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Absorbing boundary conditions for nonlinear scalar partial differential equations

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Abstract

We present two strategies dealing with the design of absorbing boundary conditions for nonlinear scalar partial differential equations. The first one relies on the linearization of the equation and the second one relies on its parolinearization. We then introduce a finite volume scheme well-suited to our absorbing boundary conditions in the case of the semilinear wave equation. We finally present numerical experiments illustrating the efficiency of these methods in the case of semilinear wave equations and of nonlinear Schrödinger equations.

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1. Introduction

Many phenomena are modeled by partial differential equations on unbounded domains (stream in the ocean, temperature in the atmosphere, etc.). Though the problem is defined in the whole space, it is often sufficient to know the solution only on a bounded domain: the domain of interest. An artificial domain which includes this region of interest is then defined. Inside the domain the equations are discretized in the usual way but there remains the question of the choice of reliable boundary conditions on the artificial

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boundary. Thus the boundary conditions have to be well-posed and accurate to be able to approximate the restriction of the solution to the domain of interest.

In the case of linear constant coefficients equations, the transparent boundary condition (the boundary condition satisfied by the exact solution) can be explicitly computed when choosing special geometries for the computational domain (half-spaces, spheres or cylinders). This boundary condition is a nonlocal operator and can be approximated by local boundary conditions [13,6,22] or fast evaluated [10,1,11,14]. One can also replace the boundary condition by a reflectionless sponge layer damping propagating waves [3,8].

In the case of linear equations with variable coefficients, the previous methods fail since the transparent boundary condition cannot be explicitly computed. A strategy has been developed to design boundary conditions which minimizes the reflection of the solution at the artificial boundary. These absorbing boundary conditions have been constructed for hyperbolic problems [6] and parabolic problems [12] with success using geometrical optics. In the case of the wave equation, the method relies on the factorization of the operator in a product of two first order operators. One operator corresponds to the incident wave and the other to the reflected wave with respect to the boundary of the computational domain. As the boundary is artificial, the transparent boundary condition consists in annihilating the operator corresponding to the reflected wave. Finally, the transparent condition is not very manageable for numerical simulation and is approximated with absorbing boundary conditions, which are easy to implement.

For nonlinear problems, very little is known. To extend the strategy for linear variable coefficients equations to nonlinear equations, a first idea is to rewrite the nonlinearity as a potential multiplied by the unknown function. The nonlinear equation can then be reinterpreted as a linear equation with variable coefficients and we can apply the method in [6,12]. We obtained good results in the case of reaction–diffusion equations [16] using this strategy. In the case of nonlinear Schrödinger equations, we showed in [17] that the solution computed with this method is significantly different from the solution of the nonlinear problem set on \mathbb{R} .

This motivates the introduction of a second method. We rely on Bony’s parilinearization theorem [4]. This consists in decomposing a nonlinearity applied to a function as the sum of a linear operator applied to this function and a smooth remainder. Using this result, we first parilinearize the nonlinear equation and we obtain a linear equation satisfied by the unknown function. Then, we can apply the method in [6,12] to this linear equation. We obtained good results in the case of semilinear wave equations [19] and in the case of nonlinear Schrödinger equations [20] using this strategy.

In this study we investigate further these two strategies in the case of the semilinear wave equation and of nonlinear Schrödinger equations. The semilinear wave equation models in particular the dislocation in crystals and laser pulses in two state media, and nonlinear Schrödinger equations are reliable models for various phenomena in plasma physics, nonlinear optic and water wave theory (see for example [23]).

The present work consists in four parts:

- In Section 2, we present the two strategies sketched above dealing with the design of absorbing boundary conditions for nonlinear scalar partial differential equations. We then recall the zero and first order absorbing boundary conditions obtained for the semilinear wave equation [19] and for nonlinear Schrödinger equations [20].
- In Section 3, we present a finite volume discretization for the semilinear wave equation with general absorbing boundary conditions. This scheme is simpler to implement and more efficient than the finite difference scheme used in [19].
- In Section 4, we present a finite element scheme well-suited to nonlinear Schrödinger equations with general absorbing boundary conditions.
- In Section 5, we compute numerically the solution of semilinear wave equations and of nonlinear Schrödinger equations using a large class of absorbing boundary conditions. We show that our absorbing boundary conditions give optimal result within this large class illustrating the efficiency of our method.

Remark 1. The zero and first order absorbing boundary conditions presented in Section 2 have been obtained by the author in [19] and [20]. Thus, the novelty of this work compared to [19] and [20] consists in the finite volume scheme of Section 3 well-suited to our absorbing boundary conditions, and in the numerical computations of Section 5 investigating the optimality of our absorbing boundary conditions within a large class of boundary conditions. Furthermore, Section 2 has its own interest as it explains without technicalities and in a unified way the strategies introduced in [19] and [20].

2. Design of absorbing boundary conditions for nonlinear problems

2.1. The potential and the paraxial strategies

We first recall the strategy of Engquist and Majda [6] used to design absorbing boundary conditions for the wave equation with variable coefficients.

The simplest case is the constant coefficients wave equation set on \mathbb{R} . Take \mathbb{R}^- as the computational domain. The problem becomes: find a boundary condition satisfied at $x = 0$ by the solution u of the wave equation $(\partial_t^2 - \partial_x^2)u = 0$. The wave operator admits the following factorization:

$$\partial_t^2 - \partial_x^2 = -(\partial_x - \partial_t)(\partial_x + \partial_t). \tag{1}$$

Now, the solutions of $(\partial_x + \partial_t)u = 0$ correspond to incident waves with respect to the boundary $x = 0$ and the solution of $(\partial_x - \partial_t)u = 0$ correspond to reflected waves (see Fig. 1). As the boundary $x = 0$ is artificial, there should not be any reflected wave. Therefore, the transparent boundary condition is $(\partial_x + \partial_t)u = 0$ as it annihilates the reflected wave.

