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Towards accurate artificial boundary conditions for nonlinear PDEs through examples

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ABSTRACT

The aim of this paper is to give a comprehensive review of current developments related to the derivation of artificial boundary conditions for nonlinear partial differential equations. The essential tools to build such boundary conditions are based on pseudodifferential and paradifferential calculus. We present various derivations and compare

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them. Some numerical results illustrate their respective accuracy and analyze the potential of each technique.

RESUMEN

La meta de este artículo es entregar una revisión comprensiva de los desarrollos actuales relacionados con la derivación de condiciones de borde artificiales para ecuaciones diferenciales parciales nolineales. Las herramientas esenciales para construir tales condiciones de borde se basan en el cálculo pseudodiferencial y paradiferencial. Presentamos varias derivaciones y las comparamos. Algunos resultados numéricos ilustran su precisión respectiva y se analiza el potencial de cada técnica.

Key words and phrases: *Nonlinear PDEs, wave equation, Schrödinger equation, artificial boundary conditions for nonlinear PDEs, numerical schemes.*

Math. Subj. Class.: *35A21, 35A27, 35L05, 35Q55, 35S50, 65M99.*

1 Introduction

The subject of designing *artificial boundary conditions for linear scalar and systems of Partial Differential Equations (PDEs)* has been studied since more than thirty years now. Essentially, the goal of these boundary conditions is to truncate an infinite domain into a finite one for computational considerations. To this end, a fictitious boundary Γ is introduced delimiting therefore a finite domain Ω. All the difficulty is then to build an accurate, robust and easy-to-implement approximate boundary condition on this fictitious boundary. These boundary conditions can be found in the literature under different names (which in fact have different subtle meanings) like artificial boundary conditions, absorbing boundary conditions, non-reflecting or transparent boundary conditions and sometimes Dirichlet-to-Neumann operators. Among the major contributions written on the topic and without being exhaustive, let us quote e.g. the papers by Engquist and Majda [9, 10], Bayliss and Turkel [4], Mur [15] or also Bérenger [5]. A few review papers have also been published to establish the current state-of-the-art on the subject (see e.g. [2, 11, 12, 22]).

While many improvements have been achieved over the past years, most of them are developed for linear equations. Practically, most available methods for linear equations do not apply to nonlinear equations since they often rely on the explicit computation of the transparent boundary condition by using the Fourier or Laplace transforms (note however that in the particular case of integrable equations, one may use the inverse scattering transform to explicitly compute the transparent boundary condition, see e.g. [23]). Now, *Nonlinear problems* have recently received some increasing special care because of their importance in applications like e.g. in wave propagation, quantum mechanics, fluid mechanics,... The aim of this paper is to give a comprehensive

introduction to possible solutions to handle such nonlinear situations. They are mainly based on pseudodifferential [21] and paradifferential operators techniques [6].

The paper is organized as follows. In Section 2, we analyze in detail the way of constructing approximate artificial boundary conditions for a general one-dimensional wave equation with variable coefficients using pseudodifferential calculus. Then, we test numerically these absorbing boundary conditions on a model problem showing that they yield accurate computations at least for small times. In a third Section, we consider a general one-dimensional nonlinear Schrödinger equation. We present several ways to extend the method of Section 2 to this nonlinear equation depending on the kind of nonlinearity involved in the equation. The various types of absorbing boundary conditions are obtained using either the pseudodifferential or the paradifferential calculus. In a fourth Section, some numerical comparisons are developed to test the accuracy of the various absorbing boundary conditions. The last Section draws a conclusion and suggests some future directions of research.

2 Artificial boundary conditions for linear variable coefficients equations: the case of the wave equation

2.1 The case of the constant coefficients wave equation

Before directly going to the case of the wave equation with variable coefficients, let us first consider the simple wave equation

$$(\partial_t^2 - \partial_x^2)u = 0, \tag{2.1}$$

with initial data $u(0,x) = u_0(x)$ and $\partial_t u(0,x) = u_1(x)$, where the field $u = u(t,x)$ is defined on the whole space $(t,x) \in [0;+\infty[\times\mathbb{R}$. For simulation purposes, it is standard to introduce a bounded spatial computational domain setting now $(t,x) \in [0;+\infty[\times[x_\ell;x_r]$, where x_ℓ (respectively x_r) is a left (respectively right) fictitious endpoint introduced to get a bounded domain $\Omega = [x_\ell;x_r]$. Let us assume that the initial data of our problem, that is u_0 and u_1, are compactly supported in Ω. Then, we can define the extension of u (which is still denoted by u) for negative times by fixing its value to zero so that u is a solution to (2.1) for all times t as long as $x \in \Omega^c$, where $\Omega^c = \mathbb{R} - \overline{\Omega}$. Let us denote by $\hat{u}_t(\tau,x) = \mathcal{F}_t(u)(\tau,x)$ the partial time-Fourier transform of u, where $\tau \in \mathbb{R}$. Applying $\mathcal{F}_t$ to (2.1) for $(t,x) \in \mathbb{R}\times\Omega^c$ leads to the Helmholtz-type constant coefficients equation

$$(\partial_x^2 + \tau^2)\hat{u}_t(\tau,x) = 0, \tag{2.2}$$

where the wavenumber is τ. The solution of this equation can be written as the superposition of two waves

$$\hat{u}_t(\tau,x) = A^+ e^{i\tau x} + A^- e^{-i\tau x}, \tag{2.3}$$

where $A^\pm$ are two smooth functions depending on τ. Computing the derivative $\partial_x \hat{u}_t$, we obtain

$$(\partial_x - i\tau)\hat{u}_t = -2i\tau e^{-i\tau x} A^-, \tag{2.4}$$

and

$$(\partial_x + i\tau)\hat{u}_t = 2i\tau e^{i\tau x} A^+, \tag{2.5}$$

and we obviously check that: $(\partial_x + i\tau)(\partial_x - i\tau)\hat{u}_t = 0$. We also have the following operator factorization

$$\partial_t^2 - \partial_x^2 = -(\partial_x + \partial_t)(\partial_x - \partial_t). \tag{2.6}$$

Equation (2.4) (respectively (2.5)) gives a characterization of the right (respectively left) traveling solution to (2.1) by setting: $A^- = 0$ (respectively $A^+ = 0$). Therefore, the following boundary condition (2.4)

$$(\partial_{\mathbf{n}} - i\tau)\hat{u}_t = 0, \quad \text{at } \Gamma, \tag{2.7}$$

acts as a filter in the time-Fourier domain and translates the property that there is no reflection back into the computational domain Ω, where $\mathbf{n}$ is the unit normal vector to $\Gamma = \{x_\ell; x_r\}$, outwardly directed to Ω. This is a constraint which forces the wave to be outgoing to Ω. In the time-space domain, the corresponding boundary condition writes down

$$(\partial_{\mathbf{n}} - \partial_t)u = 0, \quad \text{at } [0; +\infty[\times\Gamma. \tag{2.8}$$

Since there is no reflection, this boundary condition is usually called Transparent or Non-Reflecting Boundary Condition (TBC). Let us remark at this point that another interpretation of writing a transparent boundary condition is that we require $u \in \mathrm{Ker}(\partial_{\mathbf{n}} - b)$, setting $b(x, t, \partial_t) = \partial_t$.

