condition on \mathbb{Z} must be 2- or 4- periodic (or almost periodic). In particular, it will not belong to $l^2(\mathbb{Z})$, preventing us from doing a convergence analysis in $l^2(\mathbb{Z})$. Thus, we will slightly modify this program, and instead construct an initial condition on $\{-J+1,\ldots,J\}$ for J even and on $\{-2J+1,\ldots,2J\}$ for J odd and consider the scheme on these sets with *periodic boundary conditions*. The restriction to $\{1,\ldots,J\}$ yields the wanted solution and the convergence analysis is easy in the periodic context.

We denote by R the reconstruction operator. In the case where J is even, it is an operator $R : \mathbb{R}^J \to \mathbb{R}^{2J}$, and if J is odd, it is of the form $R : \mathbb{R}^J \to \mathbb{R}^{4J}$.

DEFINITION 3.1. — The operator R is defined as follows. Given $U = (U_1, \ldots, U_J) \in \mathbb{R}^J$: When J is even, $u = (u_{-J+1}, \ldots, u_J) = RU \in \mathbb{R}^{2J}$ is the unique vector such that

(a)
$$u_j = U_j$$
 for $j \in \{1, \dots, J\}$,
(b) $u_{-j+1} - u_{-j} = (-1)^{j+1} (u_{j+1} - u_j)$ for $j \in \{0, \dots, J-1\}$.

When J is odd, $u = (u_{-3J+1}, \ldots, u_J) = RU \in \mathbb{R}^{4J}$ is the unique vector such that (a) and (b) hold, and also:

(c) $u_{-J-j+1} - u_{-J-j} = (-1)^{j+1} (u_{-J+j+1} - u_{-J+j})$ for $j \in \{0, \ldots, J-1\}$, (d) $u_{-2J-j+1} - u_{-2J-j} = (-1)^{j+1} (u_{-2J+j+1} - u_{-2J+j})$ for $j \in \{0, \ldots, J-1\}$.

Remark 3.2. — Note that the above defines u by recursion, e.g. with j = 0 in (b) one gets $u_1 - u_0 = (-1)(u_1 - u_0)$ or, equivalently, $u_0 = u_1$ which precisely corresponds to the homogeneous Neumann condition. Then for j = 1 we get $u_0 - u_{-1} = (+1)(u_2 - u_1)$ from which $u_{-1} = -u_2 + u_0 + u_1 = -u_2 + 2u_1$, etc. In the odd case, also note that (c) and (d) for j = 0 imply: $u_{-J} = u_{-J+1}$ and $u_{-2J} = u_{-2J+1}$.

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The utility of the reconstruction operator will become apparent from the proposition below. In order to simplify notation and unify our expressions for J odd and even, let us introduce a vector $\hat{\alpha}(u)$ which for J odd will just be the zero vector in \mathbb{R}^{4J} but for J even and $u = RU \in \mathbb{R}^{2J}$ is given by:

$$\widehat{\alpha}(u) = \begin{pmatrix} \alpha(u) \\ 0 \\ \vdots \\ 0 \\ \alpha(u) \end{pmatrix} \in \mathbb{R}^{2J}, \text{ with } \alpha(u) = \frac{c}{2}(u_{-J+1} - u_J).$$
(3.1)

PROPOSITION 3.3. — We have

$$\begin{cases} AV + BU = 0, \\ v = RV, \end{cases} \quad if and only if \quad \begin{cases} u = RU, \\ Pv + Qu = \widehat{\alpha}(u) \end{cases}$$

Here,

$$P = I + \frac{\theta c}{2}T$$
 and $Q = -I + \frac{(1-\theta)c}{2}T$,

with T being the (periodic) difference matrix from (2.2). For the sizes of vectors and matrices: If J is even, $u, v \in \mathbb{R}^{2J}$ and $P, Q \in \mathcal{M}_{2J}(\mathbb{R})$, while if J is odd, $u, v \in \mathbb{R}^{4J}$ and $P, Q \in \mathcal{M}_{4J}(\mathbb{R})$.

The above property expresses the fact that if we reconstruct the initial condition and work with the periodical scheme then U^{n+1} solution of (2.1) will be the restriction to $\{1, \ldots, J\}$ of u^{n+1} , being a solution of

$$Pu^{n+1} + Qu^n = \widehat{\alpha}(u^0). \tag{3.2}$$

The interest is that the convergence of this extended scheme is easy to obtain by the usual consistency and stability analysis. The second hand term above will be shown to be small if the initial data is twice continuously differentiable, and equal to 0 if e.g. it is symmetric with respect to x = 1/2.