The strategy of Engquist and Majda is to extend the factorization (1) to wave equations with variable coefficients. If L denotes a wave operator with variable coefficients, it admits the following factorization:

$$L \approx -(\partial_x - a)(\partial_x - b), \tag{2}$$

where a and b are convenient operators. Again, one operator corresponds to the incident wave and the other to the reflected wave with respect to the boundary of the computational domain. Then, the transparent boundary condition is $(\partial_x - b)u = 0$ and consists in annihilating the reflected wave.

b is given by a high frequency infinite expansion which is not manageable for numerical simulations. The strategy of the absorbing boundary conditions consists in truncating this expansion after a finite number of terms. For an integer k , the absorbing boundary condition of order k is obtained by keeping the first k terms in the expansion of b . For example, for $L = (\partial_t^2 - \partial_x^2) + \partial_t$, the absorbing boundary condition of order 0 is

$$\partial_x u + \partial_t u = 0 \quad \text{at } x = 0$$

and the first order absorbing boundary condition is

$$\partial_x u + \partial_t u + u/2 = 0 \quad \text{at } x = 0.$$

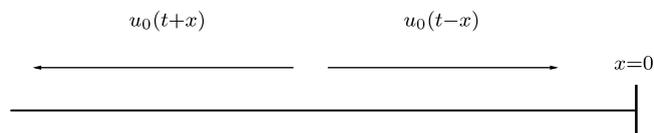


Fig. 1. The incident wave and the reflected wave with respect to the boundary $x = 0$ of the computational domain \mathbb{R}^- .

Remark 2. The absorbing boundary condition of order 0 is the transparent boundary condition of the constant coefficient case. This will also be the case for semilinear equations.

2.1.1. *The potential strategy*

Let us explain this strategy in the case of the cubic nonlinear Schrödinger equation

$$\begin{cases} (i\partial_t + \partial_x^2)u + |u|^2u = 0 & \text{in } \mathbb{R}^+ \times \mathbb{R}, \\ u = u_0 & \text{at } t = 0. \end{cases} \tag{3}$$

We take \mathbb{R}^- as a spatial computational domain and look for a boundary condition at $x = 0$.

In the sequel, we use the operators $\sqrt{-i\partial_t}$ and $\sqrt{-i\partial_t}^{-1}$ (see for example [9]) which are defined by

$$\begin{aligned} \sqrt{-i\partial_t}v(t) &= \frac{e^{-i\pi/4}}{\sqrt{\pi}} \partial_t \left(\int_0^t \frac{v(s)}{\sqrt{t-s}} ds \right), \\ \sqrt{-i\partial_t}^{-1}v(t) &= \frac{e^{i\pi/4}}{\sqrt{\pi}} \int_0^t \frac{v(s)}{\sqrt{t-s}} ds. \end{aligned} \tag{4}$$

Let $V = |u|^2$. Then (3) becomes

$$\begin{cases} (i\partial_t + \partial_x^2)u + Vu = 0 & \text{in } \mathbb{R}_t^+ \times \mathbb{R}, \\ u = u_0 & \text{at } t = 0. \end{cases} \tag{5}$$

If we neglect for a moment the dependence of V on u , we can see (5) as a linear Schrödinger equation with a potential term, hence the name of the strategy. As (5) is now a linear equation, we can use the method of Engquist and Majda in the frame of the Schrödinger equation. We obtain the zero order absorbing boundary condition

$$\partial_x u + \sqrt{-i\partial_t}u = 0 \quad \text{at } x = 0 \tag{6}$$

and the second order boundary condition

$$\partial_x u + \sqrt{-i\partial_t}u - V/2\sqrt{-i\partial_t}^{-1}u = 0 \quad \text{at } x = 0. \tag{7}$$

Now, we remember that $V = |u|^2$ and (7) becomes

$$\partial_x u + \sqrt{-i\partial_t}u - |u|^2/2\sqrt{-i\partial_t}^{-1}u = 0 \quad \text{at } x = 0. \tag{8}$$

Remark 3. We do not present the first order condition as it coincides with the zero order condition in this case.

The general case is handled in the same way. We first see the nonlinearity as a multiplication of functions with u or its derivatives. Then, we neglect the dependence of these functions on u and we use the strategy of Engquist and Majda for linear equations. Finally, we replace these functions by their expression in u in the absorbing boundary conditions, as we did to go from (7) to (8).

Remark 4. The rigorous justification of this strategy requires that u be smooth (see [19,20]). As we may want to approximate functions u with finite regularity, this justifies the introduction of a second strategy.

2.1.2. *The parilinear strategy*

Let us explain this strategy in the case of the following nonlinear Schrödinger equation:

$$\begin{cases} (i\partial_t + \partial_x^2)u + u\partial_x u = 0 & \text{in } \mathbb{R}_t^+ \times \mathbb{R}, \\ u = u_0 & \text{at } t = 0. \end{cases} \quad (9)$$

We take \mathbb{R}^- as a computational domain and look for a boundary condition at $x = 0$.

The idea is again to transform (9) into a linear equation but not in the same way. If we would use the potential strategy, we would set $V = u$ and see the nonlinearity as $V\partial_x u$. Instead, we use Bony's parilinearization theorem [4] which yields

$$u\partial_x u \approx T_u \partial_x u + T_{\partial_x u} u. \quad (10)$$

Here T_u and $T_{\partial_x u}$ are linear operator depending on u and \approx means = modulo a smooth remainder. The decomposition (10) works for functions u with finite regularity and makes it therefore interesting for our purposes. This decomposition follows from distinguishing three parts in the product $u\partial_x u$. More precisely, the Fourier transform of $u\partial_x u$ is given by a convolution and Bony considers three regions of integration. $T_u \partial_x u$ corresponds to the region where the frequencies of $\partial_x u$ are big compared to those of u . $T_{\partial_x u} u$ corresponds to the region where the frequencies of u are big compared to those of $\partial_x u$. Finally, the smooth remainder corresponds to the region where the frequencies of u and $\partial_x u$ have comparable size. For a more complete overview of the parilinearization see for example [19] where we sum up the various properties needed for the rigorous derivation of the parilinear strategy.