2.2 The case of the variable coefficients wave equation

Let us consider that α, β and γ are three $\mathcal{C}^\infty$ functions. Writing a TBC for a variable coefficient model wave equation

$$(\partial_t^2 + \beta(t,x)\partial_t - \partial_x^2 + \gamma(t,x)\partial_x + \alpha(t,x))u = 0, \tag{2.9}$$

is much more complicate than in the constant coefficients case. Indeed, in such a situation

i) directly applying a time-Fourier transform to the equation (2.9) leads to a convolution equation which is extremely difficult to write down explicitly,

ii) and even if it is possible to write an inhomogeneous Helmholtz-type equation, solving this equation for general functions associated with α, β and γ cannot be expected.

Building an accurate boundary condition which approximates the TBC can however be expected since the pioneering work of Engquist & Majda [9, 10] in the middle of the seventies using the theory of reflection of singularities at the boundary [14] and pseudodifferential calculus (see for example [21]).

Let us develop the main ideas. Like in the previous situation with constant coefficients, we assume that u as been extended by zero for negative times t and that the initial data u_0

and u_1 are compactly supported in Ω. Then, Engquist and Majda prove that there exist two classical pseudodifferential operator a and b of OPS^1 such that we get the following Nirenberg-like factorization [16]

$$-\partial_x^2+\partial_t^2+\beta(t,x)\partial_t+\gamma(t,x)\partial_x+\alpha(t,x)=-(\partial_x-a(x,t,D_t))(\partial_x-b(x,t,D_t))+R, \qquad (2.10)$$

where R is a smoothing operator of $\mathrm{OPS}^{-\infty}$. This approximate factorization can be considered as the extension to the variable coefficients case of the exact form (2.6). Actually, the smoothing operator R accounts for the fact that the factorization is now true only at high frequencies. The two pseudodifferential operators $a(x,t,D_t)$ and $b(x,t,D_t)$, with $D_t=-i\partial_t$, have respective associated symbols $a(x,t,\tau)$ and $b(x,t,\tau)$ of S^1 admitting the following asymptotic expansions in homogeneous symbols

$$a(x,t,\tau)\sim\sum_{j\geq 0}a_{1-j}(x,t,\tau) \quad \text{and} \quad b(x,t,\tau)\sim\sum_{j\geq 0}b_{1-j}(x,t,\tau), \qquad (2.11)$$

with classical homogeneous symbols a_{1-j} and b_{1-j} of order $1-j$. This means that we have e.g. $a_{1-j}(x,t,\lambda\tau)=\lambda^{1-j}a_{1-j}(x,t,\tau)$, $\forall\lambda>0$. Developing the factorization (2.10), we get

$$-\partial_x^2+\gamma(t,x)\partial_x+\partial_t^2+\beta(t,x)\partial_t+\alpha(t,x)=-\partial_x^2+(a+b)\partial_x-ab+\mathrm{Op}(\partial_x b)+R \qquad (2.12)$$

since $\partial_x(bu)=\mathrm{Op}(\partial_x b)u+b\partial_x u$. In the above equation, we designate by $\mathrm{Op}(\sigma)$ the pseudodifferential operator with symbol σ. If it is possible to compute a and b then, it can be proved that the TBC for equation (2.9) is given by

$$(\partial_{\mathbf{n}}-b(x,t,D_t))u=0, \qquad \text{at } [0;+\infty[\times\Gamma. \qquad (2.13)$$

Indeed, the results in [14] imply that (2.13) annihilates the wave reflected back in the computational domain. Generally speaking, this TBC, which extends (2.8), cannot be directly implemented since b is given by an infinite expansion, but it can however be approximated by a k-th order artificial boundary condition by truncating the series (2.11) to the first k symbolic terms and considering

$$(\partial_{\mathbf{n}}-\sum_{j=0}^{k-1}b_{1-j}(x,t,D_t))u=0, \qquad \text{at } [0;+\infty[\times\Gamma. \qquad (2.14)$$

The computation of the terms $\{b_{1-j}\}_{j=0}^{k-1}$ is therefore needed. To this end, we identify the operators on both sides of equality (2.12) and we obtain at the symbolic level the system

$$\begin{cases} a+b=\gamma \\ -a\#b+\partial_x b=-\tau^2+i\beta\tau+\alpha, \end{cases} \qquad (2.15)$$

which can also be rewritten as

$$b\#b-\gamma b+\partial_x b=-\tau^2+i\beta\tau+\alpha, \qquad (2.16)$$

by eliminating a. In the above notations, $a\#b$ designates the symbol of the composition operator ab which admits the following expansion (see for example [21]):

$$b\#b\sim\sum_{m=0}^{\infty}\frac{(-i)^m}{m!}\partial_\tau^m b\;\partial_t^m b. \qquad (2.17)$$

Since b is developable in terms of homogeneous symbols using relation (2.11), we can extract each term b_{1-j} from (2.16) by identifying the decaying order terms starting from 2 to $2-j$ using (2.17). Beginning with b_1, we get that

$$b_1(x,t,\tau) = i\tau, \tag{2.18}$$

fixing also the uniqueness of the expansion (2.11). Computing the two next terms gives

$$\begin{cases} b_0 = \dfrac{\beta+\gamma}{2}, \\ b_{-1} = \dfrac{(\gamma^2-\beta^2)+4\alpha-2(\partial_x+\partial_t)(\gamma+\beta)}{8i\tau}, \end{cases} \tag{2.19}$$

at the right point x_r. It directly gives the following proposition.

Proposition 2.1. *Let u be the solution to the generalized wave equation (2.9) with $\mathcal{C}^\infty$ variable coefficients α, β and γ. Then, the artificial boundary conditions of order k, for $k = 1, 2, 3$, are respectively given at the right endpoint x_r by*

$$\begin{aligned} &\partial_x u - \partial_t u = 0, \quad \text{at } [0;+\infty[\times\{x_r\}, \\ &\partial_x u - \partial_t u - \frac{\beta+\gamma}{2}u = 0, \quad \text{at } [0;+\infty[\times\{x_r\}, \\ &\partial_x u - \partial_t u - \frac{\beta+\gamma}{2}u - \frac{(\gamma^2-\beta^2)+4\alpha-2(\partial_x+\partial_t)(\gamma+\beta)}{8} I_t u = 0, \quad \text{at } [0;+\infty[\times\{x_r\}, \end{aligned} \tag{2.20}$$

where I_t is defined by $I_t u(t) = \displaystyle\int_0^t u(s)ds$. Similar formulas can be derived at x_ℓ.