The proof of Proposition 3.3 will make use of the following lemma:

LEMMA 3.4. — For J odd, and denoting u = RU, we have for $j \in \{0, \ldots, J-1\}$:

(i)
$$u_{-2J+j+1} - u_{-2J+j} = -(u_{j+1} - u_j),$$

(ii) $u_{-2J+j+1} - u_{-2J+j} = -(u_{j+1} - u_j),$

- (ii) $u_{-3J+j+1} u_{-3J+j} = -(u_{-J+j+1} u_{-J+j})$
- (iii) $u_{-2J+j} u_{-J+1} = u_J u_j$.

and also for $j \in \{1, ..., J - 1\}$:

(iv)
$$u_{-3J+j+1} - u_{-3J+j} = (-1)^{j+1} (u_{J-j+1} - u_{J-j}),$$

Proof. — The identities come from combining in different ways (a)–(d) from Definition 3.1. To see (i) we use (b) and substitute J - j for j in (c) to obtain:

$$u_{j+1} - u_j = (-1)^{j+1} (u_{-j+1} - u_{-j}) = (-1)^{j+1} (-1)^{J-j+1} (u_{-2J+j+1} - u_{-2J+j}) = -(u_{-2J+j+1} - u_{-2J+j}).$$

Similarly, combining (c) and (d) we get (ii) and (iii) comes from (i) by summing from j to J-1. Finally (iv) results from (b), (c) and (d) together. \Box

Proof of Proposition 3.3: Consider first the case when J is even. Given $U \in \mathbb{R}^J$, u = RU, V is obtained from U by AV + BU = 0, and v is obtained from u using $Pv + Qu = (\alpha(u), 0, \dots, 0, \alpha(u))^t$. We denote by w = RV the reconstruction from V and will show that w = v. We begin by proving that for any $j \in \{-J + 1, \dots, J\}$ we have

$$w_j - u_j + \frac{\theta c}{2} \left(w_{j+1} - w_{j-1} \right) + \frac{(1-\theta)c}{2} \left(u_{j+1} - u_{j-1} \right) = 0, \qquad (3.3)$$

provided we define $u_{-J} = u_{-J+1}$, $u_{J+1} = u_J$ and $w_{-J} = w_{-J+1}$, $w_{J+1} = w_J$. We already know the result for $j \in \{1, \ldots, J\}$ (since R is the identity operator for that range of indices) and we proceed by induction.

• We have:

$$w_{0} = w_{1} = u_{1} - \frac{\theta c}{2} (w_{2} - w_{1}) - \frac{(1 - \theta)c}{2} (u_{2} - u_{1})$$

= $u_{1} - \frac{\theta c}{2} (w_{0} - w_{-1}) - \frac{(1 - \theta)c}{2} (u_{0} - u_{-1})$
= $u_{0} - \frac{\theta c}{2} (w_{1} - w_{-1}) - \frac{(1 - \theta c)}{2} (u_{1} - u_{-1})$

which proves (3.3) for j = 0.

• We assume the result is proved for $j \in \{-k + 1, ..., J\}$ (for $k \in \{1, ..., J - 1\}$). We have

$$w_{-k} = w_{-k+1} + (-1)^{k+1} (w_k - w_{k+1})$$

= $u_{-k+1} - \frac{\theta c}{2} (w_{-k+2} - w_{-k}) - \frac{(1-\theta)c}{2} (u_{-k+2} - u_{-k})$
+ $(-1)^{k+1} (w_k - w_{k+1})$
= $u_{-k+1} - \frac{\theta c}{2} (-1)^k (w_k - w_{k-1} - (w_{k+1} - w_k))$
 $- \frac{(1-\theta)c}{2} (-1)^k (u_k - u_{k-1} - (u_{k+1} - u_k)) + (-1)^{k+1} (w_k - w_{k+1})$

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$$= u_{-k+1} - \frac{\theta c}{2} (-1)^{k+1} (w_{k+1} - 2w_k + w_{k-1}) - \frac{(1-\theta)c}{2} (-1)^{k+1} (u_{k+1} - 2u_k + u_{k-1}) + (-1)^{k+1} (w_k - w_{k+1})$$

Therefore, we deduce

$$\begin{split} w_{-k} &+ \frac{\theta c}{2} \left(w_{-k+1} - w_{-k-1} \right) + \frac{(1-\theta)c}{2} \left(u_{-k+1} - u_{-k-1} \right) \\ &= u_{-k+1} - \frac{\theta c}{2} (-1)^{k+1} \left((w_{k-1} - w_k) - (w_{k+1} - w_{k+2}) \right) \\ &- \frac{(1-\theta c)}{2} (-1)^{k+1} \left((u_{k-1} - u_k) - (u_{k+1} - u_{k+2}) \right) + (-1)^{k+1} \left(w_k - w_{k+1} \right) \\ &= u_{-k+1} + (-1)^{k+1} \left[\left(w_k + \frac{\theta c}{2} \left(w_{k+1} - w_{k-1} \right) + \frac{(1-\theta)c}{2} \left(u_{k+1} - u_{k-1} \right) \right) \\ &- \left(w_{k+1} + \frac{\theta c}{2} \left(w_{k+2} - w_k \right) + \frac{(1-\theta)c}{2} \left(u_{k+2} - u_k \right) \right) \right] \\ &= u_{-k+1} + (-1)^{k+1} \left(u_k - u_{k+1} \right) = u_{-k+1} - (u_{-k+1} - u_{-k}) = u_{-k}, \end{split}$$

which means that Formula (3.3) is true for j = -k. Formula (3.3) is proved for $j \in \{-J + 1, ..., J\}$.

