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High-order full discretization for anisotropic wave equations

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ABSTRACT

Two-dimensional linear wave equation in anisotropic media, on a rectangular domain with initial conditions and periodic boundary conditions, is considered. The energy of the problem is contemplated. The space discretization is reached by means of finite differences on a uniform grid, paying attention to the mixed derivative of the equation. The discrete energy of the semi-discrete problem is introduced. For the time integration of the system of ordinary differential equations obtained, a fourth order exponential splitting method, which is a geometric integrator, is proposed. This time integrator is efficient and easy to implement. The stability condition for time step and space step ratio is deduced. Numerical experiments displaying the good behavior in the long time integration and the efficiency of the numerical solution are provided.

1. Introduction

Anisotropic media, in which the velocity may depend on the direction, are important in several wave propagation models, as anisotropic Maxwell's equations [3] or in elastic anisotropic waves in solid-earth geophysics [11]. Anisotropy seems to be an everywhere property of earth materials and its effects on seismic data must be taken into account. Today, seismic anisotropy is considered in exploration and reservoir characterization [24]. Stability analysis of the Perfectly Matched Layer method applied to anisotropic waves in two dimensions are studied for example in [4,17,21].

In this paper we study a particular case of the equation considered in [5], the two dimensional time-dependent anisotropic and dispersive wave equation

$$\partial_{tt} u = \alpha_{11}\partial_{xx} u + 2\alpha_{12}\partial_{xy} u + \alpha_{22}\partial_{yy} u - s^2 u. \tag{1}$$

We assume that the coefficients α_{ij} and s^2 in (1) are constant satisfying

$$\alpha_{11} > 0,\ \alpha_{22} > 0,\ \alpha_{11}\alpha_{22} - \alpha_{12}^2 > 0, \tag{2}$$

so that in the steady state the equation is elliptic.

When a problem posed in an infinite domain is solved numerically, it is necessary to reduce the computational domain to a finite domain, which forces us to choose suitable boundary conditions. On physical applications, it is desirable to have numerical models that resemble the dynamics of the continuous problems. If periodic boundary conditions are taken, invariants of the original problem are preserved. Here, we consider Eq. (1) in a rectangular domain $R = [a, b] \times [c, d]$, for the unknown $u(x, y, t)$, with periodic boundary conditions,

$$u(a, y, t) = u(b, y, t), \qquad y \in [c, d], \tag{3}$$

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$$\partial_x u(a,y,t) = \partial_x u(b,y,t), \quad y \in [c,d], \tag{4}$$

$$u(x,c,t) = u(x,d,t), \qquad x \in [a,b], \tag{5}$$

$$\partial_y u(x,c,t) = \partial_y u(x,d,t), \quad x \in [a,b]. \tag{6}$$

and initial conditions,

$$u(x,y,0) = u_0(x,y), \quad \partial_t u(x,y,0) = v_0(x,y), \tag{7}$$

which satisfy the periodic boundary conditions in R.

In an isotropic medium, $\alpha_{12}=0$, $\alpha_{11}=\alpha_{22}$, we get the Klein–Gordon wave equation. If in the Eq. (1), $\alpha_{12}=0$ but $\alpha_{11}\neq\alpha_{22}$, there are different speeds on x direction and on y direction, which corresponds to the orthotropic case. However, the general anisotropic case occurs when $\alpha_{12}\neq 0$. This means the existence of a spatial mixed derivative term in (1). In the literature there are other problems containing spatial mixed derivative terms as convection–diffusion equations [8,13,14], parabolic problems with application to pricing options [12,15,26] or in numerical mathematics when coordinate transformations are applied to allow working on simple domains or on uniform grids. In [13,14] the spatial derivatives are approximated by means of second-order finite differences, whereas in [8,12] fourth order finite differences are used. Then, the semi-discrete system of ordinary differential equations (ODEs) is integrated using alternating direction implicit schemes of first and second orders. For hyperbolic problems, as (1), is less common to use implicit methods because the stability condition is less demanding and $\triangle t$ and $\triangle x$ are of similar magnitude.