2.3 Short-time vs long-time behavior

Let us now consider that we wish to compute a numerical solution to the problem

$$\begin{cases} (\partial_t^2 + \beta(t,x)\partial_t - \partial_x^2 + \gamma(t,x)\partial_x + \alpha(t,x))u = 0, \quad (t,x) \in]0;T[\times\Omega, \\ u(0,x) = u_0(x), \quad x \in \Omega, \\ \partial_t u(0,x) = u_1(x), \quad x \in \Omega, \\ (\partial_{\mathbf{n}} - \displaystyle\sum_{j=0}^{k-1} b_{1-j}^p(x,t,D_t))u = 0, \quad \text{at } [0;T]\times\{x_p\}, \end{cases} \tag{2.21}$$

for a maximal time of computation T and where the k-th artificial boundary condition is defined by operators $\{b_{1-j}^p\}_{j=0}^{k-1}$, for $p = \ell, r$, at the left or right fictitious point x_p (see e.g. Proposition 2.1). Introducing N intervals of discretization in time, we denote by Δt the time step defined by $\Delta t = T/N$. We next seek to compute an approximate solution $u^n(x) \approx u(t_n, x)$ to system (2.21), with $t_n = n\Delta t$, for $n \in \{1, ..., N\}$. We have seen before that the derivation of the artificial boundary conditions at the continuous level is made under the high frequency assumption $|\tau| \gg 1$. Since we consider discrete times t_n, for $n = 1, ..., N$, discrete time frequencies $\tau_n = \pi/t_n$ are then associated and lie in the interval $[\pi/T; \pi/\Delta t]$. Hence, the artificial boundary conditions which work well for high frequencies will be accurate if $T \ll 1$. This means that an artificial boundary

condition is accurate as long as it is used for small times of computation. They may fail for large computational times which is a known problem of artificial boundary conditions techniques (see e.g. [8] [13]).

As an illustration, we compare in Figure 1 the performances of the artificial boundary conditions of order 1, 2 and 3 in the case of the wave equation $(\partial_t^2 + \partial_t - \partial_x^2)u = 0$. We give the relative error in the $L^2(\Omega)$-norm for times between 0 and 10. As predicted by the theory, we notice indeed an improvement for small times by increasing the order. The second order condition is more efficient than the first order condition for all computed times but the third order condition is more efficient than the second order condition only for $t \leq 5.2$.

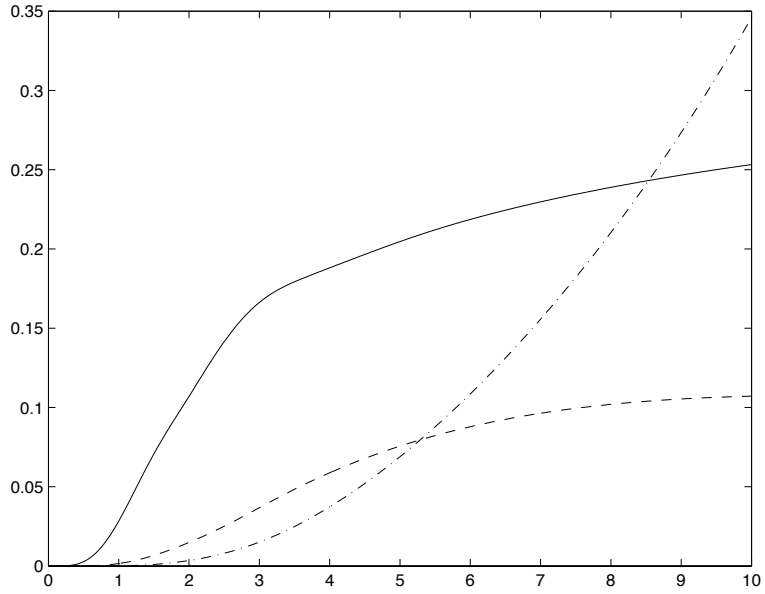


Figure 1: $(\partial_t^2 + \partial_t - \partial_x^2)u = 0$. Relative error in L^2 norm in function of time. abc — order 1, $--$ order 2 and order 3 $\cdot - \cdot$.

3 Different approaches for nonlinear equations: the case of nonlinear Schrödinger equations

3.1 Nonlinear and linear Schrödinger equations

We have seen in Section 2 that it is possible to build accurate artificial boundary conditions using techniques based on pseudodifferential calculus in the model case of the linear wave equation

with variable coefficients. The aim of the present Section is to develop some applications of the pseudodifferential calculus method and its nonlinear version, the paradifferential calculus strategy, to obtain accurate artificial boundary conditions for nonlinear equations. As a model equation, we consider the time dependent nonlinear Schrödinger equation

$$\begin{cases} i\partial_t u + \partial_x^2 u + \alpha(u)\partial_x u + \beta(u)u = 0, \quad (t,x) \in [0;+\infty[\times\mathbb{R}, \\ u(0,x) = u_0(x), \quad x \in \mathbb{R}, \end{cases} \tag{3.1}$$

where we assume again that the initial condition u_0 has compact support in Ω and that α and β are two $\mathcal{C}^\infty$ functions.

Let us now consider the following associated variable coefficients linear Schrödinger equation

$$\begin{cases} i\partial_t u + \partial_x^2 u + A(t,x)\partial_x u + B(t,x)u = 0, \quad (t,x) \in [0;+\infty[\times\mathbb{R}, \\ u(0,x) = u_0(x), \quad x \in \mathbb{R}. \end{cases} \tag{3.2}$$

Extending the previous strategy presented for the variable coefficients wave equation in section 2.2 to equation (3.2), one can prove that there exist two pseudodifferential operators $a(x,t,D_t)$ and $b(x,t,D_t)$ such that we have

$$\partial_x^2 + i\partial_t + A\partial_x + B = (\partial_x - a(x,t,D_t))(\partial_x - b(x,t,D_t)) + R, \tag{3.3}$$

where again $R \in \mathrm{OPS}^{-\infty}$. The operators a and b are elements of $\mathrm{OPS}^{1/2}$ admitting the following expansion in homogeneous symbols

$$a(x,t,\tau) \sim \sum_{j=0}^{\infty} a_{(1-j)/2}(x,t,\tau) \quad \text{and} \quad b(x,t,\tau) \sim \sum_{j=0}^{\infty} b_{(1-j)/2}(x,t,\tau), \tag{3.4}$$

where $a_{(1-j)/2}$ and $b_{(1-j)/2}$ are homogeneous symbols of order $(1-j)/2$. This means that $\forall \lambda > 0$, we have:

$$a_{(1-j)/2}(x,t,\lambda\tau) = \lambda^{(1-j)/2} a_{(1-j)/2}(x,t,\tau), \;\; b_{(1-j)/2}(x,t,\lambda\tau) = \lambda^{(1-j)/2} b_{(1-j)/2}(x,t,\tau). \tag{3.5}$$