Using the matrices ${\cal P}$ and ${\cal Q}$ defined in the statement, this can be expressed in the form

$$Pw = -Qu + \frac{\theta c}{2} \begin{pmatrix} w_{-J+1} - w_J \\ 0 \\ \vdots \\ 0 \\ w_{-J+1} - w_J \end{pmatrix} + \frac{(1-\theta)c}{2} \begin{pmatrix} u_{-J+1} - u_J \\ 0 \\ \vdots \\ 0 \\ u_{-J+1} - u_J \end{pmatrix},$$

which makes $\alpha(u)$ and $\alpha(w)$ appear. Proceeding in the same way in the odd case (we omit the details), we obtain:

$$Pw = -Qu + \frac{\theta c}{2} \begin{pmatrix} w_{-3J+1} - w_J \\ 0 \\ \vdots \\ 0 \\ w_{-3J+1} - w_J \end{pmatrix} + \frac{(1-\theta)c}{2} \begin{pmatrix} u_{-3J+1} - u_J \\ 0 \\ \vdots \\ 0 \\ u_{-3J+1} - u_J \end{pmatrix}.$$

Let us now compare $\alpha(w)$ and $\alpha(u)$.

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• If J is even:

$$w_{-J+1} = u_{-J+1} - \frac{\theta c}{2} (w_{-J+2} - w_{-J+1}) - \frac{(1-\theta)c}{2} (u_{-J+2} - u_{-J+1})$$

= $u_{-J+1} - \frac{\theta c}{2} (-1)^J (w_J - w_{J-1}) - \frac{(1-\theta)c}{2} (-1)^J (u_J - u_{J-1})$
= $u_{-J+1} - \frac{\theta c}{2} (w_J - w_{J-1}) - \frac{(1-\theta)c}{2} (u_J - u_{J-1})$
= $u_{-J+1} + w_J - u_J.$

• If J is odd:

$$\begin{split} w_{-3J+1} &= u_{-3J+1} - \frac{\theta c}{2} (w_{-3J+2} - w_{-3J+1}) - \frac{(1-\theta)c}{2} (u_{-3J+2} - u_{-3J+1}) \\ &= u_{-3J+1} - \frac{\theta c}{2} (-1)^J (-1)^J (w_{-2J+J} - w_{-2J+J-1}) \\ &- \frac{(1-\theta)c}{2} (-1)^J (-1)^J (u_{-2J+J} - u_{-2J+J-1}) \\ &= u_{-3J+1} - \frac{\theta c}{2} (-1)^J (-1)^2 (w_{-J+2} - w_{-J+1}) \\ &- \frac{(1-\theta)c}{2} (-1)^J (-1)^2 (u_{-J+2} - u_{-J+1}) \\ &= u_{-3J+1} - \frac{\theta c}{2} (-1)^J (-1)^J (w_J - w_{J-1}) \\ &- \frac{(1-\theta)c}{2} (-1)^J (-1)^J (u_J - u_{J-1}) \\ &= u_{-3J+1} + w_J - u_J \end{split}$$

Thus, whatever the parity of J, $\alpha(w) = \alpha(u)$. From Lemma 3.4 and the linearity of the reconstruction operator, we have

$$u_{-3J+j} = u_{-J+1} + u_J - u_{-J+j}$$

for any $j \in \{1, \ldots, J\}$. Thus, taking j = 1, we obtain

$$u_{-3J+1} = u_{-J+1} + u_J - u_{-J+1} = u_J,$$

which proves that $\alpha(u) = 0$ when J is odd. Thus, in any case w satisfies

$$Pw = -Qu + \widehat{\alpha}(u).$$

As the matrix P is invertible, this proves that w = v.

A consequence of the above proposition is that solving Problem (2.1) (with Neumann conditions) is equivalent to solving the problem

$$Pu^{n+1} = -Qu^n + \widehat{\alpha}(u^0)$$

when starting out with $u^0 = RU^0$ being the reconstructed vector for the initial data. The equation is in \mathbb{R}^{2J} if J is even, and in \mathbb{R}^{4J} if J is odd. Note

that the source term is $\hat{\alpha}(u^0)$ (i.e. time-independent) which is a consequence of the fact that $\alpha(u) = \alpha(w)$ in the proposition.

3.2. Step 2 : convergence of the discrete initial condition in l^{∞}

In this section, we will prove that the discrete reconstruction $u^0 = RU^0$ converges (in l^{∞}) towards the function $u^{0,*}$ which is equal to $u^{0,e}$ if J is even, and to $u^{0,o}$ if J is odd. More precisely, we will prove

PROPOSITION 3.5. — Let $u^0 \in C_c^2(0,1)$, let $U_j^0 = u^0(x_j)$ for j = 1, ..., J, $(u_j)_{j \in \mathbb{Z}} = RU^0$ and define $e_j^0 = u_j^0 - u^{0,*}(x_j)$. There exists a constant C (depending on the initial data u^0) such that

$$|e_i^0| \leq C\Delta x$$

for any $j \in \{-J+1,...,J\}$ if J is even, and $j \in \{-3J+1,...,J\}$ if J is odd.

