Accepted Manuscript

Time exponential splitting integrator for the Klein–Gordon equation with free parameters in the Hagstrom–Warburton absorbing boundary conditions

I. Alonso-Mallo, A.M. Portillo

| PII: | S0377-0427(17)30547-2 | |
|-----------------|-----------------------------------------------------|--|
| DOI: | https://doi.org/10.1016/j.cam.2017.10.02 | |
| Reference: | CAM 11368 | |
| To appear in: | Journal of Computational and Applied Mathematics | |
| Received date : | 14 December 2016 | |
| Revised date : | 28 July 2017 | |



Please cite this article as: I. Alonso-Mallo, A.M. Portillo, Time exponential splitting integrator for the Klein–Gordon equation with free parameters in the Hagstrom–Warburton absorbing boundary conditions, *Journal of Computational and Applied Mathematics* (2017), https://doi.org/10.1016/j.cam.2017.10.038

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Time exponential splitting integrator for the Klein-Gordon equation with free parameters in the Hagstrom-Warburton absorbing boundary conditions

I. Alonso-Mallo^{a,1}, A. M. Portillo^{b,1,*}

^aIMUVA, Departamento de Matemática Aplicada, Facultad de Ciencias, Universidad de Valladolid, Spain ^bIMUVA, Departamento de Matemática Aplicada, Escuela de Ingenierías Industriales, Universidad de Valladolid, Spain

Abstract

The Klein-Gordon equation on an infinite two dimensional strip is considered. Numerical computation is reduced to a finite domain by using the Hagstrom-Warburton (H-W) absorbing boundary conditions (ABCs) with free parameters in the formulation of the auxiliary variables. The spatial discretization is achieved by using fourth order finite differences and the time integration is made by means of an efficient and easy to implement fourth order exponential splitting scheme which was used in [5] considering the fixed Padé parameters in the formulation of the ABCs. Here, we generalize the splitting time technique to other choices of the parameters. To check the time integrator we consider, on one hand, four types of fixed parameters, the Newmann's parameters, the Chebyshev's parameters, the Padé's parameters and optimal parameters proposed in [13] and, on the other hand, an adaptive scheme for the dynamic control of the splitting scheme by comparing with the fourth-order four-stage Runge-Kutta method.

Keywords:

Splitting methods, Absorbing boundary conditions, Dispersive waves,

^{*}Corresponding author. Tel:+34 983184547 Fax:+34 983423490

Email addresses: isaias@mac.uva.es (I. Alonso-Mallo), anapor@mat.uva.es (A. M. Portillo)

 $^{^1{\}rm This}$ work has obtained financial support from project MTM2015-66837-P of Ministerio de Economía y Competitividad

Auxiliary variables, Artificial boundary, Finite differences 2000 MSC: 65M12, 65M20

1. Introduction

We consider dispersive waves propagating in the infinite two dimensional strip $(-\infty, \infty) \times [a, b]$. The south and north boundaries of the strip are denoted by Γ_S and Γ_N . Inside the strip, we consider the Klein-Gordon equation,

$$\partial_t^2 u - c^2 \nabla^2 u + s^2 u = f, \tag{1}$$

where c = c(x, y) is the given wave speed, s = s(x, y) is the medium dispersion coefficient, and f(x, y, t) is a given source.

On the south and north boundaries we impose periodic boundary conditions,

$$u(x, y_S, t) = u(x, y_N, t), \quad \partial_y u(x, y_S, t) = \partial_y u(x, y_N, t).$$
(2)

Finally, we consider the initial conditions,

$$u(x, y, 0) = u_0(x, y), \quad \partial_t u(x, y, 0) = v_0(x, y),$$
(3)

which satisfy the boundary conditions on Γ_S and Γ_N , and vanish outside a compact region $\Omega_0 \subset (-\infty, \infty) \times [a, b]$.

In order to obtain a numerical approximation of these problems, it is necessary to reduce the computation to a finite domain. For this, the infinite strip is truncated by introducing the west artificial boundary Γ_W , located at $x = x_W$, $a \leq y \leq b$, and the east artificial boundary Γ_E at $x = x_E$, $a \leq y \leq b$. We denote by Ω the computational domain bounded by $\Gamma_N \cup \Gamma_W \cup \Gamma_S \cup \Gamma_E$. The domain Ω must be chosen such that $\Omega_0 \subset \Omega$.

Now, we define suitable artificial boundary conditions on the artificial boundaries Γ_W and Γ_E by using ABCs, which are designed to produce small reflections inside the computational domain and to have local character. There are many works on this subject, see the works [6, 7, 10, 13, 14, 15, 16, 17] and the review papers [9, 11, 12, 25].

As an alternative, it can be first considered a space discretization of the problem and then to obtain ABCs for the discrete problem. We have worked in this sense for example in [2, 3, 4].



The H-W ABCs use auxiliary variables to avoid high derivatives in their formulation in such a way that arbitrary order of absorption P can be achieved by introducing P auxiliary variables ϕ_j , $j = 1, \ldots, P$, satisfying the recursive relations

$$\begin{aligned} &(a_0\partial_t + c\partial_x)u &= a_0\partial_t\phi_1, \\ &(a_j\partial_t + c\partial_x)\phi_j &= (a_j\partial_t - c\partial_x)\phi_{j+1}, \quad j = 1, \dots, P, \\ &\phi_{P+1} = 0, \end{aligned}$$

$$(4)$$

in the vicinity of Γ_E . The parameters a_j mean cosines of incidence angles and it is natural to take $0 < a_j \leq 1$. The choice $a_j = 1$ is associated with normal incidence. If a plane wave with incident angle θ reaches Γ_E and one of the a_j coincides with $\cos(\theta)$, the ABC is then exact and non spurious reflection is generated [13]. The problem is that, in practical applications, usually the angles of incidence are not known a priori. In [5], we built a splitting time integrator considering $a_j = 1$ for all j. In this article, we generalize this technique in order to use other choices of the parameters a_j , including the optimal and adaptive cases.

From the assumption that the initial conditions have compact support away from Γ_W and Γ_E , we have,

$$\phi_j(y,0) = 0, \quad \partial_t \phi_j(y,0) = 0 \quad \text{on} \quad \Gamma_W, \Gamma_E.$$

We choose $a_0 = 1$. In [15], it is established that the H-W ABCs of order P given by (4) may be rewritten as

$$(\partial_t + c\partial_x)u = \partial_t \phi_1, l_{11}\partial_t^2 \phi_1 + l_{12}\partial_t^2 \phi_2 = c^2(m_{10}\partial_y^2 \phi_0 + m_{11}\partial_y^2 \phi_1 + m_{12}\partial_y^2 \phi_2) -s^2(m_{10}\phi_0 + m_{11}\phi_1 + m_{12}\phi_2), l_{jj-1}\partial_t^2 \phi_{j-1} + l_{jj}\partial_t^2 \phi_j + l_{jj+1}\partial_t^2 \phi_{j+1} = c^2(m_{jj-1}\partial_y^2 \phi_{j-1} + m_{jj}\partial_y^2 \phi_j + m_{jj+1}\partial_y^2 \phi_{j+1})$$
(5)
 $-s^2(m_{jj-1}\phi_{j-1} + m_{jj}\phi_j + m_{jj+1}\phi_{j+1}),$
 $j = 2, \dots, P,$
 $u = \phi_0, \quad \phi_{P+1} = 0,$

where

$$l_{11} = (1 + a_1)^2, l_{12} = 1 - a_1^2, m_{10} = 2a_1, m_{11} = 1, m_{12} = 1, and, for $j = 2, \dots, P, l_{jj-1} = a_j(1 - a_{j-1}^2), l_{jj} = a_j(1 + a_{j-1}^2) + a_{j-1}(1 + a_j^2), l_{jj+1} = a_{j-1}(1 - a_j^2), , m_{jj-1} = a_j, m_{jj} = a_{j-1} + a_j, m_{jj-1} = a_{j-1}.$

$$(6)$$$$

We write $L = [l_{ij}]_{i,j=1}^{P}$, which is a tridiagonal strictly diagonally dominant matrix. Therefore, the Gaussian elimination can be used without pivoting to solve a linear system of equations with coefficient matrix L and it is numerically stable.