If one considers e.g. the right fictitious point x_r, then by fixing $b_{1/2}(x,t,\tau) = -\sqrt{\tau}$, where $\sqrt{\tau}$ is defined by:

$$\sqrt{\tau} = \begin{cases} \sqrt{\tau} \text{ if } \tau \geq 0, \\ -i\sqrt{-\tau} \text{ if } \tau < 0, \end{cases} \tag{3.6}$$

it can be shown (see [17, 20]) that the TBC is given by

$$(\partial_{\mathbf{n}} - b(x,t,D_t))u = 0, \quad \text{at } [0;+\infty[\times\{x_r\}, \tag{3.7}$$

and that an approximate artificial boundary condition of order k is

$$(\partial_{\mathbf{n}} - \sum_{j=0}^{k-1} b_{(1-j)/2}(x,t,D_t))u = 0, \quad \text{at } [0;+\infty[\times\{x_r\}, \tag{3.8}$$

with the convention that the artificial boundary condition of order zero corresponds to the Neumann boundary condition. The required inhomogeneous symbols can be obtained by adapting relation (2.16)

$$b\#b + Ab + \partial_x b = \tau - B, \tag{3.9}$$

using the suitable substitutions. Then, using the Leibniz symbolic rule we get the four first symbols

$$\begin{aligned} &b_{1/2} = -\sqrt{\tau}, b_0 = -\frac{A}{2}, b_{-1/2} = -\frac{1}{2\sqrt{\tau}}(\frac{A^2}{4} - B + \frac{\partial_x A}{2}), \\ &b_{-1} = -\frac{1}{8\tau}(A\partial_x A + \partial_x^2 A - 2\partial_x B + i\partial_t A). \end{aligned} \tag{3.10}$$

To explain the different strategies which can be considered, we propose now to investigate first the case $\alpha = 0$ and next to detail the situation when $\beta = 0$, where α and β are the functions in (3.1).

3.2 Case I: $\alpha = 0$

3.2.1 Potential strategy

The point of view adopted in this strategy considers that $\alpha(u)$ and $\beta(u)$ act as potential functions independent of u. More specifically, they have respectively corresponding functions A and B in Equation (3.2). If we assume that $A = 0$, then, the symbols in (3.10) simplify as

$$b_{1/2} = -\sqrt{\tau}, b_0 = 0, b_{-1/2} = \frac{B}{2\sqrt{\tau}}, b_{-1} = \frac{\partial_x B}{4\tau}. \tag{3.11}$$

Using the definition (3.8), we obtain the following artificial boundary conditions of order k at $[0; +\infty[\times\{x_r\}$

$$\begin{cases} \partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u = 0, & \text{for } k = 1, 2, \\ \partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u - e^{i\frac{\pi}{4}}\dfrac{B}{2} I_t^{1/2} u = 0, & \text{for } k = 3, \end{cases} \tag{3.12}$$

and finally

$$\partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u - e^{i\frac{\pi}{4}}\frac{B}{2} I_t^{1/2} u - i\frac{\partial_{\mathbf{n}} B}{4} I_t u = 0, \quad \text{for } k = 4. \tag{3.13}$$

In the above equations, the fractional half-order derivative operator $\partial_t^{1/2}$, with symbol $\sqrt{-i\tau}$, is given by

$$\partial_t^{1/2} f(t) = \frac{1}{\sqrt{\pi}}\partial_t \int_0^t \frac{f(s)}{\sqrt{t-s}} ds, \tag{3.14}$$

and the half-order integration operator $I_t^{1/2}$ (with symbol $(-i\tau)^{-1/2}$) is defined by

$$I_t^{1/2} f(t) = \frac{1}{\sqrt{\pi}} \int_0^t \frac{f(s)}{\sqrt{t-s}} ds. \tag{3.15}$$

Following our strategy, we replace B by the nonlinearity $\beta(u)$ which gives the three following artificial boundary conditions of order k

$$\begin{cases} \partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} \partial_t^{1/2} u = 0, \quad \text{for } k = 1, 2, \\ \partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} \partial_t^{1/2} u - e^{i\frac{\pi}{4}} \dfrac{\beta(u)}{2} I_t^{1/2} u = 0, \quad \text{for } k = 3, \\ \partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} \partial_t^{1/2} u - e^{i\frac{\pi}{4}} \dfrac{\beta(u)}{2} I_t^{1/2} u - i \dfrac{\partial_{\mathbf{n}} \beta(u)}{4} I_t u = 0, \quad \text{for } k = 4. \end{cases} \tag{3.16}$$

These conditions will be denoted by $ABC_{1,k}^{\beta}$ in the sequel of the paper.

3.2.2 Gauge change strategy

Let us remark that the artificial boundary condition (3.13) is not a transparent boundary condition even when B is a constant potential. Now, in the case of a time-dependent potential $B(x,t) = B(t)$, one can get the transparent boundary condition by using the gauge change

$$v(x,t) = e^{-i\mathcal{B}(t)} u(x,t), \tag{3.17}$$

where $\mathcal{B}(t) = I_t B(t)$, and noticing that v is now solution to the free Schrödinger equation

$$i\partial_t v + \partial_x^2 v = 0. \tag{3.18}$$

Then, the transparent boundary condition

$$\partial_{\mathbf{n}} v + e^{-i\frac{\pi}{4}} \partial_t^{1/2} v = 0 \tag{3.19}$$

holds for v and, coming back to the initial unknown u, we obtain the transparent boundary condition for u

$$\partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} e^{i\mathcal{B}(t)} \partial_t^{1/2} (e^{-i\mathcal{B}(t)} u(x,t)) = 0. \tag{3.20}$$

This boundary condition is clearly not exact if B also depends on x. Nevertheless, we can use a similar change of gauge, that is

$$v(x,t) = e^{-i\mathcal{B}(t,x)} u(x,t), \tag{3.21}$$

with $\mathcal{B}(t,x) = I_t B(t,x)$. Then, v is sought as the solution to the variable coefficients Schrödinger equation

$$i\partial_t v + \partial_x^2 v + (2i\partial_x \mathcal{B})\partial_x v + (i\partial_x^2 \mathcal{B} - (\partial_x \mathcal{B})^2) v = 0, \tag{3.22}$$

which is of the general form (3.2) with initial condition $v(x,0) = u_0(x)$. We can therefore apply the previous general derivation of artificial boundary conditions of Section 3.1 to this equation of unknown v for suitably defined variable coefficients. As a consequence, if $\left\{b_{(1-j)/2}\right\}_{j\geq 0}$ designates the symbolic asymptotic expansion of the transparent boundary condition associated with v solution to (3.22), then an artificial boundary condition of order k is given for u as

$$\partial_{\mathbf{n}} u - \sum_{j=0}^{k-1} e^{i\mathcal{B}} b_{(1-j)/2}(x,t,D_t)(e^{-i\mathcal{B}} u) - i\partial_{\mathbf{n}} \mathcal{B} u = 0, \quad \text{at } [0;+\infty[\times\{x_r\}. \tag{3.23}$$

More precisely, using (3.10), the computation of the first four symbols gives

$$b_1 = -\sqrt{\tau}, \quad b_0 = -i\partial_{\mathbf{n}}\mathcal{B}, \quad b_{-1/2} = 0, \quad b_{-1} = \frac{\partial_{\mathbf{n}} B}{4\tau}. \tag{3.24}$$

Finally, we obtain [3] the second- and fourth-order artificial boundary conditions given respectively by

$$\partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} e^{i\mathcal{B}} \partial_t^{1/2} (e^{-i\mathcal{B}} u) = 0, \qquad \text{at } [0; +\infty[\times\{x_r\}. \tag{3.25}$$

and

$$\partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} e^{i\mathcal{B}} \partial_t^{1/2} (e^{-i\mathcal{B}} u) - i\frac{\partial_{\mathbf{n}} B}{4} e^{i\mathcal{B}} I_t(e^{-i\mathcal{B}} u) = 0, \qquad \text{at } [0; +\infty[\times\{x_r\}. \tag{3.26}$$