Proof. — When J is even:

$$\begin{cases} e_j^0 = u_j^0 & \text{for } j \in \{-J+1, \dots, 0\} \\ e_j^0 = 0 & \text{for } j \in \{1, \dots, J\}, \end{cases}$$

and if J is odd:

$$\begin{cases} e_j^0 = u_j^0 & \text{for } j \in \{-3J + 1, \dots, -2J\} \\ e_j^0 = u_j^0 + u_0(x_j + 2) & \text{for } j \in \{-2J + 1, \dots, -J\} \\ e_j^0 = u_j^0 & \text{for } j \in \{-J + 1, \dots, 0\} \\ e_j^0 = 0 & \text{for } j \in \{1, \dots, J\}. \end{cases}$$

Thanks to Lemma 3.4, if J is odd,

$$\begin{cases} e_j^0 = u_j^0 & \text{for } j \in \{-3J+1, \dots, -2J\} \\ e_j^0 = u_{-J+1} + u_J - u_{J+2J} + u_0(x_j+2) & \text{for } j \in \{-2J+1, \dots, -J\} \\ e_j^0 = u_j^0 & \text{for } j \in \{-J+1, \dots, 0\} \\ e_j^0 = 0 & \text{for } j \in \{1, \dots, J\}. \end{cases}$$

• For $j \in \{1, \ldots, J\}$, the result is trivial.

• For
$$j \in \{-J+1, ..., 0\}$$
, we have $j = -J+k$ with $k \in \{1, ..., J\}$ and

$$\begin{split} u^0_{-J+k} &= u^0_{-J+k+1} - (-1)^{J-k+1} (u^0_{J-k+1} - u^0_{J-k}) \\ &= u^0_{-J+k+2} - (-1)^{J-k} (u^0_{J-k} - u^0_{J-k-1}) - (-1)^{J-k+1} (u^0_{J-k+1} - u^0_{J-k}) \\ &= u^0_{-J+k+2} + (-1)^{J-k} (u^0_{J-k+1} - 2u^0_{J-k} + u^0_{J-k-1}), \\ & \text{thus } |u^0_{-J+k}| \leqslant |u^0_{-J+k+2}| + C\Delta x^2 \text{ if } u^0 \text{ is twice continuously differentiable. By induction, } |u^0_j| \leqslant + C\Delta x, \text{ since } u^0_1 = 0. \end{split}$$

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• For $j \in \{-2J+1, \ldots, -J\}$ (if J is odd), we have j = -2J + k with $k \in \{1, \ldots, J\}$ and, from Lemma 3.4,

$$u_{-2J+k}^{0} = u_{-J+1}^{0} + u_{J}^{0} - u_{k}^{0} = u_{-J+1}^{0} - u_{k}^{0}$$

since $u_J^0 = 0$. Thus, as $|u_{-J+1}^0| \leq C\Delta x$, $|e_j^0| \leq C\Delta x$.

• For $j \in \{-3J + 1, \dots, -2J\}$, we can repeat the arguments in the second item above.

The result is proved.

3.3. Step 3 : convergence of e^n in $l^{\infty}(0, T, l^2)$

In this section we show the convergence of e^n towards 0 in l^{∞} in time and l^2 in space, i.e. Theorem 2.1.

LEMMA 3.6 (stability of the scheme). — Scheme 3.2 is stable in a strong sense, i.e. one has

$$|P^{-1}Q|_2 \leqslant 1$$

if and only if $\theta \leq 1/2$.

The lemma expresses the fact that the amplification matrix of the scheme is of l^2 norm less than 1 (without any condition on Δt).

Proof. — Recall that $P = I + \frac{\theta_C}{2}T$, $Q = -I + \frac{(1-\theta)_C}{2}T$ with T being the (antisymmetric) matrix from (2.2). Thus, P and Q are normal and commuting so $P^{-1}Q$ is also normal and $|||P^{-1}Q|||_{l^2} = \sqrt{\rho((P^{-1}Q)(P^{-1}Q)^*)} = \rho(P^{-1}Q)$.

Also, P and Q are simultaneously diagonalizable. The eigenvalues for T (being antisymmetric), τ_j (for $j \in \{1, \ldots, 2J\}$ if J is even, and $j \in \{1, \ldots, 4J\}$ if J is odd) are therefore purely imaginary and the eigenvalues of $P^{-1}Q$ will be given by $\left(-1 + \frac{(1-\theta)c}{2}\tau_j\right)/\left(1 + \frac{\theta c}{2}\tau_j\right)$. It follows that $(\rho(P^{-1}Q))^2 = \sup_j \left(1 + \frac{(1-\theta)^2\tau_j^2c^2}{4}\right)/\left(1 + \frac{\theta^2\tau_j^2c^2}{4}\right) \leqslant 1$ if and only if $\theta \geqslant \frac{1}{2}$. This ends the proof.