Using (10), we can see (9) as a linear Schrödinger equation with variable coefficients

$$\begin{cases} (i\partial_t + \partial_x^2)u + T_u \partial_x u + T_{\partial_x u} u = 0 & \text{in } \mathbb{R}_t^+ \times \mathbb{R}, \\ u = u_0 & \text{at } t = 0. \end{cases} \quad (11)$$

If we neglect for a moment the dependence of T_u and $T_{\partial_x u}$ on u , we can see (5) as a linear Schrödinger equation with variable coefficients. We can therefore use the method of Engquist and Majda in the frame of the Schrödinger equation. We obtain the zero order absorbing boundary condition

$$\partial_x u + \sqrt{-i\partial_t} u = 0 \quad \text{at } x = 0 \quad (12)$$

and the first order boundary condition

$$\partial_x u + \sqrt{-i\partial_t} u + T_u u / 2 = 0 \quad \text{at } x = 0. \quad (13)$$

Now, we want to get rid of the tricky operator T_u . Therefore, we use once again Bony's parilinearization theorem [4] which yields

$$u^2 \approx T_u u + T_u u. \quad (14)$$

This allows us to replace $T_u u$ by $u^2/2$ and (13) becomes

$$\partial_x u + \sqrt{-i\partial_t} u + u^2/4 = 0 \quad \text{at } x = 0. \quad (15)$$

The general case is handled in the same way. We first use Bony's parilinearization theorem to transform the nonlinearity into linear operators applied to u and its derivatives. Then, we neglect the dependence of these operators on u and we use the strategy of Engquist and Majda for linear equations. Finally, we replace these operators using again Bony's parilinearization theorem, as we did to go from (13)–(15).

Remark 5. The decomposition (10) is different from the decomposition used in the potential strategy and does not lead to the same boundary conditions as we will see in the next paragraph. The reader interested in the rigorous derivation of this strategy is referred to [19–21,18].

2.2. The absorbing boundary conditions

Here, we present the zero and first order absorbing boundary conditions obtained using the potential and the parilinear strategies. We focus on four examples studied in Section 5:

$$\begin{cases} (\partial_t^2 - \partial_x^2)u + u^2\partial_t u = 0 & \text{in } \mathbb{R}_t^+ \times \mathbb{R}, \\ u = u_0, \quad \partial_t u = u_1 & \text{at } t = 0, \end{cases} \tag{16}$$

$$\begin{cases} (\partial_t^2 - \partial_x^2)u - u^2\partial_x u = 0 & \text{in } \mathbb{R}_t^+ \times \mathbb{R}, \\ u = u_0, \quad \partial_t u = u_1 & \text{at } t = 0, \end{cases} \tag{17}$$

$$\begin{cases} (i\partial_t + \partial_x^2)u + |u|^2 u = 0 & \text{in } \mathbb{R}_t^+ \times \mathbb{R}, \\ u = u_0 & \text{at } t = 0, \end{cases} \tag{18}$$

and

$$\begin{cases} (i\partial_t + \partial_x^2)u + u\partial_x u = 0 & \text{in } \mathbb{R}_t^+ \times \mathbb{R}, \\ u = u_0 & \text{at } t = 0. \end{cases} \tag{19}$$

We consider the computational domain (a, b) , where $a < b$. We sum up the various absorbing boundary conditions at $x = a$ and $x = b$ in Tables 1–4.

Table 1
Zero and first order abc for $(\partial_t^2 - \partial_x^2)u + u^2\partial_t u = 0$ at $x = a$ and $x = b$

	Potential strategy	Parilinear strategy
Zero order abc at $x = a$	$\partial_x u - \partial_t u = 0$	$\partial_x u - \partial_t u = 0$
First order abc at $x = a$	$\partial_x u - \partial_t u - u^3/2 = 0$	$\partial_x u - \partial_t u - u^3/6 = 0$
Zero order abc at $x = b$	$\partial_x u + \partial_t u = 0$	$\partial_x u + \partial_t u = 0$
First order abc at $x = b$	$\partial_x u + \partial_t u + u^3/2 = 0$	$\partial_x u + \partial_t u + u^3/6 = 0$

Table 2
Zero and first order abc for $(\partial_t^2 - \partial_x^2)u - u^2\partial_x u = 0$ at $x = a$ and $x = b$

	Potential strategy	Parilinear strategy
Zero order abc at $x = a$	$\partial_x u - \partial_t u = 0$	$\partial_x u - \partial_t u = 0$
First order abc at $x = a$	$\partial_x u - \partial_t u + u^3/2 = 0$	$\partial_x u - \partial_t u + u^3/6 = 0$
Zero order abc at $x = b$	$\partial_x u + \partial_t u = 0$	$\partial_x u + \partial_t u = 0$
First order abc at $x = b$	$\partial_x u + \partial_t u + u^3/2 = 0$	$\partial_x u + \partial_t u + u^3/6 = 0$

Table 3
Zero and second order abc for $(i\partial_t + \partial_x^2)u + |u|^2 u = 0$ at $x = a$ and $x = b$

	Potential strategy
Zero order abc at $x = a$	$\partial_x u - \sqrt{-i\partial_t} u = 0$
Second order abc at $x = a$	$\partial_x u - \sqrt{-i\partial_t} u + u ^2/2\sqrt{-i\partial_t}^{-1} u = 0$
Zero order abc at $x = b$	$\partial_x u + \sqrt{-i\partial_t} u = 0$
Second order abc at $x = b$	$\partial_x u + \sqrt{-i\partial_t} u - u ^2/2\sqrt{-i\partial_t}^{-1} u = 0$

Table 4

Zero and first order *abc* for $(i\partial_t + \partial_x^2)u + u\partial_x u = 0$ at $x = a$ and $x = b$

	Potential strategy	Paralinear strategy
Zero order <i>abc</i> at $x = a$	$\partial_x u - \sqrt{-i\partial_t}u = 0$	$\partial_x u - \sqrt{-i\partial_t}u = 0$
First order <i>abc</i> at $x = a$	$\partial_x u - \sqrt{-i\partial_t}u + u^2/2 = 0$	$\partial_x u - \sqrt{-i\partial_t}u + u^2/4 = 0$
Zero order <i>abc</i> at $x = b$	$\partial_x u + \sqrt{-i\partial_t}u = 0$	$\partial_x u + \sqrt{-i\partial_t}u = 0$
First order <i>abc</i> at $x = b$	$\partial_x u + \sqrt{-i\partial_t}u + u^2/2 = 0$	$\partial_x u + \sqrt{-i\partial_t}u + u^2/4 = 0$

Remark 6. In the case of the cubic nonlinear Schrödinger equation, the zero and first order absorbing boundary conditions are the same. Therefore, we give in this case the second order absorbing boundary condition. Moreover, we are not able to design absorbing boundary conditions using the paralinear strategy in this case (see [20]). The reason is that the cubic nonlinear Schrödinger equation should be considered as a system in (u, \bar{u}) and not as a scalar equation, due to the term in \bar{u} contained in the nonlinearity (the analog of (10) in this case is $|u|^2 u \approx 2T_{|u|^2}u + T_{u^2}\bar{u}$). Therefore, Table 3 gives the zero and second order absorbing boundary conditions obtained by the potential strategy.