On the boundary Γ_W , the first equation in (5) has to be replaced by $(\partial_t - c\partial_x)u = \partial_t\phi_1$, but all other conditions are the same.

The space discretization is reached by means of fourth order finite differences. For the time discretization, we propose a fourth order exponential splitting method which improves the computational efficiency of the time integration. We show the improvement by comparing the splitting scheme with the standard fourth-order four-stage Runge-Kutta method used in [17]. Useful overviews of splitting methods can be found in the review papers [8, 22].

The paper is organized as follows. Section 2 is devoted to show the feasibility of the time and space discretization when it is applied to the simple case of finite domain with periodic boundary conditions. In Section 3, the ABCs are added in the one dimensional case, and the full discretization is modified in a suitable way. A similar full discretization for the two dimensional case, also with ABCs, is studied in Section 4. Numerical experiments for the latter two dimensional case are presented in Section 5.

2. Two dimensional Klein-Gordon equation with periodic boundary conditions.

We consider the problem with periodic boundary conditions,

$$u(a, y, t) = u(b, y, t), \quad y \in [c, d],$$
 (7)

$$\partial_x u(a, y, t) = \partial_x u(b, y, t), \quad y \in [c, d],$$
(8)

$$u(x, c, t) = u(x, d, t), \qquad x \in [a, b],$$
(9)

$$\partial_y u(x,c,t) = \partial_y u(x,d,t), \quad x \in [a,b].$$
(10)

The initial conditions, $u_0(x, y)$ and $v_0(x, y)$, satisfy periodic boundary conditions in $[a, b] \times [c, d]$.

2.1. Spatial discretization

We take the same size step in both directions x and y, that is, for a value of N, $h = \frac{b-a}{N}$ and $M = \frac{d-c}{h}$. Let $x_j = a + (j-1)h$, $j = 1, \ldots, N+1$, and $y_l = c + (l-1)h$, $l = 1, \ldots, M+1$, be the nodes of the spatial discretization. This produces a uniform grid in the computational domain with M+1 rows and N+1 columns. We denote $u_{jl}(t) = u(x_j, y_l, t)$.

Second order spatial derivatives in the direction x and in the direction y are approximated by fourth order central finite differences

$$\partial_{xx} u_{jl} \approx \frac{1}{h^2} \left(-\frac{1}{12} u_{j-2,l} + \frac{4}{3} u_{j-1,l} - \frac{5}{2} u_{jl} + \frac{4}{3} u_{j+1,l} - \frac{1}{12} u_{j+2,l} \right),$$

$$\partial_{yy} u_{jl} \approx \frac{1}{h^2} \left(-\frac{1}{12} u_{j,l-2} + \frac{4}{3} u_{j,l-1} - \frac{5}{2} u_{jl} + \frac{4}{3} u_{j,l+1} - \frac{1}{12} u_{j,l+2} \right),$$

or, equivalently, in stencil form,

respectively.

We consider \mathbf{u}_j the approximations to the unknowns $(u(x_j, y_1), \ldots, u(x_j, y_{M+1}))^T$, for fixed x_j , and we denote $\mathbf{u}_h = [\mathbf{u}_1^T, \ldots, \mathbf{u}_{N+1}^T]^T$. Then, the spatial semidiscrete problem is

$$\frac{d^2 \mathbf{u}_h}{dt^2} = A \mathbf{u}_h,\tag{11}$$

where
$$A = \frac{c^2}{12h^2}B - s^2I$$
, with

$$B = \begin{bmatrix} B_1 & B_2 & B_3 & B_3 & B_2 \\ B_2 & B_1 & B_2 & B_3 & B_3 \\ B_3 & B_2 & B_1 & B_2 & B_3 & B_3 \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & B_3 & B_2 & B_1 & B_2 & B_3 \\ B_3 & & & B_3 & B_2 & B_1 & B_2 \\ B_2 & B_3 & & & B_3 & B_2 & B_1 \end{bmatrix}.$$
(12)

Notice that B is a circulant block matrix

$$B = circ(B_1, B_2, B_3, 0, \dots, 0, B_3, B_2),$$

whose blocks are, in turn, circulant matrices of dimension $(M+1) \times (M+1)$.

$$B = circ(B_1, B_2, B_3, 0, \dots, 0, B_3, B_2),$$

$$B_1 = circ(-60, 16, -1, 0, \dots, 0, -1, 16),$$

$$B_2 = circ(16, 0, \dots, 0),$$

$$B_3 = circ(-1, 0, \dots, 0).$$

Lemma 1. The eigenvalues of matrix B in (12), satisfy

$$\sigma(B) \subset [-128, 0]. \tag{13}$$

 $\mathit{Proof.}$ We consider the following polynomials associated to the blocks of matrix B

$$h_1(z) = -60 + 16z - z^2 - z^{M-1} + 16z^M,$$

$$h_2(z) = 16,$$

$$h_3(z) = -1,$$

$$h_N(z) = -1,$$

$$h_{N+1}(z) = 16.$$

Then, the eigenvalues of matrix B are (see [20, 21])

$$\lambda_{l,k} = \tilde{\varepsilon}_l^0 h_1(\tilde{\omega}_k) + \tilde{\varepsilon}_l h_2(\tilde{\omega}_k) + \tilde{\varepsilon}_l^2 h_3(\tilde{\omega}_k) + \tilde{\varepsilon}_l^{N-1} h_N(\tilde{\omega}_k) + \tilde{\varepsilon}_l^N h_{N+1}(\tilde{\omega}_k),$$

for l = 1, ..., N + 1, k = 1, ..., M + 1, where

$$\omega_{M+1} = \exp(\frac{2\pi i}{M+1}), \quad \tilde{\omega}_k = (\omega_{M+1})^k,$$

$$\varepsilon_{N+1} = \exp(\frac{2\pi i}{N+1}), \quad \tilde{\varepsilon}_l = (\varepsilon_{N+1})^l.$$

That is,

$$\lambda_{l,k} = -60 + 16 \exp(\frac{2\pi i k}{M+1}) - \exp(\frac{2\pi i k}{M+1}2) - \exp(\frac{2\pi i k}{M+1}(M-1)) + 16 \exp(\frac{2\pi i k}{M+1}M) + 16 \exp(\frac{2\pi i l}{N+1}) - \exp(\frac{2\pi i l}{N+1}2) - \exp(\frac{2\pi i l}{N+1}(N-1)) + 16 \exp(\frac{2\pi i l}{N+1}N) = -60 + 32 \cos(\frac{2\pi k}{M+1}) - 2 \cos(\frac{2\pi k}{M+1}2) + 32 \cos(\frac{2\pi l}{N+1}) - 2 \cos(\frac{2\pi l}{N+1}2).$$

Now, by using that $\cos(2z) = 2\cos^2(z) - 1$,

$$\lambda_{l,k} = -56 + 32\cos(\frac{2\pi k}{M+1}) - 4\cos^2(\frac{2\pi k}{M+1}) + 32\cos(\frac{2\pi l}{N+1}) - 4\cos^2(\frac{2\pi l}{N+1})$$

We deduce that $\lambda_{l,k} \in D = \{ f(x,y) : (x,y) \in [-1,1] \times [-1,1] \}$, where

$$f(x,y) = -56 + 32x + 32y - 4x^2 - 4y^2.$$

We are going to prove that $D \subset [-128, 0]$. For that, we calculate the absolute extrema of the continuous function f(x, y) on the compact domain $[-1, 1] \times [-1, 1]$.