We write the evolution formula for the error: $Pe^{n+1} = -Qe^n + \hat{\alpha}(u^0) + \Delta t\epsilon_n$ with ϵ_n being the consistency error of Scheme (3.2). We may rewrite this as follows:

$$e^{n+1} = -P^{-1}Qe^n + P^{-1}\widehat{\alpha}(u^0) + \Delta t P^{-1}\epsilon_n$$

= $(-P^{-1}Q)^{n+1}e^0$
+ $\Delta t \sum_{k=0}^n (-P^{-1}Q)^{n-k}P^{-1}\epsilon_k + \sum_{k=0}^n (-P^{-1}Q)^{n-k}P^{-1}\widehat{\alpha}(u^0)$

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Thus

$$|e^{n}|_{2} = |(P^{-1}Q)^{n}e^{0}|_{2} + \sum_{k=0}^{n-1} |(P^{-1}Q)^{n-1-k}P^{-1}\widehat{\alpha}(u^{0})|_{2}$$
$$+ \Delta t \sum_{k=0}^{n-1} |(P^{-1}Q)^{n-1-k}P^{-1}\epsilon_{k}|_{2}$$
$$\leqslant |e^{0}|_{2} + \sum_{k=0}^{n-1} |\widehat{\alpha}(u^{0})|_{2} + \Delta t \sum_{k=0}^{n-1} |\epsilon_{k}|_{2}$$

thanks to Lemma (3.6), and, finally,

 $|e^{n}|_{2} \leq |e^{0}|_{2} + n\sqrt{2}|\alpha(u^{0})|\Delta x^{\frac{1}{2}} + n\Delta t||\epsilon||_{\infty}.$

We already know that $|e^0|_2 \leq |e^0|_{\infty} \xrightarrow{\Delta x \to 0} 0$, thus it remains to show that $n|\alpha(u^0)|\Delta x^{\frac{1}{2}}$ and $\|\epsilon\|_{\infty}$ converge towards 0.

We here prove an estimate that is actually finer as in the theorem. We know that the solution of (2.5) is $u^*(t,x) = u^{0,*}(x - ct)$. So, thanks to the assumption $u^0 \in \mathcal{C}^2_c(0,1)$, $u^{0,*}$ and u^* are of class $\mathcal{C}^2(\mathbb{R})$ too, and we have the following consistency estimate :

$$\|\epsilon_{n}\|_{\infty} = \left\|\frac{u^{*}(x_{i}, t_{n+1}) - u^{*}(x_{i}, t_{n})}{\Delta t} + \theta c \frac{u^{*}(x_{i+1}, t_{n+1}) - u^{*}(x_{i-1}, t_{n+1})}{2\Delta x} + (1 - \theta) c \frac{u^{*}(x_{i+1}, t_{n}) - u^{*}(x_{i-1}, t_{n})}{2\Delta x}\right\|_{\infty} \leq C \|u_{0}^{'''}\|_{\infty} (\Delta t + \Delta x).$$
(3.4)

Moreover, if we assume $u^0 \in \mathcal{C}^3_c(0,1)$, $u^{0,*}$ and u^* are of class $\mathcal{C}^3(\mathbb{R})$ too, and we have the following more precise consistency estimate :

$$\|\epsilon_{n}\|_{\infty} = \left\|\frac{u^{*}(x_{i}, t_{n+1}) - u^{*}(x_{i}, t_{n})}{\Delta t} + \theta c \frac{u^{*}(x_{i+1}, t_{n+1}) - u^{*}(x_{i-1}, t_{n+1})}{2\Delta x} + (1 - \theta) c \frac{u^{*}(x_{i+1}, t_{n}) - u^{*}(x_{i-1}, t_{n})}{2\Delta x}\right\|_{\infty}$$
$$\leqslant C \|u_{0}^{'''}\|_{\infty} (|1 - 2\theta|\Delta t + \Delta t^{2} + \Delta x^{2}). \tag{3.5}$$

In the case where J is odd, we have seen that $\alpha(u^0) = 0$, thus the result is proved. In the case where J is even we have to bound this quantity. By definition, $\alpha(u^0) = c/2(u^0_{-J+1} - u^0_J) = cu^0_{-J+1}/2$ as $u^0_J = 0$, and we have already seen that due to the assumption on the regularity of u^0 , $u^0_{-J+1} \leq C\Delta x$.

Finally, we have the following inequality, valid whatever the parity of J: $|e^n|_2 \leq C\Delta x + Cn\Delta t(\Delta t + \Delta x + ((J+1) \mod 2)\Delta x^{1/2}),$ or even, in the case where $u_0 \in \mathcal{C}^3_c(0,1)$,

$$|e^n|_2 \leq C\Delta x + Cn\Delta t(|1 - 2\theta|\Delta t + \Delta t^2 + \Delta x^2 + ((J+1) \mod 2)\Delta x^{1/2}).$$

This proves the theorem

nis proves the theorem.