Remark 7. The reader interested in the design of first and second order absorbing boundary conditions in more general cases is referred to [19,20].

3. A finite volume discretization for semilinear wave equations

In [19], we used a finite differences scheme to compute the semilinear wave equation with the boundary conditions given in Tables 1 and 2. Here, we construct a finite volume scheme which is simpler to implement and more efficient.

We extend to the nonlinear case the finite volume scheme described in [7]. Let $\Omega = (a, b)$. We discretize the wave equation on $\Omega \times (0, T)$, using a finite volume discretization on a rectangular grid with the mesh size Δx and Δt . There are $J + 1$ points in space, numbered from 0 up to J with $\Delta x = (b - a)/J$, and $N + 1$ grid points in time, numbered from 0 up to N , with $\Delta t = T/N$. We denote the numerical approximation to $u(a + j\Delta x, n\Delta t)$ by $U(j, n)$.

We discretize the following semilinear wave equation:

$$\begin{cases} (\partial_t^2 - \partial_x^2)u = f(u, \partial_t u, \partial_x u) & \text{in } \Omega \times (0, T), \\ \partial_t u - \partial_x u + g^-(u) = 0, & \text{at } x = a, \\ \partial_t u + \partial_x u + g^+(u) = 0, & \text{at } x = b, \\ u(\cdot, 0) = p, \quad \partial_t u(\cdot, 0) = q. \end{cases} \tag{20}$$

Remark 8. The boundary conditions in Table 1 correspond to $g^+(u) = u^3/2$ and $g^-(u) = u^3/2$ for the potential strategy and to $g^+(u) = u^3/6$ and $g^-(u) = u^3/6$ for the paralinear strategy. The boundary conditions in Table 2 correspond to $g^+(u) = u^3/2$ and $g^-(u) = -u^3/2$ for the potential strategy and to $g^+(u) = u^3/6$ and $g^-(u) = -u^3/6$ for the paralinear strategy.

3.1. Interior points

Denoting by D the volume around a grid point $(x = a + j\Delta x, t = n\Delta t)$ in the interior of $\Omega \times (0, T)$ given by $D = (x - \Delta x/2, x + \Delta x/2) \times (t - \Delta t/2, t + \Delta t/2)$, we obtain the finite volume scheme by integrating the equation over the volume D and applying the divergence theorem

$$\begin{aligned}
 0 &= \int_{x-\Delta x/2}^{x+\Delta x/2} \partial_t u(\zeta, t + \Delta t/2) d\zeta - \int_{x-\Delta x/2}^{x+\Delta x/2} \partial_t u(\zeta, t - \Delta t/2) d\zeta \\
 &\quad - \int_{t-\Delta t/2}^{t+\Delta t/2} \partial_x u(x + \Delta x/2, \tau) d\tau + \int_{t-\Delta t/2}^{t+\Delta t/2} \partial_x u(x - \Delta x/2, \tau) d\tau \\
 &\quad - \int_{x-\Delta x/2}^{x+\Delta x/2} \int_{t-\Delta t/2}^{t+\Delta t/2} f(u, \partial_t u, \partial_x u) d\zeta d\tau.
 \end{aligned}$$

We use finite differences to approximate the integrals.

$$\begin{aligned}
 D_t^+ U(j, n) &= \frac{U(j, n + 1) - U(j, n)}{\Delta t}, & D_t^- U(j, n) &= \frac{U(j, n) - U(j, n - 1)}{\Delta t}, \\
 D_x^+ U(j, n) &= \frac{U(j + 1, n) - U(j, n)}{\Delta x}, & D_x^- U(j, n) &= \frac{U(j, n) - U(j - 1, n)}{\Delta x}, \\
 D_x^0 U(j, n) &= \frac{U(j + 1, n) - U(j - 1, n)}{2\Delta x}, & D_t^0 U(j, n) &= \frac{U(j, n + 1) - U(j, n - 1)}{2\Delta t},
 \end{aligned} \tag{21}$$

$$\begin{aligned}
 D_x^{--} U(j, n) &= \frac{3U(j, n) - 4U(j - 1, n) + U(j - 2, n)}{2\Delta x}, \\
 D_x^{++} U(j, n) &= \frac{3U(j, n) - 4U(j + 1, n) + U(j + 2, n)}{2\Delta x}, \\
 D_t^{--} U(j, n) &= \frac{3U(j, n) - 4U(j, n - 1) + U(j, n - 2)}{2\Delta t}, \\
 D_t^{*} U(j, n) &= \begin{cases} D_t^{--} U(j, n) & \text{for } n \geq 2, \\ D_t^- U(j, n) & \text{for } n = 1. \end{cases}
 \end{aligned} \tag{22}$$

The numerical approximation to $\partial_t u$ in the finite volume scheme is a piecewise constant and given by $D_t^+ U(j, n)$ for $t \in [t_n, t_{n+1})$. Similarly the numerical approximation to $\partial_x u$ is piecewise constant in the finite volume scheme and given by $D_x^+ U(j, n)$ for $x \in [x_j, x_{j+1})$. The last finite derivatives are second order approximation of $\partial_x u$ and $\partial_t u$ we shall use for the nonlinear term, in order to design an explicit scheme. We now write

$$\int_{x-\Delta x/2}^{x+\Delta x/2} \partial_t u(\zeta, t \pm \Delta t/2) d\zeta \approx \Delta x D_t^\pm U(j, n), \quad \int_{t-\Delta t/2}^{t+\Delta t/2} \partial_x u(x \pm \Delta x/2, \tau) d\tau \approx \Delta t D_x^\pm U(j, n)$$

and the scheme in the interior writes

$$(D_t^+ D_t^- - D_x^+ D_x^-) U(j, n) - f(U(j, n), D_t^* U(j, n), D_x^0 U(j, n)) = 0, \quad 1 \leq j \leq J - 1, \quad 1 \leq n \leq N - 1. \tag{23}$$