Firstly, we look for the possible extrema of f(x, y) in $(-1, 1) \times (-1, 1)$, which have to satisfy

$$\frac{\partial f}{\partial x}(x,y) = 32 - 8x = 0, \tag{14}$$

$$\frac{\partial f}{\partial y}(x,y) = 32 - 8y = 0, \tag{15}$$

but the unique solution of (14) and (15) is the point (4,4), which does not belong to $(-1,1) \times (-1,1)$.

Now, we study the function f(x, y) on the boundary. The possible extrema of f(x, y) in $\{x \in (-1, 1), y = -1\}$, are the critic points of the Lagrange

auxiliary function $F(x, y) = f(x, y) + \lambda(y + 1)$, which have to satisfy

$$\frac{\partial F}{\partial x}(x,y) = 32 - 8x = 0, \tag{16}$$

$$\frac{\partial F}{\partial y}(x,y) = 32 - 8y + \lambda = 0, \tag{17}$$

$$y = -1. \tag{18}$$

Equation (16) does not have any solution in (-1, 1). A similar study can be done when $\{x \in (-1, 1), y = 1\}$, $\{y \in (-1, 1), x = -1\}$ and $\{y \in (-1, 1), x =$ 1 $\}$. Therefore, the extrema of f(x, y) in $[-1, 1] \times [-1, 1]$ are achieved in some of the points (-1, -1), (-1, 1), (1, -1), (1, 1). As f(-1, -1) = -128, f(-1, 1) = -64, f(1, -1) = -64, f(1, 1) = 0, the absolute minimum of f(x, y) in $[-1, 1] \times [-1, 1]$ is -128 and the absolute maximum is 0. We conclude (13).

Proposition 2. The matrix

$$A = \frac{c^2}{12h^2}B - s^2I$$

is symmetric negative definite and

$$\sigma(A) \subset \left[-\frac{128c^2}{12h^2} - s^2, -s^2\right].$$
(19)

Proof. As the matrix B in (12) is symmetric, this is also true for the matrix A. Moreover, (19) is a direct consequence of Lemma 1.

Now, the discrete energy

$$E_h(t) = \frac{h^2}{2} \left(\mathbf{v}_h^T \mathbf{v}_h - \mathbf{u}_h^T A \mathbf{u}_h \right), \qquad (20)$$

where $\mathbf{v}_h = \begin{bmatrix} \frac{d}{dt} \mathbf{u}_1^T, \dots, \frac{d}{dt} \mathbf{u}_{N+1}^T \end{bmatrix}^T$, is conserved because $\frac{dE_h}{dt}(t) = 0$ and we deduce that the semidiscrete problem (11) is well posed.

2.2. Time integration

We rewrite the problem (11) as a first order ordinary differential system,

$$\frac{d}{dt} \begin{bmatrix} \mathbf{u}_h \\ \mathbf{v}_h \end{bmatrix} = \begin{bmatrix} 0 & I \\ A & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_h \\ \mathbf{v}_h \end{bmatrix}, \qquad (21)$$

where $\mathbf{v}_h = [\frac{d}{dt}\mathbf{u}_1^T, \dots, \frac{d}{dt}\mathbf{u}_{N+1}^T]^T.$

We want to discretize in time the problem (21). For this, we now define a time numerical scheme which will be used to advance a time step size k > 0. We begin by splitting

$$\begin{bmatrix} 0 & I \\ A & 0 \end{bmatrix} = \begin{bmatrix} 0 & I \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ A & 0 \end{bmatrix} := M_1 + M_2.$$
(22)

Since M_1 and M_2 are nilpotent matrices with degree 2 (that is, $M_i^2 = 0$, for i = 1, 2), we can obtain the exact flows of the problems

$$\frac{d}{dt} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = M_i \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}, \quad i = 1, 2,$$

which are given by,

$$\Psi_{k}^{[1]} : \exp(kM_{1}) \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{u} + k\mathbf{v} \\ \mathbf{v} \end{bmatrix},$$
$$\Psi_{k}^{[2]} : \exp(kM_{2}) \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} + kA\mathbf{u} \end{bmatrix}.$$

Now, we combine these intermediate flows to obtain a numerical approximation of the solution of (21). First, we consider the second order Strang scheme splitting

$$\mathcal{S}_{k}^{[2]} = \Psi_{k/2}^{[1]} \circ \Psi_{k}^{[2]} \circ \Psi_{k/2}^{[1]}, \tag{23}$$

and, in turn, we combine $\mathcal{S}_{k}^{[2]}$ to obtain the fourth order scheme [24, 26],

$$\mathcal{S}_{k}^{[4]} = \mathcal{S}_{\alpha k}^{[2]} \circ \mathcal{S}_{\beta k}^{[2]} \circ \mathcal{S}_{\alpha k}^{[2]}, \qquad (24)$$

where $\alpha = (2 - 2^{1/3})^{-1}$ and $\beta = 1 - 2\alpha$.

We remark that it is possible to save some computational cost in (24) by join together the last step in the composition of $S_{\alpha k}^{[2]}$ and the first one in $S_{\beta k}^{[2]}$ and, similarly, the last one in the composition of $S_{\beta k}^{[2]}$ and the first one in $S_{\alpha k}^{[2]}$. That is,

$$\mathcal{S}_{k}^{[4]} = \psi_{\alpha k/2}^{[1]} \circ \psi_{\alpha k}^{[2]} \circ \psi_{\alpha k/2}^{[1]} \circ \psi_{\beta k/2}^{[2]} \circ \psi_{\beta k}^{[2]} \circ \psi_{\beta k/2}^{[1]} \circ \psi_{\alpha k/2}^{[2]} \circ \psi_{\alpha k}^{[2]} \circ \psi_{\alpha k/2}^{[1]},
= \psi_{\alpha k/2}^{[1]} \circ \psi_{\alpha k}^{[2]} \circ \psi_{(\alpha + \beta) k/2}^{[1]} \circ \psi_{\beta k}^{[2]} \circ \psi_{(\alpha + \beta) k/2}^{[1]} \circ \psi_{\alpha k}^{[2]} \circ \psi_{\alpha k/2}^{[1]}.$$
(25)

In a similar way, if many steps are performed without output, only three evaluations of $\psi^{[1]}$ and $\psi^{[2]}$ are required per time step.

In this way, we have obtained a full discretization whose order of consistency is four in space and time. Moreover, the time integration method $S_k^{[4]}$ is explicit and easily implementable. However, it is not unconditionally stable and the stability must be studied. As it is shown in [23], the stability interval of the splitting scheme (24) is $[0, \omega_*]$, where

$$\omega_* = \sqrt{\frac{-1 + \sqrt{1 + 1152\gamma}}{48\gamma}}, \ \gamma = \frac{6 + 5 \cdot 2^{1/3} + 4 \cdot 2^{2/3}}{36}.$$

A necessary condition for stability is that [1],

$$k(-\lambda)^{1/2} \in [0, \omega_*],$$

for all $\lambda \in \sigma(A)$.