4. Dirichlet boundary condition

In this section, we take $J \in \mathbb{N}^*$, let $\Delta x = 1/(J+1)$ and define the nodes of the grid $y_i = j\Delta x$, and we consider the following θ -scheme, that corresponds formally with imposing homogeneous boundary conditions on both sides:

$$\begin{cases} \frac{U_{j}^{n+1} - U_{j}^{n}}{\Delta t} + a\theta \frac{U_{j+1}^{n+1} - U_{j-1}^{n+1}}{2\Delta x} + a(1-\theta) \frac{U_{j+1}^{n} - U_{j-1}^{n}}{2\Delta x} = 0, & n \ge 0, \\ \frac{U_{1}^{n+1} - U_{1}^{n}}{\Delta t} + a\theta \frac{U_{2}^{n+1}}{2\Delta x} + a(1-\theta) \frac{U_{2}^{n}}{2\Delta x} = 0, & n \ge 0, \\ \frac{U_{j}^{n+1} - U_{j}^{n}}{\Delta t} - a\theta \frac{U_{j-1}^{n+1}}{2\Delta x} - a(1-\theta) \frac{U_{j-1}^{n+1}}{2\Delta x} = 0, & n \ge 0, \\ U_{j}^{0} = U^{0}(y_{j}), & j \in \{1, \dots, J\}. \end{cases}$$
(4.1)

Second and third equations above can also be obtained by defining the boundary (fictive) values $U_0^n = U_{J+1}^n = 0$, which is consistent with the homogeneous Dirichlet conditions.

Setting $U^n = (U_j^n)_{j=1}^J$, this system also takes the following matrix form:

$$\overline{A}U^{n+1} + \overline{B}U^n = 0,$$

with $\overline{A} = I + \frac{\theta c}{2}\overline{D}, \ \overline{B} = I + \frac{(1-\theta)c}{2}\overline{D}$ and $\overline{D} = \begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & 0 \\ -1 & 0 & 1 & & & \vdots \\ 0 & -1 & 0 & 1 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & 0 & 1 & 0 \\ \vdots & & & -1 & 0 & 1 \\ 0 & \cdots & \cdots & 0 & -1 & 0 \end{pmatrix} \in \mathcal{M}_J(\mathbb{R}).$

With these "boundary conditions", we also observe a strange numerical behavior with a periodical in time phenomenon, but with very oscillating intermediate solutions: see Figures 5.3 and 5.4. We can prove a similar theorem. We use the same notations as in Section 2 for $u^{0,e}$, $u^{0,o}$, u^e and u^o and we define

$$f_j^n = \begin{cases} U_j^n - u^o(t^n, y_j) & \text{if J is even,} \\ U_j^n - u^e(t^n, y_j) & \text{if J is odd,} \end{cases} \quad \forall j \in \{0, \dots, J+1\},$$

where it is understood that $U_0^n = 0$, and

$$\widetilde{f}_J(t,x) = \sum_{j=0}^J \sum_{n=0}^{+\infty} f_j^n \chi_{[j\Delta x, (j+1)\Delta x)}(x) \chi_{[n\Delta t, (n+1)\Delta t)}(t).$$

THEOREM 4.1. — Assume $u^0 \in C_c^2(0,1)$. Then, for any Courant number c and any parameter $\theta \ge 1/2$, we have

- (case where J is even) for any $g \in L^2(-1,1)$, $\lim_{\Delta x \to 0} \| \langle u_{2K} - u^o, g \rangle_{L^2(-1,1)} \|_{L^{\infty}(0,T)} = 0;$
- (case where J is odd) for any $g \in L^2(-2,2)$,

$$\lim_{\Delta x \to 0} \| \langle u_{2K+1} - u^e, g \rangle_{L^2(-2,2)} \|_{L^{\infty}(0,T)} = 0.$$

Here it is understood that, as in the whole paper, $\Delta t = c\Delta x/a$, thus Δt tends to 0 at the same velocity as Δx .

Observe that the (here weak) limits are not the same as in the Neumann case: the convergence is towards u^o as J is even and towards u^e when J is odd.

As it is very similar to the proof of the result in the Neumann case, we do not reproduce it here (actually it is even simpler because there is no source term $\alpha(u^0)$). We only give the reconstruction operator that has to be used here.

DEFINITION 4.2. — The operator \overline{R} is defined in the following way. If J is odd, $u = (u_{-(J+1)}, \ldots, u_J) = \overline{R}U \in \mathbb{R}^{2(J+1)}$ is the unique vector such that

•
$$u_0 = 0, u_{-(J+1)} = 0,$$

• $u_j = U_j, \ u_{-j} = (-1)^j U_j \text{ for } j \in \{1, \dots, J\}.$

If J is even, $u = (u_{-3(J+1)}, \dots, u_J) = \overline{R}U \in \mathbb{R}^{4(J+1)}$, is the unique vector such that

- $u_0 = 0, u_{-(J+1)} = 0, u_{-2(J+1)} = 0, u_{-3(J+1)} = 0.$
- $u_j = U_j, \ u_{-j} = (-1)^j U_j, \ u_{-(J+1)-j} = (-1)^j u_{-(J+1)+j}, \ u_{-2(J+1)-j} = (-1)^j u_{-2(J+1)+j}$ for $j \in \{1, \dots, J\}$.