Replacing B by $\beta(u)$, the associated nonlinear artificial boundary conditions are then given by

$$\partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} e^{i\mathbb{B}(u)} \partial_t^{1/2} (e^{-i\mathbb{B}(u)} u) = 0, \qquad \text{at } [0; +\infty[\times\{x_r\}. \tag{3.27}$$

and

$$\partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} e^{i\mathbb{B}(u)} \partial_t^{1/2} (e^{-i\mathbb{B}(u)} u) - i\frac{\partial_{\mathbf{n}} \beta(u)}{4} e^{i\mathbb{B}(u)} I_t(e^{-i\mathbb{B}(u)} u) = 0, \qquad \text{at } [0; +\infty[\times\{x_r\}, \tag{3.28}$$

setting $\mathbb{B}(u)(x,t) = I_t(\beta(u))(x,t)$. These conditions will be referred to as $\mathrm{ABC}_{2,j}^{\beta}$ in the sequel, for $j = 2, 4$.

Let us develop the connection existing between the artificial boundary conditions $\mathrm{ABC}_{m,j}^{\beta}$, for $m = 1, 2$ and $j = 2, 4$. To this end, let us recall the following Leibniz formula for computing the fractional derivative of the product of two functions

$$\partial_t^p (fg) = \sum_{k=0}^{\infty} \frac{\Gamma_s(p+1)}{k!\Gamma_s(p-k+1)} \partial_t^k f \partial_t^{p-k} g, \tag{3.29}$$

for $p > 0$. The real-valued function f is supposed to be $\mathcal{C}^\infty$ and g is a continuous function. The notation Γ_s designates the Gamma special function. For $p = 1/2$, we obtain

$$\partial_t^{1/2} (fg) = f\partial_t^{1/2} g + \frac{1}{2}\partial_t f I_t^{1/2} g + R, \tag{3.30}$$

where R is an error operator in $\mathrm{OPS}^{-3/2}$. Using a similar formula for the integral operator gives $I_t(fg) = fI_t g + S$ (with $S \in \mathrm{OPS}^{-2}$). Using these two relations to approximate the half-order operator in (3.26) by setting $f = e^{-i\mathcal{B}}$ and $g = u$, we see that (3.26) exactly corresponds to (3.13) up to an operator in $\mathrm{OPS}^{-3/2}$. This error may be not negligible since is involves time derivatives of the potential, and, in the nonlinear case, of $\beta(u)$. This difference can therefore be significant between the two kinds of artificial boundary conditions. This will be more deeply investigated during the numerical simulations.

3.3 Case II: $\beta = 0$

3.3.1 Potential strategy

Let us now consider the second case where $\beta = 0$. Then, the potential strategy consists in replacing $B = 0$ in (3.10) leading to

$$\begin{aligned} &b_{1/2} = -\sqrt{\tau}, b_0 = -\frac{A}{2}, b_{-1/2} = -\frac{1}{2\sqrt{\tau}}(\frac{A^2}{4} + \frac{\partial_x A}{2}), \\ &b_{-1} = -\frac{1}{8\tau}(A\partial_x A + \partial_x^2 A + i\partial_t A). \end{aligned} \tag{3.31}$$

This gives the following artificial boundary conditions

$$\begin{cases} \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u = 0, \\ \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \dfrac{A}{2}u = 0, \\ \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \dfrac{A}{2}u + \dfrac{e^{i\frac{\pi}{4}}}{2}(\dfrac{A^2}{4} + \dfrac{\partial_x A}{2}) I_t^{1/2} u = 0, \end{cases} \tag{3.32}$$

and

$$\partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \frac{A}{2}u + \frac{e^{i\frac{\pi}{4}}}{2}(\frac{A^2}{4} + \frac{\partial_x A}{2}) I_t^{1/2} u + \frac{i}{8}(A\partial_x A + \partial_x^2 A + i\partial_t A) I_t u = 0, \tag{3.33}$$

at $[0; +\infty[\times\{x_r\}$. Again, replacing A by $\alpha(u)$ yields the nonlinear artificial boundary conditions of order k

$$\begin{cases} \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u = 0, \quad \text{for } k = 1, \\ \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \dfrac{\alpha(u)}{2}u = 0, \quad \text{for } k = 2, \\ \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \dfrac{\alpha(u)}{2}u + \dfrac{e^{i\frac{\pi}{4}}}{2}(\dfrac{\alpha(u)^2}{4} + \dfrac{\partial_x \alpha(u)}{2}) I_t^{1/2} u = 0, \quad \text{for } k = 3, \\ \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \dfrac{\alpha(u)}{2}u + \dfrac{e^{i\frac{\pi}{4}}}{2}(\dfrac{\alpha(u)^2}{4} + \dfrac{\partial_x \alpha(u)}{2}) I_t^{1/2} u \\ \qquad + \dfrac{i}{8}(\alpha(u)\partial_x \alpha(u) + \partial_x^2 \alpha(u) + i\partial_t \alpha(u)) I_t u = 0, \quad \text{for } k = 4. \end{cases} \tag{3.34}$$

The set of above j-th order artificial boundary conditions will be called $\mathrm{ABC}_{1,j}^{\alpha}$ is the sequel, for $j = 1, ..., 4$.

3.3.2 Linearization strategy

We linearize equation (3.1) with $\beta = 0$ around a mean state u and call v its linearization. We obtain

$$i\partial_t v + \partial_x^2 v + \alpha(u)\partial_x v + \alpha'(u)\partial_x u v = 0, \tag{3.35}$$

which is of the form (3.2) with $A = \alpha(u)$ and $B = \alpha'(u)\partial_x u$. Equations (3.10) give

$$\begin{aligned} &b_{1/2} = -\sqrt{\tau}, b_0 = -\frac{\alpha(u)}{2}, b_{-1/2} = -\frac{1}{2\sqrt{\tau}}\left(\frac{\alpha(u)^2}{4} - \frac{\alpha'(u)\partial_x u}{2}\right), \\ &b_{-1} = -\frac{1}{8\tau}(\alpha(u)\partial_x \alpha(u) - \partial_x^2 \alpha(u) + i\partial_t \alpha(u)). \end{aligned} \tag{3.36}$$

This yields absorbing boundary conditions for the linearized problem. To go back to the original problem, we now need to "unlinearize" these boundary conditions.