3.2. Points on the initial line

For $x = a + j\Delta x$ in the interior of Ω , we integrate the equation on the half-cell $(x - \Delta x/2, x + \Delta x/2) \times (0, \Delta t/2)$, and get

$$\begin{aligned}
 0 &= \int_{x-\Delta x/2}^{x+\Delta x/2} \partial_t u(\zeta, \Delta t/2) d\zeta - \int_{x-\Delta x/2}^{x+\Delta x/2} \partial_t u(\zeta, 0) d\zeta - \int_0^{\Delta t/2} \partial_x u(x + \Delta x/2, \tau) d\tau \\
 &\quad + \int_0^{\Delta t/2} \partial_x u(x - \Delta x/2, \tau) d\tau - \int_{x-\Delta x/2}^{x+\Delta x/2} \int_0^{\Delta t/2} f(u, \partial_t u, \partial_x u) d\zeta d\tau.
 \end{aligned}$$

Now the remaining derivatives can be approximated by finite differences (21), except the term $\partial_t u(\xi, 0)$. But this derivative is given explicitly by the initial condition

$$\int_{x-\Delta x/2}^{x+\Delta x/2} \partial_t u(\xi, 0) d\xi = \int_{x-\Delta x/2}^{x+\Delta x/2} q(\xi) d\xi \approx \Delta x q(x).$$

We define the discrete initial conditions as

$$P(j) = p(a + j\Delta x), \quad Q(j) = q(a + j\Delta x). \quad (24)$$

The nonlinear term is approximated by $\Delta x \frac{\Delta t}{2} f(p(x), q(x), \partial_x p(x))$, and we obtain the scheme

$$\left(D_t^+ - \frac{\Delta t}{2} D_x^+ D_x^- \right) U(j, 0) - Q(j) = \frac{\Delta t}{2} f(P(j), Q(j), D_x^0 Q(j)), \quad \text{for } 1 \leq j \leq J. \quad (25)$$

3.3. Boundary points

Suppose the point $(x = a, t = n\Delta t)$ is on the left boundary of $\Omega \times (0, T)$, for $n \geq 1$. We integrate on the half-cell $(x, x + \Delta x/2) \times (t - \Delta t/2, t + \Delta t/2)$ and proceed as before

$$\begin{aligned} 0 &= \int_x^{x+\Delta x/2} \partial_t u(\xi, t + \Delta t/2) d\xi - \int_x^{x+\Delta x/2} \partial_t u(\xi, t - \Delta t/2) d\xi \\ &\quad - \int_{t-\Delta t/2}^{t+\Delta t/2} \partial_x u(x + \Delta x/2, \tau) d\tau + \int_{t-\Delta t/2}^{t+\Delta t/2} \partial_x u(x, \tau) d\tau \\ &\quad - \int_x^{x+\Delta x/2} \int_{t-\Delta t/2}^{t+\Delta t/2} f(u, \partial_t u, \partial_x u) d\xi d\tau. \end{aligned}$$

Again we can approximate $\partial_t u$ and $\partial_x u$ by the finite differences given in (21), except on the left side of the control volume, where we apply the boundary condition. For the nonlinear term, we use the one-sided approximations of $\partial_x u$, and $\partial_t u$

$$\int_x^{x+\Delta x/2} \int_{t-\Delta t/2}^{t+\Delta t/2} f(u, \partial_t u, \partial_x u) d\xi d\tau \approx \Delta t \frac{\Delta x}{2} f(U(0, n), D_t^- U(0, n), D_x^{++} U(0, n))$$

and we obtain

$$\begin{aligned} 0 &= \left(\frac{\Delta x}{2} (D_t^+ - D_t^-) - \Delta t D_x^+ \right) U(0, n) + \int_{t-\Delta t/2}^{t+\Delta t/2} \partial_x u(x, \tau) d\tau \\ &\quad - \Delta t \frac{\Delta x}{2} f(U(0, n), D_t^- U(0, n), D_x^{++} U(0, n)). \end{aligned} \quad (26)$$

We now introduce the left boundary condition

$$\partial_t u - \partial_x u + g^-(u) = 0.$$

We integrate it over $(t - \Delta t/2, t + \Delta t/2)$, and extract the boundary term

$$\int_{t-\Delta t/2}^{t+\Delta t/2} \partial_x u(x, \tau) d\tau \approx \Delta t D_t^0 U(0, n) + \int_{t-\Delta t/2}^{t+\Delta t/2} g^-(u)(x, \tau) d\tau \approx \Delta t D_t^0 U(0, n) + \Delta t g^-(U(0, n)),$$

which together with (26) yields

$$0 = \left(D_t^0 - D_x^+ + \frac{\Delta x}{2} D_t^+ D_t^- \right) U(0, n) - \frac{\Delta x}{2} f(U(0, n), D_t^- U(0, n), D_x^{++} U(0, n)) + g^-(U(0, n)). \quad (27)$$

The treatment of the right boundary condition is the same

$$0 = \left(D_t^0 + D_x^- + \frac{\Delta x}{2} D_t^+ D_t^- \right) U(J, n) - \frac{\Delta x}{2} f(U(J, n), D_t^{-*} U(J, n), D_x^{-} U(J, n)) + g^+(U(J, n)) \quad n \geq 1. \tag{28}$$

3.4. Corner points

For the corner points on the initial line, there is only a quarter of the original finite volume left to integrate over. For example on the left corner we obtain for $x = a$,

$$0 = \int_x^{x+\Delta x/2} \partial_t u(\xi, \Delta t/2) d\xi - \int_x^{x+\Delta x/2} \partial_t u(\xi, 0) d\xi - \int_0^{\Delta t/2} \partial_x u(x + \Delta x/2, \tau) d\tau + \int_0^{\Delta t/2} \partial_x u(x, \tau) d\tau - \int_x^{x+\Delta x/2} \int_0^{\Delta t/2} f(u, \partial_t u, \partial_x u) d\xi d\tau.$$