Given $u = \overline{R}U$, we define the associated piecewise affine function $u_{\Delta x}$ in the way we defined $f_{\Delta x}$, but here on [-3, 1] if J is even, and on [-1, 1] if Jis odd. Remark that if the initial data is smooth in (0, 1), the reconstructed initial function $u_{\Delta x}^0$ is oscillating with large amplitude around 0 in (-1, 0), and also in (-3, -2) is J if even. More precisely, it is easy to prove that the restriction of $u_{\delta x}^0$ to (-1, 0) converges weakly to 0 on this interval, and the same for the restriction of $u_{\delta x}^0$ to (-3, -2) if J is even. This explains that the convergence is only weak. The rest of the proof follows the line of the preceding analysis (multiplying the error function $f_{\Delta x}$ by an arbitrary function in L^2).

5. Numerical results

In all this section, devoted to a more precise observation of numerical results, the chosen initial condition remains

$$u_0(x) = \begin{cases} \frac{1}{\exp(-9)} \exp\left(\frac{1}{(x-1/2)^2 - \frac{1}{9}}\right) & \text{if } \frac{1}{6} < x < \frac{5}{6};\\ 0 & \text{otherwise,} \end{cases}$$

and we take a = 1 and J = 1000 or J = 1001. All the simulations are done with a Courant number c = 1/2. The numerical results obtained with the implicit scheme ($\theta = 1$) and Neumann conditions has been exposed in Section 1. Here, we zoom in on the numerical solution at time 1, to see the small oscillations around 0.

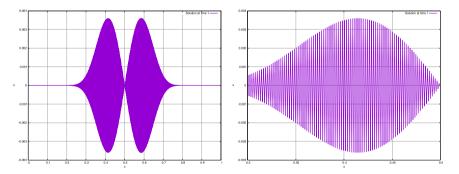


Figure 5.1. Zoom on the solution at time 1 for J = 1000 (see the y and x scales).

These small perturbations, which amplitude are of order Δx and that are strongly related to the small oscillations of the *reconstructed* initial data in the proof of the convergence theorem (with the operator R of Definition 3.1; the fact that the oscillations have an amplitude of order Δx is guaranteed by the result of Proposition 3.5), are moving to the left with velocity -a. Actually, this fact is easy to understand, because if $(U_j^n)_{j,n}$ denotes the numerical solution to the implicit centered scheme and is "smooth", then, posing $V_j^n = (-1)^j U_j^n$ gives

$$\frac{V_j^{n+1} - V_j^n}{\Delta t} - a \frac{V_{j+1}^{n+1} - V_{j-1}^{n+1}}{2\Delta x} = 0,$$

what means that V has velocity -a. This of course remains true for any $\theta \in$ [1/2, 1]. The scheme has a group velocity -a and allow perturbations from the right boundary to go to the left, and when they arrive at position x = 0. they interact with the left boundary in a "constructive" manner. See [11] for a study of the links between instability and group velocities. Remark that, as in the continuous problem (1.1), the *inflow* boundary condition is responsible for this kind of instability phenomenon (namely, starting from the solution at time 1 that has a small l^{∞} norm, we recover in finite time a solution with an l^{∞} norm that is typically 1). This lack of stability is the reason why the ghost phenomenon occurs, and is also the reason why a classical numerical analysis in terms of consistency and stability has not been performed directly on the scheme (but has been used only after the reconstruction procedure) to prove the convergence. The fact that the homogeneous Neumann *inflow* boundary condition (and not the *outflow* one) is responsible for the phenomenon is proved by the convergence results in the case of a Dirichlet inflow boundary condition and an extrapolation (of any order) on the outflow boundary: see [5] (and also [8] for the stability theory) and [3].

Similar results are observed with $\theta = 1/2$. However, we note that while diffusion was quite important with the first scheme, it essentially disappears with the Crank–Nicolson scheme. We only show the result at time 100 and see that the amplitude remains almost constant, but the positivity is not preserved (what can be viewed as a consequence of the dispersive behavior of the scheme, that is to say that the Crank–Nicolson scheme is consistent, at the third order in Δt and Δx , with a dispersive equation (see [10] for an insight on these so-called modified equations)).