The first order absorbing boundary condition for v does not involve u and we immediately obtain for u

$$\partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u = 0, \text{ for } k = 1. \tag{3.37}$$

The second order absorbing boundary condition for v reads

$$\partial_x v + e^{-i\frac{\pi}{4}}\partial_t^{1/2} v + \frac{1}{2}\alpha(u)v = 0, \tag{3.38}$$

where $\alpha(u)v$ is the linearization of $\gamma(u)$, where γ is the primitive of α vanishing at 0. Thus, the unlinearization of (3.38) is:

$$\partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \frac{1}{2}\gamma(u) = 0, \text{ for } k = 2. \tag{3.39}$$

The unlinearization of the third and fourth order absorbing boundary conditions of v are far more challenging. We have to unlinearize:

$$\partial_x v + e^{-i\frac{\pi}{4}}\partial_t^{1/2} v + \frac{1}{2}\alpha(u)v + \frac{e^{i\frac{\pi}{4}}\alpha(u)^2}{8} I_t^{1/2}(v) - \frac{e^{i\frac{\pi}{4}}\alpha'(u)\partial_x u}{4} I_t^{1/2}(v) = 0, \tag{3.40}$$

and

$$\begin{aligned}\partial_x v + e^{-i\frac{\pi}{4}}\partial_t^{1/2} v + \frac{1}{2}\alpha(u)v + \frac{e^{i\frac{\pi}{4}}\alpha(u)^2}{8} I_t^{1/2}(v) - \frac{e^{i\frac{\pi}{4}}\alpha'(u)\partial_x u}{4} I_t^{1/2}(v) \\ + \frac{i(\alpha(u)\partial_x\alpha(u) - \partial_x^2\alpha(u) + i\partial_t\alpha(u))}{8} I_t(v).\end{aligned} \tag{3.41}$$

To achieve this goal, we rely on the paradifferential operators of J. M. Bony [6] which are generalization of pseudodifferential operators well-suited to nonlinear problems. We refer to [17] [20] for details about these operators and about the rigorous unlinearization of (3.40) and (3.41). We finally obtain the following nonlinear artificial boundary conditions of order k for u at $[0; +\infty[\times\{x_r\}$:

$$\begin{cases} \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u = 0, & \text{for } k = 1, \\ \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \dfrac{\gamma(u)}{2} = 0, & \text{for } k = 2, \\ \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u + \dfrac{\gamma(u)}{4} - \dfrac{e^{i\frac{\pi}{4}}}{4} I_t^{1/2}(\alpha(u)\partial_x u) = 0, & \text{for } k = 3, \\ \partial_x u + e^{-i\frac{\pi}{4}}\partial_t^{1/2} u - \dfrac{e^{i\frac{\pi}{4}}}{2} I_t^{1/2}(\alpha(u)\partial_x u) \\ \qquad + \dfrac{i}{8} I_t\left(-\alpha'(u)(\partial_x u)^2 + \alpha(u)^2\partial_x u\right) = 0, & \text{for } k = 4, \end{cases} \tag{3.42}$$

where γ is the primitive of α vanishing at 0. From now, these j-th order artificial boundary conditions will be referred to as $\mathrm{ABC}_{2,j}^{\alpha}$, for $j = 1, ..., 4$.

Remark 1. *The unlinearization step of the linearization strategy has been successful not only in the case of* (3.1) *with* $\beta = 0$*, but also in the case of the semilinear wave equation with various nonlinearities (see [19]). However, the unlinearization step of the linearization strategy is not always successful, as shown by the case of the cubic nonlinear Schrödinger equation (see [20]).*

4 Numerical examples

We consider the model Schrödinger equation (3.1) for the two specific cases I ($\alpha = 0$) and II ($\beta = 0$) of section 3. More specifically, we choose to present results in Case I for the nonlinearity $\beta(u) = |u|^2$, which corresponds to the well-known one-dimensional cubic nonlinear Schrödinger equation, and in Case II for $\alpha(u) = u$. We therefore will focus on systems (4.1) and (4.2) respectively given by

$$\begin{cases} i\partial_t u + \partial_x^2 u + |u|^2 u = 0, & (t,x) \in [0;+\infty[\times\mathbb{R}, \\ u(0,x) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{4.1}$$

and

$$\begin{cases} i\partial_t u + \partial_x^2 u + u\partial_x u = 0, & (t,x) \in [0;+\infty[\times\mathbb{R}, \\ u(0,x) = u_0(x), & x \in \mathbb{R}. \end{cases} \tag{4.2}$$

In both cases, we have to our disposal explicit solutions. Concerning system (4.1), we consider the so-called *soliton* solution computed by using the inverse scattering theory and given by

$$u_{\mathrm{ex},\alpha=0}(x,t) = \sqrt{2a}\,\mathrm{sech}(\sqrt{a}(x-ct))\exp(i\frac{c}{2}(x-ct))\exp(i(a+\frac{c^2}{4})t). \tag{4.3}$$

Concerning system (4.2), adapting the Cole-Hopf transform [20] , we have the explicit solution

$$\begin{aligned} u_{\mathrm{ex},\beta=0}(x,t) \;=\; & \int_0^2 \exp\left(i\frac{(x-y)^2}{4t}\right) u_0(y)\exp(\int_0^y \frac{u_0(s)}{2}ds)dy \\ & \times\left(\sqrt{i\pi t} - \int_0^x \exp(i\frac{y^2}{4t})dy + \int_0^2 \exp(i\frac{(x-y)^2}{4t})\exp(\int_0^y \frac{u_0(s)}{2}ds)dy\right. \\ & \left. + \exp(\int_0^2 \frac{u_0(s)}{2}ds)(\sqrt{i\pi t} - \int_0^{2-x} \exp(i\frac{y^2}{4t})dy)\right)^{-1}, \end{aligned} \tag{4.4}$$

which has a compact support in $[0,2]$ at time $t = 0$.

In the two situations, we have to solve a nonlinear equation coupled with nonlinear boundary conditions. The Schrödinger equations are discretized at time $t_{n+1/2} = (t_{n+1} + t_n)/2$ by a second-order approximation. In the sequel, if δt designates the time step, then $t_n = n\delta t$ stands for the n-th time step, where $n \in \mathbb{N}$. The Crank-Nicolson schemes are adapted from the one proposed by Durán and Sanz-Serna [7] and are given by

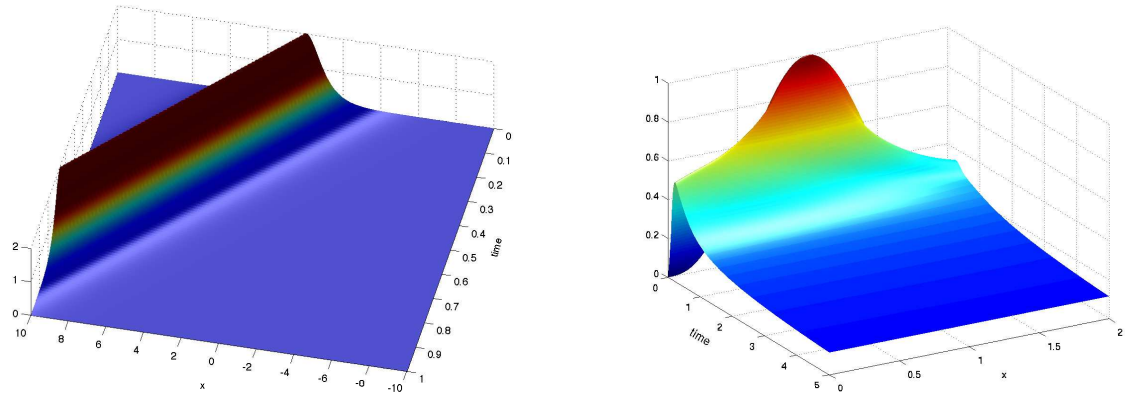
$$i\frac{u^{n+1}-u^n}{\delta t} + \partial_x^2\frac{u^{n+1}+u^n}{2} + \left|\frac{u^{n+1}+u^n}{2}\right|^2\frac{u^{n+1}+u^n}{2} = 0 \tag{4.5}$$