Here two of the remaining derivatives can be approximated by the finite differences (21)

$$\int_x^{x+\Delta x/2} \partial_t u(\xi, \Delta t/2) d\xi \approx \frac{\Delta x}{2} D_t^+ U(0, 0), \quad \int_0^{\Delta t/2} \partial_x u(x + \Delta x/2, \tau) d\tau \approx \frac{\Delta t}{2} D_x^+ U(0, 0),$$

whereas $\frac{\partial u}{\partial t}(\xi, 0)$ is given by the initial condition

$$\int_x^{x+\Delta x/2} \partial_t u(\xi, 0) d\xi \approx \frac{\Delta x}{2} Q(0),$$

where Q is defined in (24), and $\frac{\partial u}{\partial x}(0, \tau)$ has to be obtained from the boundary condition by proceeding as before: we integrate the left boundary condition over $(0, \Delta t/2)$ and extract the boundary term

$$\int_0^{\Delta t/2} \partial_x u(x, \tau) d\tau \approx \frac{\Delta t}{2} D_t^+ U(0, n) + \int_0^{\Delta t/2} g^-(u)(x, \tau) d\tau.$$

The nonlinear term in the former equation is approximated by

$$\frac{\Delta t}{2} g^-(P(0))$$

and we obtain the discrete scheme

$$0 = \left(\frac{\Delta x}{2} D_t^+ - \frac{\Delta t}{2} D_x^+ + \frac{\Delta t}{2} D_t^+ \right) U(0, 0) - \frac{\Delta x}{2} Q(0) - \frac{\Delta x \Delta t}{4} f(P(0), Q(0), D_x^{++} P(0)) + \frac{\Delta t}{2} g^-(P(0)).$$

Dividing by $\Delta t/2$ yields

$$0 = \left(D_t^+ - D_x^+ + \frac{\Delta x}{\Delta t} D_t^+ \right) U(0, 0) - \frac{\Delta x}{\Delta t} Q(0) - \frac{\Delta x}{2} f(P(0), Q(0), D_x^{++} P(0)) + g^-(P(0)). \tag{29}$$

The treatment of the right boundary is the same

$$0 = \left(D_t^+ + D_x^- + \frac{\Delta x}{\Delta t} D_t^+ \right) U(J, 0) - \frac{\Delta x}{\Delta t} Q(J) - \frac{\Delta x}{2} f(P(J), Q(J), D_x^{--} P(J)) + g^+(P(J)). \tag{30}$$

Remark 9. Our numerical computations indicate that this scheme is second order both in space and time.

4. The numerical scheme for nonlinear Schrödinger equations

In order to compute nonlinear Schrödinger equations with absorbing boundary conditions, we take the interval $]a, b[$ as computational domain. We want to compute the solution u of

$$\begin{cases} (i\partial_t + \partial_x^2)u + f(u, \bar{u}, \partial_x u, \partial_x \bar{u}) = 0, \\ \partial_x u = T_a u, \quad \text{at } x = a, \\ \partial_x u = T_b u, \quad \text{at } x = b, \end{cases} \quad (31)$$

where T_a and T_b are operators corresponding to our absorbing boundary conditions. For the time discretization, we use the scheme of Durán and Sanz-Serna [5]

$$i \frac{u^{n+1} - u^n}{\Delta t} + \partial_{xx} u^{n+1/2} + f\left(u^{n+1/2}, \overline{u^{n+1/2}}, \partial_x u^{n+1/2}, \partial_x \overline{u^{n+1/2}}\right) = 0, \quad (32)$$

where $u^{n+1/2} = (u^{n+1} + u^n)/2$ and $n = 0, \dots, T/\Delta t - 1$. We solve the nonlinear system with a fixed point method giving $u^{n+1/2}$

$$Z = \left(1 - i \frac{\Delta t}{2} \partial_{xx}\right)^{-1} \left(u^n + i \frac{\Delta t}{2} f(Z, \bar{Z}, \partial_x Z, \partial_x \bar{Z})\right).$$

We initialize the fixed point method with u^n . Then $u^{n+1} = 2Z - u^n$. For the space discretization, we use P1 finite elements based on the following weak formulation:

$$\begin{aligned} i \int_a^b \frac{u^{n+1} - u^n}{\Delta t} \bar{v} \, dx - \int_a^b \partial_x u^{n+1/2} \partial_x \bar{v} \, dx + T_b u^{n+1/2}(b) \bar{v}(b) - T_a u^{n+1/2}(a) \bar{v}(a) \\ + \int_a^b f\left(u^{n+1/2}, \overline{u^{n+1/2}}, \partial_x u^{n+1/2}, \partial_x \overline{u^{n+1/2}}\right) \bar{v} \, dx = 0, \end{aligned}$$

where v is a test function. It remains to discretize the operators T_a and T_b . It suffices to discretize $\sqrt{\partial_t}$ and $\sqrt{\partial_t}^{-1}$. In [2], Antoine and Besse proposed to approximate these operators by

$$\begin{aligned} (\sqrt{\partial_t}^{-1} \varphi)(t_{n+1/2}) &\approx \sqrt{\frac{\Delta t}{2}} \sum_{k=0}^n \alpha_k \varphi^{n+1/2-k}, \\ (\sqrt{\partial_t} \varphi)(t_{n+1/2}) &\approx \sqrt{\frac{2}{\Delta t}} \sum_{k=0}^n \beta_k \varphi^{n+1/2-k}, \end{aligned}$$

where $\varphi^{n+1/2-k}$ is an approximation of $\varphi(t_{n+1/2-k})$ and where

$$\alpha_0 = \alpha_1 = 1, \quad \text{and} \quad \alpha_{2k} = \prod_{j=1}^k \frac{2j-1}{2j} = \alpha_{2k+1}, \quad k \geq 1,$$

$$\beta_k = (-1)^k \alpha_k, \quad k \geq 0.$$

5. Numerical results

5.1. The frame of the experiments for semilinear wave equations

We compute the semilinear wave equation with absorbing boundary conditions using the finite volume scheme of Section 3. We take the interval $]0, 2[$ as computational domain. We choose the stepsizes small in order to see the errors due to the various boundary conditions and not to the discretization: $\Delta t = 0.01$ and $\Delta x = 0.001$. We choose u_0 in $H^4(\mathbb{R})$ and u_1 in $H^3(\mathbb{R})$ with compact support in $]0, 2[$

$$\begin{cases} u_0(x) = x^3(2-x)^3 & \text{on }]0, 2[, \\ u_0(x) = 0 & \text{on }]-\infty, 0] \cup [2, +\infty[, \\ u_1(x) = 3x^2(2-x)^2(x-1) & \text{on }]0, 2[, \\ u_1(x) = 0 & \text{on }]-\infty, 0] \cup [2, +\infty[. \end{cases} \tag{33}$$

The solution of the semilinear wave equation on \mathbb{R} propagates at speed 1 (see for instance [15]). In order to compute this solution with initial data (33) and for t between 0 and 10, we compute the equation in $] -10, 12[$ with Dirichlet boundary conditions.