At last, we here propose some results obtained with the implicit scheme and Dirichlet boundary conditions, to illustrate Theorem 4.1. Remark that with these Dirichlet conditions, the oscillating perturbations created by the outflow boundary condition, that propagate with velocity -a, do not have a small amplitude (and notice that this is consistent with the reconstruction operator \overline{R} defined in Definition 4.2). This is responsible for the fact that the convergence is only weak in Theorem 4.1. Once the perturbation has reached

Ghost solutions with centered schemes

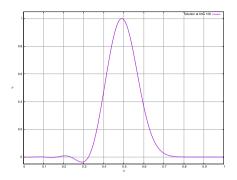


Figure 5.2. Solution with the Crank–Nicolson scheme $(\theta=1/2)$ at time 100 for J=1000

the inflow boundary, it also interacts with it, in a constructive manner, to recreate an approximation of the initial profile. At times 2 and 4, one recover approximations of u^0 or of $-u^0$. As for the Neumann conditions case, the amplitude has decreased, but if one refines the mesh one observes, as stated in the above theorems, the convergence.

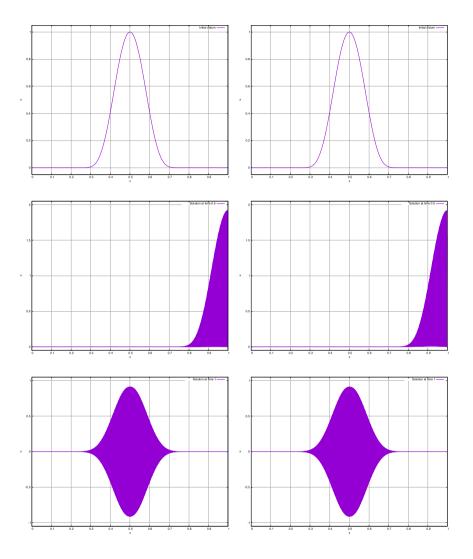


Figure 5.3. Numerical results: with 1000 cells on the left, 1001 cells on the right. From top to bottom: time 0, 0.5, 1.

Ghost solutions with centered schemes

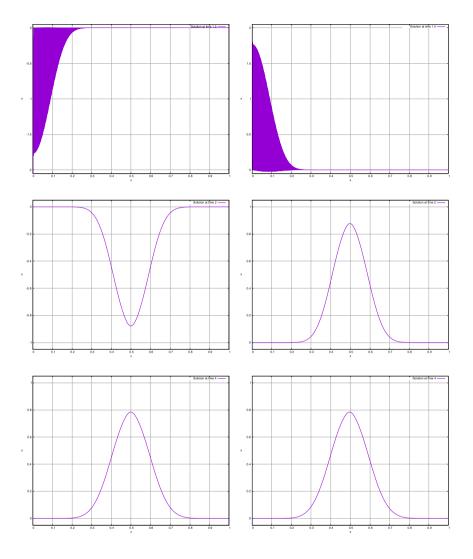


Figure 5.4. Numerical results: with 1000 cells on the left, 1001 cells on the right. From top to bottom: time 1.5, 2, 4.

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Bibliography

- X. ANTOINE, A. ARNOLD, C. BESSE, M. EHRHARDT & A. SCHÄDLE, "A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations", *Commun. Comput. Phys.* 4 (2008), no. 4, p. 729-796.
- [2] B. BOUTIN & J. F. COULOMBEL, "Stability of finite difference schemes for hyperbolic initial boundary value problems: Numerical boundary layers", Numer. Math., Theory Methods Appl. 10 (2017), no. 3, p. 489-519.
- [3] J.-F. COULOMBEL & F. LAGOUTIÈRE, "The Neumann numerical boundary condition for transport equations", https://hal.archives-ouvertes.fr/hal-01902551, 2018.
- [4] M. EHRHARDT, "Absorbing boundary conditions for hyperbolic systems", Numer. Math., Theory Methods Appl. 3 (2010), no. 3, p. 295-337.
- [5] B. GUSTAFSSON, "The convergence rate for difference approximations to mixed initial boundary value problems", *Math. Comput.* 29 (1975), p. 396-406.
- [6] —, "The convergence rate for difference approximations to general mixed initialboundary value problems", SIAM J. Numer. Anal. 18 (1981), no. 2, p. 179-190.
- [7] B. GUSTAFSSON, H.-O. KREISS & J. OLIGER, Time dependent problems and difference methods, Pure and Applied Mathematics, John Wiley & Sons, 1995, xii+642 pages.
- [8] B. GUSTAFSSON, H.-O. KREISS & A. SUNDSTRÖM, "Stability theory of difference approximations for mixed initial boundary value problems. II", *Math. Comput.* 26 (1972), p. 649-686.
- [9] H.-O. KREISS & E. LUNDQVIST, "On difference approximations with wrong boundary values", Math. Comput. 22 (1968), p. 1-12.
- [10] R. J. LEVEQUE, Finite difference methods for ordinary and partial differential equations. Steady-state and time-dependent problems, Society for Industrial and Applied Mathematics, 2007, xvi+341 pages.
- [11] L. N. TREFETHEN, "Instability of difference models for hyperbolic initial-boundary value problems", Commun. Pure Appl. Math. 37 (1984), no. 3, p. 329-367.