From Proposition 2, we deduce the stability condition

$$\frac{ck}{h}\sqrt{\frac{128}{12} + \frac{s^2h^2}{c^2}} < \omega_* \approx 0.9711.$$

If we suppose that sh is small enough, we obtain the simpler stability condition

$$\frac{ck}{h} < \frac{\sqrt{12}\,\omega^*}{\sqrt{128}} \approx 0.2973.$$
 (26)

3. One dimensional Klein-Gordon equation with H-W ABCs

To make it easier, we start considering the full discretization of the one dimensional Klein-Gordon equation with H-W ABCs. We will translate the method to the two-dimensional case in the following section.

The problem in one dimension reduces to

$$\partial_t u(x_W, t) = c \partial_x u(x_W, t) + \partial_t \phi_1^W, \qquad (27)$$

$$\partial_t^2 u(x,t) = c^2 \partial_x^2 u(x,t) - s^2 u(x,t), \quad x_W < x < (28),$$

$$\partial_t u(x_E, t) = -c \partial_x u(x_E, t) + \partial_t \phi_1^E,$$
 (29)

$$l_{11}\frac{d^2}{dt^2}\phi_1^W + l_{12}\frac{d^2}{dt^2}\phi_2^W = -s^2(m_{10}\phi_0^W + m_{11}\phi_1^W + m_{12}\phi_2^W), \quad (30)$$

$$l_{jj-1}\frac{d^2}{dt^2}\phi_{j-1}^W + l_{jj}\frac{d^2}{dt^2}\phi_j^W + l_{jj+1}\frac{d^2}{dt^2}\phi_{j+1}^W = -s^2(m_{jj-1}\phi_{j-1}^W + m_{jj}\phi_j^W + m_{jj+1}\phi_{j+1}^W)$$

$$i = 2, \dots, P.$$
(32)

$$l_{11}\frac{d^2}{dt^2}\phi_1^E + l_{12}\frac{d^2}{dt^2}\phi_2^E = -s^2(m_{10}\phi_0^E + m_{11}\phi_1^E + m_{12}\phi_2^E), \quad (33)$$

$$l_{jj-1}\frac{d^2}{dt^2}\phi_{j-1}^E + l_{jj}\frac{d^2}{dt^2}\phi_j^E + l_{jj+1}\frac{d^2}{dt^2}\phi_{j+1}^E = -s^2(m_{jj-1}\phi_{j-1}^E + m_{jj}\phi_j^E + m_{jj+1}\phi_{j+1}^E) + j = 2, \dots, P,$$
(35)

$$u(x_W, t) = \phi_0^W, \quad \phi_{P+1}^W = 0, \qquad u(x_E, t) = \phi_0^E, \quad \phi_{P+1}^E = 0,$$
 (36)

with the initial conditions

$$u(x,0) = u_0(x), \quad \partial_t u(x,0) = v_0(x),$$

$$\phi_j^W(0) = 0, \quad \phi_j^E(0) = 0, \quad \partial_t \phi_j^W(0) = 0, \quad \partial_t \phi_j^W(0) = 0.$$

3.1. Spatial discretization

Let N be a positive integer number and let $h = \frac{x_E - x_W}{N}$ be the size step of the spatial grid. Then, $x_j = x_W + (j-1)h$, $j = 1, \ldots, N+1$, are the nodes of the spatial discretization, and $u_j(t) \approx u(x_j, t)$ are the semidiscrete approximations of the solution of (28).

Fourth order central finite differences are used to approximate spatial derivatives in (28) from u_3 to u_{N-1} and fourth order one-sided finite differences are used for u_2 and u_N . Finally, for u_1 and u_{N+1} , fourth order one-sided finite differences are used to approximate spatial derivatives in (27) and (29).

In this way, we obtain a semidiscrete ordinary differential problem given by,

$$\frac{d}{dt}u_{1} = \frac{c}{h}\left(-\frac{25}{12}u_{1} + 4u_{2} - 3u_{3} + \frac{4}{3}u_{4} - \frac{1}{4}u_{5}\right) + \frac{d}{dt}\phi_{1}^{W},$$

$$\frac{d^{2}}{dt^{2}}u_{2} = \frac{c^{2}}{h^{2}}\left(\frac{11}{12}u_{1} - \frac{5}{3}u_{2} + \frac{1}{2}u_{3} + \frac{1}{3}u_{4} - \frac{1}{12}u_{5}\right) - s^{2}u_{2},$$

$$\frac{d^{2}}{dt^{2}}u_{j} = \frac{c^{2}}{h^{2}}\left(-\frac{1}{12}u_{j-2} + \frac{4}{3}u_{j-1} - \frac{5}{2}u_{j} + \frac{4}{3}u_{j+1} - \frac{1}{12}u_{j+2}\right) - s^{2}u_{j}, j = 3, \dots, N-1,$$

$$\frac{d^{2}}{dt^{2}}u_{N} = \frac{c^{2}}{h^{2}}\left(-\frac{1}{12}u_{N-3} + \frac{1}{3}u_{N-2} + \frac{1}{2}u_{N-1} - \frac{5}{3}u_{N} + \frac{11}{12}u_{N+1}\right) - s^{2}u_{N},$$

$$\frac{d}{dt}u_{N+1} = \frac{c}{h}\left(-\frac{1}{4}u_{N-3} + \frac{4}{3}u_{N-2} - 3u_{N-1} + 4u_{N} - \frac{25}{12}u_{N+1}\right) + \frac{d}{dt}\phi_{1}^{E},$$

along with the ordinary differential equations (30)-(34) for the auxiliary variables.

3.2. Time integration

First, we rewrite the semidiscrete problem of Subsection 3.1 as the first order ordinary differential system

$$\frac{d}{dt} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \boldsymbol{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix} = M \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \boldsymbol{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \boldsymbol{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix}, \quad (37)$$

where $\mathbf{u} = [u_1, \dots, u_{N+1}]^T$, $\mathbf{u}' = [\frac{d}{dt}u_2, \dots, \frac{d}{dt}u_N]^T$, $\boldsymbol{\phi}^W = [\phi_1^W, \dots, \phi_P^W]^T$, $\boldsymbol{\phi}^E = [\phi_1^E, \dots, \phi_P^E]^T$, $(\boldsymbol{\phi}^W)' = [\frac{d}{dt}\phi_1^W, \dots, \frac{d}{dt}\phi_P^W]$, $(\boldsymbol{\phi}^E)' = [\frac{d}{dt}\phi_1^E, \dots, \frac{d}{dt}\phi_P^E]^T$ and M a square matrix of dimension 2N + 4P, based on the submatrices

$$M_{11} = \begin{bmatrix} \frac{c}{h}A_1 & 0 & 0\\ 0 & 0 & 0\\ \hline 0 & 0 & 0 \end{bmatrix}, M_{12} = \begin{bmatrix} A_2 & A_3 & A_4\\ \hline 0 & I_P & 0\\ \hline 0 & 0 & I_P \end{bmatrix}, M_{21} = \begin{bmatrix} A_5 & 0 & 0\\ \hline -s^2A_6 & -s^2A_7 & 0\\ \hline -s^2A_8 & 0 & -s^2A_7 \end{bmatrix}$$