Remark 10. In order to implement the semilinear wave equation with the absorbing boundary conditions, the support of the initial data must be included in the computational domain. In order to implement the method using the Dirichlet boundary conditions, the support of the solution must be included in the computational domain on the whole time interval. Therefore, the method using the absorbing boundary conditions approaches the semilinear wave equation on \mathbb{R} with a low numerical cost compared to the method using Dirichlet boundary conditions.

5.2. The frame of the experiments for nonlinear Schrödinger equations

The equation $(i\partial_t + \partial_x^2)u + |u|^2u = 0$ has a family of solitons as solutions

$$u(t, x) = \sqrt{2a} \operatorname{sech}(\sqrt{a}(x - ct)) \exp\left(i\frac{c}{2}(x - ct) + i\theta_0\right) \exp\left(i\left(a + \frac{c^2}{4}\right)t\right). \tag{34}$$

To approximate this soliton, we take $] -5, 5[$ as computational domain. We fix the parameters of the soliton as $a = 27$, $c = 15$ and $\theta_0 = \pi/4$. This solution is a good test because it has almost compact support in $] -5, 5[$ at $t = 0$ (it remains under 10^{-10} on the boundary), and crosses the boundary $x = 5$ between $t = 0$ and $t = 1$. We take the time step $\Delta t = 0.001$ and the space step $\Delta x = 0.025$.

In the case of the nonlinear Schrödinger equation (9), we take $]0, 2[$ as computational domain. We take the time step $\Delta t = 0.001$ and the space step $\Delta x = 0.025$. We choose u_0 in $H^4(\mathbb{R})$ with support in $[0, 2]$

$$\begin{cases} u_0(x) = x^3(2-x)^3 & \text{in }]0, 2[, \\ u_0(x) = 0 & \text{in }]-\infty, 0] \cup [2, +\infty[. \end{cases} \tag{35}$$

5.3. Comments on the results

We call relative error in the L^2 norm at time t the expression

$$\frac{\|u(t, \cdot) - v(t, \cdot)\|_{L^2}}{\|u_0\|_{L^2}},$$

where v is the solution of (16), (17), (18) or (19) i.e. the solution on \mathbb{R} that we want to approximate, u is the solution computed with one of the various absorbing boundary conditions, and where we take the L^2 norm on the computational domain.

In each case, we introduce a large class of absorbing boundary conditions depending on a parameter α coinciding with our absorbing boundary conditions for a particular value of α , and we look for an α giving optimal results.

5.3.1. The case of the equation $(\partial_t^2 - \partial_x^2)u + u^2 \partial_t u = 0$

We want to approximate the solution of the semilinear wave equation (16) by the solution u of

$$\begin{cases} (\partial_t^2 - \partial_x^2)u + u^2 \partial_t u = 0 & \text{in }]0, T[\times]0, 2[, \\ \partial_x u - \partial_t u - \alpha u^3 = 0 & \text{at } x = 0, \\ \partial_x u + \partial_t u + \alpha u^3 = 0 & \text{at } x = 2. \end{cases} \quad (36)$$

The zero order absorbing boundary conditions correspond to $\alpha = 0$, the first order absorbing boundary conditions obtained with the potential strategy correspond to $\alpha = 1/2$, and the first order absorbing boundary conditions obtained with the parilinear strategy correspond to $\alpha = 1/6$.

In Table 5, we give the maximum of the relative error in the L^2 norm for times between 0 and T for various T and various choices of α . We notice that for all choices of T , the first order absorbing boundary conditions obtained with the parilinear strategy give the best results, except for $T = 10$ where it is only slightly improved by $\alpha = 1/12$. The results given by the parilinear first order condition are very satisfactory: the error remains under 1.7% on the whole time interval $[0, 10]$.

5.3.2. The case of the equation $(\partial_t^2 - \partial_x^2)u - u^2 \partial_x u = 0$

We want to approximate the solution of the semilinear wave equation (17) by the solution u of

$$\begin{cases} (\partial_t^2 - \partial_x^2)u - u^2 \partial_x u = 0 & \text{in }]0, T[\times]0, 2[, \\ \partial_x u - \partial_t u + \alpha u^3 = 0 & \text{at } x = 0, \\ \partial_x u + \partial_t u + \alpha u^3 = 0 & \text{at } x = 2. \end{cases} \quad (37)$$

The zero order absorbing boundary conditions correspond to $\alpha = 0$, the first order absorbing boundary conditions obtained with the potential strategy correspond to $\alpha = 1/2$, and the first order absorbing boundary conditions obtained with the parilinear strategy correspond to $\alpha = 1/6$.

In Table 6, we give the maximum of the relative error in the L^2 norm for times between 0 and T for various T and various choices of α . We notice that for all choices of T , the first order absorbing boundary conditions obtained with the parilinear strategy give the best results. The results given by this first order condition are very satisfactory: the error remains under 1.5% on the whole time interval $[0, 10]$.