and

$$i\frac{u^{n+1}-u^n}{\delta t} + \partial_x^2\frac{u^{n+1}+u^n}{2} + \frac{u^{n+1}+u^n}{2}\partial_x\left(\frac{u^{n+1}+u^n}{2}\right) = 0 \tag{4.6}$$

respectively for Cases I and II. We denote here by u^n the approximate value of u at time t_n. In order to reduce the computational time, we set $2v^{n+1} = u^{n+1} + u^n$, and the schemes read for $n \geq 0$

$$2i\frac{v^{n+1}-u^n}{\delta t} + \partial_x^2 v^{n+1} + |v^{n+1}|^2 v^{n+1} = 0, \tag{4.7}$$



(a) Case I, $a = 2$, $c = 15$, $\theta = 0$ (b) Case II

Figure 2: Exact solutions representations.

and

$$2i\frac{v^{n+1}-u^n}{\delta t}+\partial_x^2 v^{n+1}+v^{n+1}\partial_x v^{n+1}=0, \tag{4.8}$$

imposing in both cases that $v^0 = 0$. Clearly, a general form of the previous schemes is

$$2i\frac{v^{n+1}-u^n}{\delta t}+\partial_x^2 v^{n+1}+v^{n+1}f(v^{n+1})=0, \tag{4.9}$$

where f designates the map $|\cdot|^2$ or ∂_x according to the equation. The Crank-Nicolson approximation must be coupled to the boundary conditions (3.16), (3.27), (3.28), (3.34) and (3.42). Since the Jacobian of the maps associated to these nonlinear problems is difficult to obtain, we choose to use a classical fixed-point method based on the semi-discrete Crank-Nicolson schemes. The choice of a variational approximation method is thus obvious. Here, we specifically use a $\mathbb{P}_1$ linear Lagrange finite element approximation. The bounded computational domain is the open set $\Omega =]x_l, x_r[$. The fictitious boundary is limited to the two endpoints $\Gamma = \{x_l, x_r\}$. At this point, let us note that the boundary conditions for the case $\beta = 0$ have been given explicitly only at the right endpoint. The left boundary conditions differ. Concerning the potential strategy, the system of equations (3.34) is transformed on $[0; +\infty[\times\{x_l\}$ as:

$$\begin{cases}
\partial_x u - e^{-i\frac{\pi}{4}}\partial_t^{1/2}u = 0, \quad \text{for } k=1,\\
\partial_x u - e^{-i\frac{\pi}{4}}\partial_t^{1/2}u + \dfrac{\alpha(u)}{2}u = 0, \quad \text{for } k=2,\\
\partial_x u - e^{-i\frac{\pi}{4}}\partial_t^{1/2}u + \dfrac{\alpha(u)}{2}u - \dfrac{e^{i\frac{\pi}{4}}}{2}\left(\dfrac{\alpha(u)^2}{4}+\dfrac{\partial_x\alpha(u)}{2}\right)I_t^{1/2}u = 0, \quad \text{for } k=3,\\
\partial_x u - e^{-i\frac{\pi}{4}}\partial_t^{1/2}u + \dfrac{\alpha(u)}{2}u - \dfrac{e^{i\frac{\pi}{4}}}{2}\left(\dfrac{\alpha(u)^2}{4}+\dfrac{\partial_x\alpha(u)}{2}\right)I_t^{1/2}u\\
\qquad\qquad +\dfrac{i}{8}(\alpha(u)\partial_x\alpha(u)+\partial_x^2\alpha(u)+i\partial_t\alpha(u))I_t u = 0, \quad \text{for } k=4.
\end{cases} \tag{4.10}$$

Concerning the linearization strategy, we get on $[0;+\infty[\times\{x_l\}$:

$$\begin{cases} \partial_x u - e^{-i\frac{\pi}{4}}\partial_t^{1/2}u = 0, \quad \text{for } k=1, \\ \partial_x u - e^{-i\frac{\pi}{4}}\partial_t^{1/2}u + \dfrac{\gamma(u)}{2} = 0, \quad \text{for } k=2, \\ \partial_x u - e^{-i\frac{\pi}{4}}\partial_t^{1/2}u + \dfrac{\gamma(u)}{4} + \dfrac{e^{i\frac{\pi}{4}}}{4} I_t^{1/2}(\alpha(u)\partial_x u) = 0, \quad \text{for } k=3, \\ \partial_x u - e^{-i\frac{\pi}{4}}\partial_t^{1/2}u + \dfrac{e^{i\frac{\pi}{4}}}{2} I_t^{1/2}(\alpha(u)\partial_x u) \\ \qquad + \dfrac{i}{8} I_t\left(-\alpha'(u)(\partial_x u)^2 + \alpha(u)^2\partial_x u\right) = 0, \quad \text{for } k=4, \end{cases} \tag{4.11}$$

where γ is the primitive of α vanishing at 0.

The boundary conditions are of memory-type and involve half-order fractional derivatives and integrals. To preserve the second-order approximation and the unconditional stability of the Crank-Nicolson schemes, the operators $\partial_t^{1/2}$ and $I_t^{1/2}$ are approximated through quadrature rules which are well suited to the Crank-Nicolson schemes. Namely, we choose the quadrature formulas derived in [1], which read for the sequence of complex values $\{f_n\}_{n\in\mathbb{N}}$ approximating $\{f(t_n)\}_{n\in\mathbb{N}}$,

$$I_t^{1/2} f(t_n) \approx \frac{\sqrt{2\delta t}}{2}\sum_{k=0}^{n}\alpha_k f^{n-k} \text{ and } \partial_t^{1/2} f(t_n) \approx \frac{2}{\sqrt{2\delta t}}\sum_{k=0}^{n}\beta_k f^{n-k}, \tag{4.12}$$

where $(\alpha_k)_{k\in\mathbb{N}}$ and $(\beta_k)_{k\in\mathbb{N}}$ designate the sequences defined by

$$\begin{cases} (\alpha_0,\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5,\cdots) = \left(1,1,\dfrac{1}{2},\dfrac{1}{2},\dfrac{1\cdot 3}{2\cdot 4},\dfrac{1\cdot 3}{2\cdot 4},\cdots\right), \\ \beta_k = (-1)^k\alpha_k, \ \forall k \geq 0. \end{cases}$$