,

where the $(N+1) \times (N+1)$ matrix A_1 given by

$$A_{1} = \begin{bmatrix} -\frac{25}{12} & 4 & -3 & \frac{4}{3} & -\frac{1}{4} \\ & & & 0 \\ & & & -\frac{1}{4} & \frac{4}{3} & -3 & 4 & -\frac{25}{12} \end{bmatrix}$$

has nonzero elements only in the first and last rows; the $(N + 1) \times (N - 1)$ matrix A_2 is given by

$$A_2 = \left[\begin{array}{c} 0\\I_{N-1}\\0 \end{array} \right],$$

where 0 denotes a row vector of N-1 zeros and I_{N-1} is the identity matrix of dimension N-1; the $(N+1) \times P$ matrix A_3 has the value 1 in the position (1,1) and the remaining elements are zero; the $(N+1) \times P$ matrix A_4 has the value 1 in the position (N+1,1) and the remaining elements are zero; the matrix A_5 is given by

$$A_5 = \frac{c^2}{h^2} M_x - s^2 A_2^T,$$

where the $(N-1) \times (N+1)$ matrix M_x is

$$M_x = \begin{bmatrix} \frac{11}{12} & \frac{5}{3} & \frac{1}{2} & \frac{1}{3} & -\frac{1}{12} \\ -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} \\ & & -\frac{1}{12} & \frac{1}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} \\ & & -\frac{1}{12} & \frac{1}{3} & \frac{1}{2} & -\frac{5}{3} & \frac{11}{12} \end{bmatrix};$$

 $A_6 = L^{-1}\tilde{A}_6$, where \tilde{A}_6 is the $P \times (N+1)$ matrix with all elements zero except the position (1, 1) which is equal to $2a_1$; $A_7 = L^{-1}\tilde{A}_7$, where \tilde{A}_7 is a

 $P \times P$ given by

ven by

$$\tilde{A}_{7} = \begin{bmatrix} 1 & 1 & & & \\ a_{2} & a_{1} + a_{2} & a_{1} & & \\ & \ddots & \ddots & \ddots & \\ & a_{j} & a_{j-1} + a_{j} & a_{j-1} & & \\ & & \ddots & \ddots & \\ & & & a_{P} & a_{P-1} + a_{P} \end{bmatrix},$$

and, finally, $A_8 = L^{-1}\tilde{A}_8$, where \tilde{A}_8 is the $P \times (N+1)$ matrix with all elements zero except the position (1, N+1) which is equal to $2a_1$.

With the same idea of obtaining intermediate problems with simple exponential matrices that we have carried in Subsection 2.2, we now propose a similar splitting. The step 1 is

$$\frac{d}{dt} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \mathbf{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix} = M_{1} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \mathbf{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \mathbf{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix}$$

As distinct of the case in Subsection 2.2, the matrix M_1 is not nilpotent, but it is very similar to the one in Subsection 2.2 because it has changed only in few elements related to the boundary nodes and the auxiliary functions. In fact, in Subsection 3.2 of [5] we have proved that

$$\exp(kM_1) = \begin{bmatrix} \frac{I_{N+1} + \eta_k A_1 & 0 & 0}{0 & I_P & 0} & \frac{B_k & \frac{h}{c} \eta_k A_3 & \frac{h}{c} \eta_k A_4}{0 & kI_P & 0} \\ 0 & 0 & I_P & 0 & 0 & kI_P \\ \hline 0 & 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 & 0 & kI_P & 0 \\ \hline 0 &$$

Therefore, flow $\psi_k^{[1]}$ (its non constant part) is

$$\begin{aligned}
\mathbf{u}(t+k) &= \mathbf{u}(t) + \eta_k A_1 \mathbf{u}(t) + B_k \mathbf{u}'(t) + \frac{h}{c} \eta_k A_3(\boldsymbol{\phi}^W)'(t) + \frac{h}{c} \eta_k A_4(\boldsymbol{\phi}^E)'(t), \\
\boldsymbol{\psi}_k^{[1]} &: \quad \boldsymbol{\phi}^W(t+k) &= \boldsymbol{\phi}^W(t) + k(\boldsymbol{\phi}^W)'(t), \\
\boldsymbol{\phi}^E(t+k) &= \boldsymbol{\phi}^E(t) + k(\boldsymbol{\phi}^E)'(t).
\end{aligned}$$

The step 2 corresponds to

$$\frac{d}{dt} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^W \\ \boldsymbol{\phi}^E \\ \mathbf{u}' \\ (\boldsymbol{\phi}^W)' \\ (\boldsymbol{\phi}^E)' \end{bmatrix} = M_2 \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^W \\ \boldsymbol{\phi}^E \\ \mathbf{u}' \\ (\boldsymbol{\phi}^W)' \\ (\boldsymbol{\phi}^E)' \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ M_{21} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^W \\ \boldsymbol{\phi}^E \\ \mathbf{u}' \\ (\boldsymbol{\phi}^W)' \\ (\boldsymbol{\phi}^E)' \end{bmatrix}.$$

In this case, M_2 is again a nilpotent matrix of degree 2 and we have

$$\exp\left(k\left[\begin{array}{c|c}0&0\\\hline M_{21}&0\end{array}\right]\right) = \left[\begin{array}{c|c}I_{N+1+2P}&0\\\hline kM_{21}&I_{N-1+2P}\end{array}\right].$$

Hence, the flow $\psi_k^{[2]}$ means

$$\begin{aligned}
\mathbf{u}'(t+k) &= \mathbf{u}'(t) + kA_5\mathbf{u}(t), \\
\psi_k^{[2]}: & (\boldsymbol{\phi}^W)'(t+k) &= (\boldsymbol{\phi}^W)'(t) + k(-s^2)A_6\mathbf{u}(t) + k(-s^2)A_7\boldsymbol{\phi}^W(t), \\
& (\boldsymbol{\phi}^E)'(t+k) &= (\boldsymbol{\phi}^E)'(t) + k(-s^2)A_8\mathbf{u}(t) + k(-s^2)A_7\boldsymbol{\phi}^E(t).
\end{aligned}$$

The flow $\psi_k^{[2]}$ can be rewritten as

$$\mathbf{u}'(t+k) = \mathbf{u}'(t) + kA_{5}\mathbf{u}(t),
 L\rho^{W} = -s^{2}(\tilde{A}_{6}\mathbf{u}(t) + \tilde{A}_{7}\boldsymbol{\phi}^{W}(t)),
 \psi_{k}^{[2]}: (\boldsymbol{\phi}^{W})'(t+k) = (\boldsymbol{\phi}^{W})'(t) + k\rho^{W},
 L\rho^{E} = -s^{2}(\tilde{A}_{8}\mathbf{u}(t) + \tilde{A}_{7}\boldsymbol{\phi}^{E}(t)),
 (\boldsymbol{\phi}^{E})'(t+k) = (\boldsymbol{\phi}^{E})'(t) + k\rho^{E}.$$

Then, two systems with the tridiagonal matrix L of size $P \times P$ have to be solved in step 2.

Once we have chosen the steps and we have solved exactly each step, there is still missing combining these solutions to obtain a high order approximation of the solution of (37). As in Subsection 2.2, we first consider the second order Strang splitting (23) and we obtain a fourth order numerical scheme by using the composition (24).

4. Two dimensional Klein-Gordon equation with H-W ABCs

We approach here the two dimensional case, taking advantage of the results obtained for the one dimensional case considered in the previous section.

4.1. Spatial discretization

For the sake of simplicity, we consider the same size step in both directions x and y, that is, for a value of N, $h = \frac{x_E - x_W}{N}$ and $M = \frac{b-a}{h}$. Let $x_j = x_W + (j-1)h$, $j = 1, \ldots, N+1$, and $y_l = a + (l-1)h$, $l = 1, \ldots, M+1$, be the nodes of the spatial discretization. This produces a uniform grid in the computational domain with M + 1 rows and N + 1 columns. We denote $u_{jl}(t) = u(x_j, y_l, t)$. In this way, there is a matrix of unknowns. On the other hand, we consider $\phi_{rl} = \phi_r(y_l)$, $r = 1, \ldots, P$, and $l = 1, \ldots, M+1$, on west and east boundaries.