5.3.3. The case of the equation $(i\partial_t + \partial_x^2)u + |u|^2 u = 0$

We want to approximate the solution of the cubic nonlinear Schrödinger equation (18) by the solution u of

Table 5

Maximum of the relative error in the L^2 norm for times between 0 and T for various T and various choices of α in (36)

T	$\alpha = 0$	$\alpha = \frac{1}{12}$	$\alpha = \frac{1}{6}$	$\alpha = \frac{1}{3}$	$\alpha = \frac{1}{2}$	$\alpha = 1$	$\alpha = 2$	$\alpha = 5$	$\alpha = -\frac{1}{6}$	$\alpha = -\frac{1}{2}$
1	0.0015	0.0007	9.73e-06	0.0015	0.0029	0.0070	0.0145	0.0331	0.0030	0.0061
2	0.0188	0.0088	0.0008	0.0192	0.0364	0.0824	0.1561	0.3005	0.0399	0.0875
5	0.0362	0.0158	0.0086	0.0460	0.0806	0.1711	0.3088	0.5468	0.0804	0.1855
10	0.0362	0.0158	0.0170	0.0544	0.0886	0.1788	0.3108	0.5468	0.0804	0.2032

Table 6

Maximum of the relative error in the L^2 norm for times between 0 and T for various T and various choices of α in (37)

T	$\alpha = 0$	$\alpha = \frac{1}{12}$	$\alpha = \frac{1}{6}$	$\alpha = \frac{1}{3}$	$\alpha = \frac{1}{2}$	$\alpha = 1$	$\alpha = 2$	$\alpha = 5$	$\alpha = -\frac{1}{6}$	$\alpha = -\frac{1}{2}$
1	0.0015	0.0007	1.29e-05	0.0014	0.0028	0.0067	0.0139	0.0311	0.0029	0.0060
2	0.0181	0.0093	0.0008	0.0153	0.0302	0.0695	0.1300	0.2343	0.0368	0.0796
5	0.0421	0.0245	0.0077	0.0276	0.0562	0.1298	0.2366	0.3862	0.0800	0.1700
10	0.0498	0.0322	0.0154	0.0276	0.0562	0.1298	0.2366	0.4651	0.0877	0.1778

$$\begin{cases} (i\partial_t^2 + \partial_x^2)u + |u|^2u = 0 & \text{in }]0, T[\times] - 5, 5[, \\ \partial_x u - \sqrt{-i\partial_t}u + \alpha|u|^2\sqrt{-i\partial_t}^{-1}u = 0 & \text{at } x = -5, \\ \partial_x u + \sqrt{-i\partial_t}u - \alpha|u|^2\sqrt{-i\partial_t}^{-1}u = 0 & \text{at } x = 5. \end{cases} \tag{38}$$

The zero order absorbing boundary conditions correspond to $\alpha = 0$ and the second order absorbing boundary conditions obtained with the potential strategy correspond to $\alpha = 1/2$.

In Table 7, we give the maximum of the relative error in the L^2 norm for times between 0 and 10 and for various choices of α . The maximum of the relative error in the L^2 norm occurs before $T = 1$, so we do not display the results obtained for $T = 1$, $T = 2$ or $T = 5$ since they are identical with those obtained for $T = 10$. We notice that the second order absorbing boundary conditions obtained with the potential strategy give the best results. The results given by this second order condition are satisfactory: the error remains under 12% on the whole time interval $[0, 10]$. However, further improvements are possible. One could for instance use the third order condition given by the potential strategy (see [20]).

5.3.4. *The case of the equation $(i\partial_t + \partial_x^2)u + u\partial_x u = 0$*

We want to approximate the solution of the nonlinear Schrödinger equation (19) by the solution u of

$$\begin{cases} (i\partial_t^2 + \partial_x^2)u + u\partial_x u = 0 & \text{in }]0, T[\times]0, 2[, \\ \partial_x u - \sqrt{-i\partial_t}u + \alpha u^2 = 0 & \text{at } x = 0, \\ \partial_x u + \sqrt{-i\partial_t}u + \alpha u^2 = 0 & \text{at } x = 2. \end{cases} \tag{39}$$

The zero order absorbing boundary conditions correspond to $\alpha = 0$, the first order absorbing boundary conditions obtained with the potential strategy correspond to $\alpha = 1/2$, and the first order absorbing boundary conditions obtained with the paralignar strategy correspond to $\alpha = 1/4$.

In Table 8, we give the maximum of the relative error in the L^2 norm for times between 0 and 10 and for various choices of α . The maximum of the relative error in the L^2 norm occurs before $T = 1$, so we do not display the results obtained for $T = 1$, $T = 2$ or $T = 5$ since they are identical with those obtained for

Table 7

Maximum of the relative error in the L^2 norm for times between 0 and 10 and for various choices of α in (38)

T	$\alpha = 0$	$\alpha = \frac{1}{4}$	$\alpha = \frac{1}{2}$	$\alpha = 1$	$\alpha = 2$	$\alpha = 5$	$\alpha = -\frac{1}{4}$	$\alpha = -\frac{1}{2}$	$\alpha = -1$
10	0.3046	0.1759	0.1178	0.1307	0.2456	0.3967	0.6135	7.0525e+93	2.1852e+68

Table 8

Maximum of the relative error in the L^2 norm for times between 0 and 10 and for various choices of α in (39)

T	$\alpha = 0$	$\alpha = \frac{1}{8}$	$\alpha = \frac{1}{4}$	$\alpha = \frac{1}{2}$	$\alpha = 1$	$\alpha = 2$	$\alpha = 5$	$\alpha = -\frac{1}{4}$	$\alpha = -\frac{1}{2}$	$\alpha = -1$
10	0.0231	0.0136	0.0042	0.0155	0.0551	0.1390	0.3463	0.0418	0.0601	0.0949

$T = 10$. We notice that the first order absorbing boundary conditions obtained with the parilinear strategy give the best results. The results given by this first order condition are very satisfactory: the error remains under 0.4% on the whole time interval $[0, 10]$.

Remark 11. Tables 5–8 clearly illustrate the improvement of the first order condition with respect to the zero order condition. There is an improvement of a factor 2 in Table 5, a factor 3 in Table 6, a factor 2.5 in Table 7 and a factor 55 in Table 8 for $T = 10$. There is an improvement of more than a factor 100 in Tables 5 and 6 for $T = 1$. Moreover, our numerical computations indicate that these improved results are obtained at no additional cost in numerical stability or efficiency. Finally, we notice that the first order conditions are as easy to implement as the zero order conditions (see Tables 1–4).

6. Conclusion

The potential and the parilinear strategies are two ways of designing absorbing boundary conditions for nonlinear scalar partial differential equations. We have derived a finite volume scheme well-suited to these absorbing boundary conditions in the case of semilinear wave equations. We have also shown that these absorbing boundary conditions give optimal results within a large class of boundary conditions in the case of semilinear wave equations and of nonlinear Schrödinger equations. Therefore, these two strategies are efficient to approximate nonlinear scalar partial differential equations on unbounded domains with a low numerical cost.

All the results in this work are for the one dimensional case only. The multidimensional study contains in addition difficulties due to the geometry and should be the heart of a forthcoming paper.

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