The composition of the approximation of $I_t^{1/2}$ with itself gives the approximation of I_t by the trapezoidal rule, which is coherent with the underlying Crank Nicolson scheme. Using these quadratures formulas, the numerical versions of the boundary conditions (3.16), (3.27), (3.28), (3.34) and (3.42) are discrete convolutions which may be represented by the following formulation

$$\partial_{\mathbf{n}} v^{n+1} + e^{-i\frac{\pi}{4}}\sqrt{\frac{2}{\delta t}}v^{n+1} + g(v^{n+1},v^n,v^{n-1},\cdots,v^0) = 0,$$

where g is a function giving information on the construction of the approximation. For example, the approximation of $ABC_{1,3}^{\beta}$ is given by

$$\partial_{\mathbf{n}} v^{n+1} + e^{-i\frac{\pi}{4}}\sqrt{\frac{2}{\delta t}}\sum_{k=0}^{n+1}\beta_k v^{n+1-k} - \frac{e^{i\frac{\pi}{4}}}{2}|v^{n+1}|\frac{\sqrt{2\delta t}}{2}\sum_{k=0}^{n+1}\alpha_k|v^{n+1-k}|v^{n+1-k} = 0.$$

The other approximations of $ABC_{j,k}^{\alpha,\beta}$, $j=1,2$, $k=1,2,3$ can be found in [3] and [20]. The complete Crank Nicolson scheme with fixed point procedure therefore takes the form given in Table 1.

let $w^0 = u^n$
$s = 0$
while $\|w^{s+1} - w^s\|_{L^2(\Omega_i)} > \varepsilon$ do
solve the linear boundary-value problem

$$\int_\Omega \frac{2i}{\delta t} w^{s+1}\psi dx - \int_\Omega \partial_x w^{s+1}\partial_x \psi dx - \int_\Gamma e^{-i\frac{\pi}{4}}\sqrt{\frac{2}{\delta t}} w^{s+1}\psi d\Gamma = - \int_\Omega f(w^s)w^s\psi dx + \int_\Omega \frac{2i}{\delta t} u^n \psi dx + \int_\Gamma g^s \psi d\Gamma,$$

setting
$g^s = g(w^s, v^n, v^{n-1}, \cdots, v^0)$
and ψ is one of the basis functions of the P1 finite element set.
end while
$v^{n+1} = w^{s+1}$
$u^{n+1} = 2v^{n+1} - u^n$

Table 1: Fixed-point algorithm for solving the nonlinear Schrödinger equation with nonlinear ABC.

We present below some numerical experiments to show the effectiveness of the different boundary conditions. Since we have an exact solution in Cases I and II, we choose to evaluate the schemes on the solutions with initial data (4.3) and (4.4) respectively. Concerning Case I, the computational domain is limited to the open set $(-10, 10)$ discretized with 4000 points. The time step is fixed to $\delta t = 10^{-3}$. In Case II, the finite domain is $(0, 2)$ discretized with 2000 points. The time step δt is equal to $2 \cdot 10^{-3}$. To analyze the accuracy of the different boundary conditions, we compute the relative error for the $L^2(\Omega)$-norm

$$\frac{\|u_{\text{ex}} - u_{\text{num}}\|_{0,\Omega}(t)}{\|u_{\text{ex}}\|_{0,\Omega}(t=0)},$$

where u_{num} denotes the numerical solution.

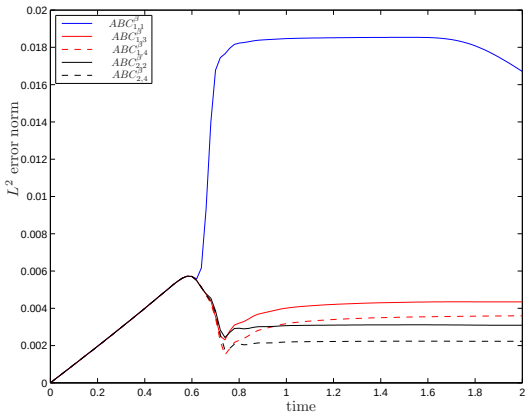


Figure 3: Evolution of the relative error for Case I, $a = 2$, $c = 15$, $\theta = 0$.

For case I, we compare in Figure 3 the ABCs obtained with the potential strategy and the gauge change strategy for various orders. We can see that increasing the order improves the accuracy. Moreover, the gauge change strategy ($ABC^{\beta}_{2,k}$) provides better accuracy compared to the potential strategy ($ABC^{\beta}_{1,k}$). Finally, let us also notice that the long-time behaviour of the various ABCs seems correct. To analyze the accuracy behaviour of the computed solution with respect to the velocity parameter, we plot on Fig. 4 the evolution of the relative error with respect to c for the most accurate ABC: $ABC^{\beta}_{2,2}$. We see that the relative error increases with lower velocities. This is in agreement with the theory developed in the paper since the boundary conditions are constructed under a high-frequency assumption.

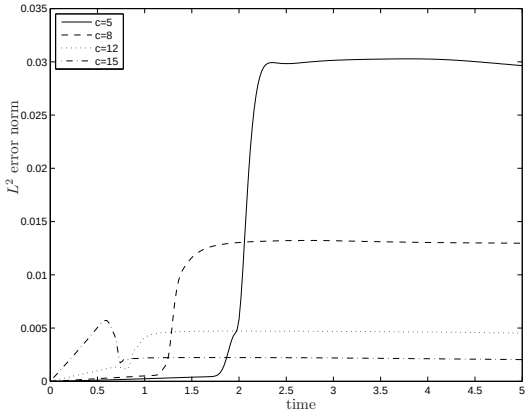


Figure 4: Evolution of the relative error for the simulation of the soliton solution with respect to the velocity c for $ABC^{\beta}_{2,2}$.

In our last experiment, we focus on case II. We compare in Figure 5 the ABCs obtained with the potential strategy and the linearization strategy for various orders. Generally, the linearization strategy leads to the most accurate solutions. Increasing the order of the ABC improves the accuracy for small times ($t \leq 2.5$ in the experiments). After this time, the relative errors cross and the best results are obtained for $ABC^{\alpha}_{2,2}$. The potential strategy is accurate and competitive for $ABC^{\alpha}_{1,3}$ but only for sufficiently large computational times. This shows that each strategy has his own strengths and weaknesses. Finally, let us mention that $ABC^{\alpha}_{2,2}$ has been shown to give optimal results within a large class of ABCs (see [18]).

5 Conclusion

We presented an analysis of the construction and some numerical validations of ABCs for nonlinear PDEs considering the example of the nonlinear Schrödinger equation. The methods are mainly based on pseudo- and paradifferential operator techniques. We show that each strategy can lead to powerful solutions. However, much work remains to be done. In particular, developing rigorous extensions for higher dimensions, coupled problems and systems is a complete open problem.

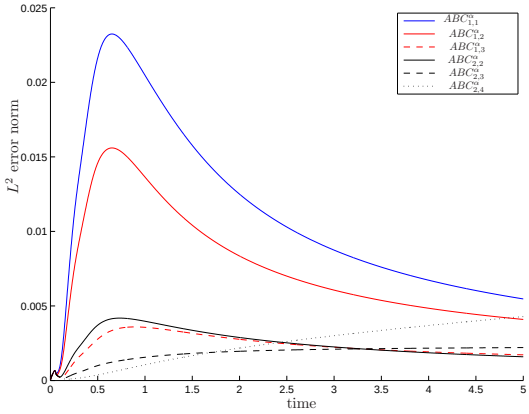


Figure 5: Relative error for Case II.

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