As in the one dimensional case, second order spatial derivatives in the direction x, $\partial_x^2 u_{jl}$, from j = 3 to N - 1, are approximated by fourth order central finite differences and, for j = 2 and N, by fourth order one-sided finite differences. First order spatial derivatives $\partial_x u_{1l}$ and $\partial_x u_{N+1,l}$ are approximated by fourth order one-sided finite differences.

Spatial derivatives in the direction y are approximated by fourth order central finite differences. Near the south and north boundaries, periodic boundary conditions are considered.

4.2. Time integration

Let it be \mathbf{u}_j the column $j, \boldsymbol{\phi}_j^W$ and $\boldsymbol{\phi}_j^E$ the column vectors corresponding to the auxiliary variable j on west and east boundary respectively. We consider $\mathbf{u} = [\mathbf{u}_1^T, \dots, \mathbf{u}_{N+1}^T]^T, \mathbf{u}' = [\frac{d}{dt}\mathbf{u}_2^T, \dots, \frac{d}{dt}\mathbf{u}_N^T]^T, \boldsymbol{\phi}^W = [(\boldsymbol{\phi}_1^W)^T, \dots, (\boldsymbol{\phi}_P^W)^T]^T,$ $\boldsymbol{\phi}^E = [(\boldsymbol{\phi}_1^E)^T, \dots, (\boldsymbol{\phi}_P^E)^T]^T, (\boldsymbol{\phi}^W)' = [\frac{d}{dt}(\boldsymbol{\phi}_1^W)^T, \dots, \frac{d}{dt}(\boldsymbol{\phi}_P^W)^T]^T$ and finally $(\boldsymbol{\phi}^E)' = [\frac{d}{dt}(\boldsymbol{\phi}_1^E)^T, \dots, \frac{d}{dt}(\boldsymbol{\phi}_P^E)^T]^T.$

Rewriting the problem of Subsection 4.1 as a first order ordinary differ-

ential system

$$\frac{d}{dt} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \boldsymbol{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix} = \mathcal{M} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \boldsymbol{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix} = \begin{bmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ \mathcal{M}_{21} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi}^{W} \\ \boldsymbol{\phi}^{E} \\ \mathbf{u}' \\ (\boldsymbol{\phi}^{W})' \\ (\boldsymbol{\phi}^{E})' \end{bmatrix}, \quad (38)$$

and \mathcal{M} a square matrix of dimension (2N + 4P)(M + 1), with submatrices

$$\mathcal{M}_{11} = \begin{bmatrix} \frac{c}{h} \mathcal{A}_1 & 0 & 0\\ 0 & 0 & 0\\ \hline 0 & 0 & 0 \end{bmatrix}, \\ \mathcal{M}_{12} = \begin{bmatrix} \mathcal{A}_2 & \mathcal{A}_3 & \mathcal{A}_4\\ \hline 0 & I_{P(M+1)} & 0\\ \hline 0 & 0 & I_{P(M+1)} \end{bmatrix}, \\ \mathcal{M}_{21} = \begin{bmatrix} \mathcal{A}_5 & 0 & 0\\ \hline \mathcal{A}_6 & \mathcal{A}_7 & 0\\ \hline \mathcal{A}_8 & 0 & \mathcal{A}_7 \end{bmatrix},$$

where, by denoting \otimes to the Kronecker product of matrices, $\mathcal{A}_1 = A_1 \otimes I_{M+1}$, $\mathcal{A}_2 = A_2 \otimes I_{M+1}, \mathcal{A}_3 = A_3 \otimes I_{M+1}, \mathcal{A}_4 = A_4 \otimes I_{M+1}$ and $\mathcal{A}_5 = \frac{c^2}{h^2} M_x \otimes I_{M+1} + A_2^T \otimes A_9, \mathcal{A}_6 = A_6 \otimes A_9, \mathcal{A}_7 = A_7 \otimes A_9, \mathcal{A}_8 = A_8 \otimes A_9,$

$$A_9 = \frac{c^2}{h^2} M_y - s^2 I_{M+1},$$

In order to obtain an explicit method with intermediate problems with simple exponentials, we consider an exponential splitting method based in two steps similar to the one dimensional case in Section 3.

$$\begin{aligned}
\psi_k^{[1]} : & \\
\mathbf{u}(t+k) &= \mathbf{u}(t) + \eta_k \mathcal{A}_1 \mathbf{u}(t) + \mathcal{B}_k \mathbf{u}'(t) + \frac{h}{c} \eta_k \mathcal{A}_3(\boldsymbol{\phi}^W)'(t) + \frac{h}{c} \eta_k \mathcal{A}_4(\boldsymbol{\phi}^E)'(t), \\
\boldsymbol{\phi}^W(t+k) &= \boldsymbol{\phi}^W(t) + k(\boldsymbol{\phi}^W)'(t), \\
\boldsymbol{\phi}^E(t+k) &= \boldsymbol{\phi}^E(t) + k(\boldsymbol{\phi}^E)'(t), \\
\psi_k^{[2]} : & \\
\mathbf{u}'(t+k) &= (\boldsymbol{\phi}^W)'(t) + k \mathcal{A}_5 \mathbf{u}(t), \\
(\boldsymbol{\phi}^W)'(t+k) &= (\boldsymbol{\phi}^W)'(t) + k \mathcal{A}_6 \mathbf{u}(t) + k \mathcal{A}_7 \boldsymbol{\phi}^W(t), \\
(\boldsymbol{\phi}^E)'(t+k) &= (\boldsymbol{\phi}^E)'(t) + k \mathcal{A}_8 \mathbf{u}(t) + k \mathcal{A}_7 \boldsymbol{\phi}^E(t),
\end{aligned}$$
(39)

where $\mathcal{B}_k = B_k \otimes I_{M+1}$. We remark that the formulas (39) are very similar to the ones displayed in the one dimensional case.

Now, taking into account that

$$L^{-1}\tilde{A} \otimes A_9 = (L^{-1} \otimes I_{M+1})(\tilde{A} \otimes A_9), \text{ and } (L^{-1} \otimes I_{M+1}) = (L \otimes I_{M+1})^{-1},$$

the flow of step 2 can be rewritten as

$$\psi_{k}^{[2]}: = \mathbf{u}'(t) + k\mathcal{A}_{5}\mathbf{u}(t),
(L \otimes I_{M+1})\rho^{W} = (\tilde{A}_{6} \otimes A_{9})\mathbf{u}(t) + (\tilde{A}_{7} \otimes A_{9})\boldsymbol{\phi}^{W}(t),
(\boldsymbol{\phi}^{W})'(t+k) = (\boldsymbol{\phi}^{W})'(t) + k\rho^{W},
(L \otimes I_{M+1})\rho^{E} = (\tilde{A}_{8} \otimes A_{9})\mathbf{u}(t) + (\tilde{A}_{7} \otimes A_{9})\boldsymbol{\phi}^{E}(t),
(\boldsymbol{\phi}^{E})'(t+k) = (\boldsymbol{\phi}^{E})'(t) + k\rho^{E}.$$
(40)

Then, two systems with dimension matrix $P(M+1) \times P(M+1)$ have to be solved in step 2. However, $L \otimes I_{M+1}$ is a block diagonal matrix and L is the unique diagonal block. Therefore, it suffices to solve 2(M+1) linear systems with the same coefficient matrix L.

Finally, we combine the previous steps to obtain a fourth order in time splitting method by using the same formulas (23), (24) and (25) used for the periodic case in Section 2.

4.3. Analysis of the efficiency of the algorithm

In this analysis, we only take into account the matrix vector products in the algorithm described in Subsection 4.2. Step 1 requires (N+2P+19)(M+1) products, that is NM + 2PM + O(N) + O(M) + O(P) products.

Regarding step 2, $\mathcal{A}_5 \mathbf{u}$, 10(N-1)(M+1) products are needed. As for $(\tilde{A}_6 \otimes A_9) \mathbf{u}(t) + (\tilde{A}_7 \otimes A_9)$ and $(\tilde{A}_8 \otimes A_9) \mathbf{u}(t) + (\tilde{A}_7 \otimes A_9) \boldsymbol{\phi}^E(t)$, (6P-2)5(M+1) products are necessary.

The factorization of matrix L as a product of a lower matrix and an upper matrix is done once at the beginning. Then, in step 2 we only consider the products required to do the forward substitution and backward substitution to solve the systems. One system needs (P-1)(M+1)+(1+2(P-1))(M+1)products, consequently to solve two systems 2(3P-2)(M+1) products are necessary. Altogether, step 2 requires 10NM+36PM+O(N)+O(M)+O(P)products.

When we combine steps 1 and 2 using the second order Strang splitting (23) and (24) to obtain fourth order in time, using the formula (25), we repeat four times step 1 and three times the step 2. Therefore, we need 34NM + 116PM + O(N) + O(M) + O(P) products for every step in time.

If many steps are performed without output, only three evaluation of $\psi^{[1]}$ and $\psi^{[2]}$ are required per time step and then only 33NM + 114PM + O(N) + O(M) + O(P) products for every step in time are necessary.

Now, we study the efficiency of the splitting scheme by comparing with the fourth-order four-stage Runge-Kutta method. For the Runge-Kutta the computational cost of the product of one stage requires 11NM + 38PM + O(N) + O(M) + O(P) products, but in this case it is necessary do it four times for each step, that is 44NM + 152PM + O(N) + O(M) + O(P) products.

Basically, the computational cost relation between the Runge-Kutta method and the splitting scheme is four to three.

5. Numerical experiments

We consider the problem described in Section 4 with initial conditions

$$u_0(x,y) = \begin{cases} \frac{(1+10\sqrt{x^2+y^2})(\sqrt{x^2+y^2}-0.2)^2}{(0.2)^2}, & -0.2 < x, y < 0.2, \\ 0, & \text{otherwise}, \end{cases}$$

and $v_0(x, y) = 0$, with compact support contained in the computational domain $[-1/4, 1/4] \times [-1/4, 1/4]$. The function in u_0 is chosen so that $u_0 \in C^1([-1/4, 1/4] \times [-1/4, 1/4])$. In the following experiments we set c = 1 and s = 1. In this way, the solution reaches the boundary in a relative short time $t_0 = 0.05$ and the ABCs are soon involved. In order to check the full

discretization introduced in Section 4, it is enough to consider final time T = 1.

To test the proposed discretization, we have used five types of choices for the parameters a_j , j = 1, ..., P, considered in [13]: Newmann's parameters $a_j = \exp(-j/P)$; Chebyshev's parameters $a_j = \frac{1}{2}(1 + \cos\frac{(2j-1)\pi}{2P})$; Padé's parameters $a_j = 1$; optimal parameters for order P = 5,

$$a_1 = 0.91, a_2 = 0.41, a_3 = 0.12, a_4 = 0.029, a_5 = 0.0038,$$
 (41)

taken from Table 1 of [13], obtained by a Genetic Algorithm based on the minimization of

$$I^{P}[a_{1},\ldots,a_{P}] = \int_{0}^{\pi/2} \prod_{j=1}^{P} \left(\frac{a_{j}-\cos\theta}{a_{j}+\cos\theta}\right)^{2};$$

and, finally, an adaptive scheme to select the parameters.

The first issue is if the suggested discretization in Section 4 requires an admissible size of the time step. The periodic case studied in Section 2 can be used as reference. In that case, the ratio between the stability limit time step k_l and the space step h is 0.2973. We have examined the stability condition for the five types of choices of the parameters a_j , $j = 1, \ldots, P$, here considered. We have computed numerically the stability limit time step k_l for several values of P and N. In all cases the stability ratio k_l/h has turned out to be 0.4831, which is even better than the obtained for the periodic case. Therefore this allows to use the proposed discretization in Section 4.

The discrete energy (20) remains constant for the solution of the problem with periodic boundary conditions introduced in Section 2. Now, we test the discrete energy (20) for the numerical solution of the problem described in Section 4. Figure 1 displays $E_h(t)$ for Padé's coefficients for P = 10, N = 200 and $k = 10^{-4}$. It can be seen that, while the solution keeps inside the computational domain the discrete energy remains constant. But, when the solution reaches the boundary and the ABCs are working, the discrete energy diminishes.

Next, we focus on the absorption error. In order to achieve a time integration error negligible we take $k = 1/80000 = 1.25 \times 10^{-5}$. The reflections committed by the ABCs are measured comparing the numerical solution u^h on the computational domain $[-1/4, 1/4] \times [-1/4, 1/4]$ with the numerical solution $u^{h,ref}$ on a longer domain $[-1/4-5/2, 1/4+5/2] \times [-1/4, 1/4]$ for the



Figure 1: E_h for Padé's coefficients for P = 10, N = 200 and $k = 10^{-4}$.

same step size h. In the time interval [0, 1], there are no reflections of $u^{h, ref}$ on the computational domain. We denote by Emax the maximum of the absolute value of the difference between u^h and $u^{h, ref}$ on the computational domain.

Since the solution reaches the boundary at $t_0 = 0.05$, for $t < t_0$, the last step in the composition of $S_{\alpha k}^{[2]}$ for one step and the first one in $S_{\alpha k}^{[2]}$ for the next step are joined together $(\psi_{\alpha k/2}^{[1]} \circ \psi_{\alpha k/2}^{[1]} = \psi_{\alpha k}^{[1]})$, only three times of step 1 are needed.

Figures 2, 3 and 4 show, respectively, the values of Emax obtained using the splitting scheme with the Newmann's, Chebyshev's and Padé's coefficients for P = 10 and N = 200. It can be observed that the error of



Figure 2: *Emax* for Newmann's coefficients for P = 10 and N = 200.



Figure 3: *Emax* for Chebyshev's coefficients for P = 10 and N = 200.



Figure 4: *Emax* for Padé's coefficients for P = 10 and N = 200.

absorption obtained with the Padé's parameters is smaller than the error of absorption with Chebyshev's parameters. In turn, the error of absorption with Chebyshev's parameters is smaller than the error of absorption with the Newmann's ones. This agrees with the experiments displayed in [13], where, for P = 10 and short times, Padé's parameters produce the best results, following by Chebyshev's parameters and finally by Newmann's parameters.

Figure 5 displays *Emax* using the splitting scheme with the optimal coefficients (41) for N = 200. The use of optimal coefficients (41) with P = 5does not maintain small error of absorption along the time.

Then, we consider an adaptive scheme for the dynamic control of the order P and the parameters a_i similar to the one in [13]:



Figure 5: *Emax* for optimal coefficients for P = 5 and N = 200.

- 1. Determine δ , the minimum distance between the artificial boundary and the source region (in this case $\delta = 0.05$). Define $t_0 = \delta/c$. Choose a refining tolerance ϵ .
- 2. Initialize the order P = 2 and set $a_1 = a_2 = 1$.
- 3. For $t \leq t_0$, do not alter the initial parameters.
- 4. For $t > t_0$, if $\|\phi_P\| > \epsilon \|u\|_{\mathcal{B}}$, add a new auxiliary function, i.e., $P \leftarrow P+1$, with $a_{P+1} = 0.25/(c(t+0.2))$.



Figure 6 shows *Emax* using the adaptive scheme for N = 200 and $\epsilon = 10^{-3}$ and Figure 7 for N = 200 and $\epsilon = 10^{-4}$. It seems that the adaptive



Figure 7: *Emax* for $N = 200, \epsilon = 10^{-4}$.

algorithm keeps the error of absorption along the time increasing the number of auxiliary variables with the corresponding coefficients a_i .

Finally, we study the efficiency of the splitting scheme by comparing with the fourth-order four-stage Runge-Kutta method. We have ran both algorithms with Chebyshev's parameters in the formulation of the ABCs, for N = 100, 200 and 400, for several values of P and $k = 10^{-4}$, and we have measured the computational cost in terms of CPU time. The own structure of the splitting method carries to consider six vectors of unknowns: \mathbf{u}, \mathbf{u}' $\phi^W, \phi^E, (\phi^W)'$ and $(\phi^E)'$. However, the natural way to implement the Runge-Kutta method is considering all the variables in a single vector, this supposes to work with a larger matrix. Even if the number of the operations is the same, the CPU time is longer because it is more expensive to locate the elements of the matrix. Nevertheless, it is possible to perform the Runge-Kutta method with the same six vectors of unknowns as the splitting method. In this way, both methods work with matrices with the same dimension. Figure 8 displays *Emax* at t = 1 versus CPU time for the exponential splitting method and the Runge-Kutta method, for $N = 200, k = 10^{-4}$ using Chebyshev's parameters with P = 10 and P = 40. It can be observed that, for the same level of accuracy the splitting scheme is cheaper than the Runge-Kutta method. Table 1 shows the CPU ratio r for the Runge-Kutta method and the splitting method with the same partition of the variables. It can be seen, either in Figure 8 or in Table 1, that the relative behavior of both methods is



Figure 8: *Emax* at t = 1 versus CPU time, for N = 200, $k = 10^{-4}$, using Chebyshev's parameters with P = 10 and P = 40.

| $N \backslash P$ | 10 | 20 | 40 |
|------------------|--------|--------|--------|
| 100 | 1.4888 | 1.4699 | 1.4465 |
| 200 | 1.5005 | 1.4779 | 1.4482 |
| 400 | 1.4309 | 1.4815 | 1.4893 |

Table 1: CPU ratio for the Runge-Kutta method and the splitting method.

more or less 1.4, near of the expected 1.3, from the analysis of the products required, done in Section 4.3. The splitting method is advantageous over the Runge-Kutta method, especially when N increases and the needed CPU time do too.

As conclusion, the splitting time integrator proposed can be implemented for different choices of the parameters a_j and, moreover, it is computationally more efficient than the fourth order Runge-Kutta method.

References

I. Alonso-Mallo, B. Cano, M. J. Moreta, The stability of rational approximations of cosine functions on Hilbert spaces, Appl. Numer. Math. 59 (2009), no. 1, 21–38.

- [2] I. Alonso-Mallo, A. M. Portillo, A proof of the well posedness of discretized wave equation with an absorbing boundary condition, J. Numer. Math. 22 (2014), no. 4, 271–287.
- [3] I. Alonso-Mallo, A. M. Portillo, Absorbing boundary conditions and geometric integration: A case study for the wave equation, Math. Comput. Sim. 111 (2015), 1–16.
- [4] I. Alonso-Mallo, A. M. Portillo, High order full discretizations of coupled wave equations with absorbing boundary conditions and geometric integration, J. Comput. Phys. 265 (2014), 16–33.
- [5] I. Alonso-Mallo, A. M. Portillo, Time exponential splitting technique for the Klein-Gordon equation with Hagstrom-Warburton high-order absorbing boundary conditions, J. Comput. Phys. 311 (2016), 196-212.
- [6] I. Alonso-Mallo, N. Reguera, Weak Ill-posedness of spatial Discretizations of Absorbing Boundary Conditions for Schrödinger-type Equations, SIAM J. Numer. Anal. 40 (2002), 134–158.
- [7] I. Alonso-Mallo, N. Reguera, Discrete Absorbing Boundary Conditions for Schrödinger-type Equations. Construction and Error Analysis, SIAM J. Numer. Anal. 41 (2003), 1824–1850.
- [8] S. Blanes, F. Casas, A. Murua, Splitting and composition methods in the numerical integration of differential equations, Bol. Soc. Esp. Mat. Apl. 45 (2008), 89–145.
- [9] D. Givoli, High-order local non-reflecting boundary conditions: A review, Wave Motion 39 (2004), 319–326.
- [10] T. Hagstrom, On high-order radiation boundary conditions, Computational wave propagation, IMA Vol. Math. Appl. 86 (1997), 1–21.
- [11] T. Hagstrom, Radiation boundary conditions for the numerical simulation of waves, Acta Numer. 8 (1999), 47–106.
- [12] T. Hagstrom, New results on absorbing layers and radiation boundary conditions. Topics in computational wave propagation, Lect. Notes Comput. Sci. Eng. 31 (2003), 1–42.

- [13] T. Hagstrom, M. de Castro, D. Givoli, D. Tzemach, Local high order absorbing boundary conditions for time-dependent waves in guides, J. Comput. Acoust. 15 (2007), 1–22.
- [14] T. Hagstrom, D. Givoli, D. Rabinovich, J. Bielak, The double absorbing boundary method, J. Comput. Phys. 259 (2014), 220–241.
- [15] T. Hagstrom, A. Mar-Or, D. Givoli, High-order local absorbing conditions for the wave equation: extensions and improvements, J. Comput. Phys. 227 (2008), 3322–3357.
- [16] T. Hagstrom, T. Warburton A new auxiliary variable formulation of high-order local radiation boundary conditions: corner compatibility conditions and extensions to first order systems, Wave Motion 39 (2004), 327–338.
- [17] T. Hagstrom, T. Warburton Complete radiation boundary conditions: minimizing the long time error growth of local methods, SIAM J. Numer. Anal. 47 (2009), 3678–3704.
- [18] R.L. Higdon, Numerical absorbing boundary conditions for the wave equation, Math. Comput. 49 (1987), 65–90.
- [19] R.L. Higdon, Radiation boundary conditions for dispersive waves, SIAM J. Numer. Anal. 31 (1994), 64–100.
- [20] I. Kra, S.R. Simanca, On circulant matrices, Notices Amer. Math. Soc. 59 (2012), 368–377.
- [21] T. Lara, Circulant Matrices, Divulgaciones Matemáticas, 9 1(2001), 85– 102.
- [22] R.I. McLachlan, R. Quispel, Splitting methods, Acta Numerica, 11(2002), 341–434.
- [23] A. M. Portillo, *High order full discretization for anisotropic wave equations*, submitted.
- [24] M. Suzuki, Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations, Phys. Lett. A, 146 (1990), 319–323.

- [25] S.V. Tsynkov, Numerical solution of problems on unbounded domains. A review, Appl. Numer. Math. 27 (1998), 465–532.
- [26] H. Yoshida, Construction of higher order symplectic integrators, Phys. Lett. A, 150 (1990), 262–268.

28