We are interested in obtaining efficient high order in space and time schemes for the numerical solution of Eq. (1), with periodic boundary conditions (3)–(6) and initial conditions (7). In this paper, the spatial derivatives are approximated using second and fourth order finite differences. As the boundary conditions are periodic, the matrix in the ODE system achieved is a block circulant matrix where each block is too a circulant matrix. For second order approximation of the spatial derivatives we prove that this matrix is symmetric negative definite and we locate the interval that contains its eigenvalues. We study well-posedness by using the discrete energy associated to the problem. For fourth order approximation of the spatial derivatives we compute numerically the eigenvalues of the corresponding symmetric matrix for moderate values of the dimension of the matrix, and the eigenvalues obtained are negative values.

We rewrite the semi-discrete problem as first order in time and the resulting ODE system is a Hamiltonian problem. This ODE system is split in two intermediate problems which are solved exactly. A fourth order splitting scheme is achieved by the flow composition of the two intermediate problems chosen. In stead of using alternating directions as in [8], the contribution of all spatial derivatives are regarded together because that the splitting obtained is computationally more efficient. A similar splitting method is considered in [2] for an isotropic problem with absorbing boundary conditions. The stability interval of the splitting method and the stability condition for the ratio between the time step and the space step are studied.

Useful overviews of splitting methods can be found in the review papers [6,20]. Splitting schemes are especially useful in the scope of geometric integration. Actually, splitting integrators preserve structural properties of the original problem's flow as long as the intermediate problems' flow do. The good performance of the geometric integrators in the long time integration of Hamiltonian ODE systems is well showed in [10,22].

The paper is organized as follows. The energy of the continuous problem is introduced in Section 2. In Section 3, second order approximation of the spatial derivatives are considered and the corresponding discrete energy is regarded. Section 4 is devoted to the exponential splitting time integrator. In Section 5 fourth order approximation of the spatial derivatives are introduced. Numerical experiments are conducted in Section 6. The good long time behavior as well as the efficiency of the splitting scheme by comparing with the fourth-order four-stage Runge–Kutta method in terms of CPU time are displayed.

2. Energy of the continuous problem

Knowing the energy of the system is important because it allows knowing an amount that is conserved over time without solving the equation. Moreover, when the continuous problem is discretized in space, we can compare the energy of the continuous problem with the energy of the semi-discrete problem.

An energy,

$$E(t)=\frac{1}{2}\iint_R ((\partial_t u(x,y,t))^2+\alpha_{11}(\partial_x u(x,y,t))^2+2\alpha_{12}\partial_x u(x,y,t)\partial_y u(x,y,t)+\alpha_{22}(\partial_y u(x,y,t))^2+s^2u(x,y,t)^2)dxdy,$$

can be introduced. Here

$$(u,v) = \iint_R v^* u \, dxdy, \quad \|u\|^2 = (u,u).$$

Then,

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$$E(t) = \frac{1}{2}(\|\partial_t u)\|^2 + \alpha_{11}\|\partial_x u\|^2 + 2\alpha_{12}(\partial_x u, \partial_y u) + \alpha_{22}\|\partial_y u\|^2 + s^2\|u\|^2).$$

From ellipticity condition (2), it is deduced that $E(t)$ is non-negative. It can be shown that solutions of (1) with periodic boundary conditions conserve $E(t)$. Multiplying Eq. (1) by $\partial_t u$, the equation can be rewritten as a divergence. Then, considering the integral over the rectangle R, it can be seen that $E'(t) = 0$, from the divergence theorem and the periodic conditions. Therefore the energy $E(t)$ is constant with time and

$$E(t) = E(0) = \frac{1}{2}\iint_R (v_0(x,y)^2 + \alpha_{11}(\partial_x u_0(x,y))^2 + 2\alpha_{12}\partial_x u_0(x,y)\partial_y u_0(x,y) + \alpha_{22}(\partial_y u_0(x,y))^2 + s^2 u_0(x,y)^2)dxdy. \tag{8}$$

In this way, we can compute the energy of the problem calculating the initial energy through the initial condition.

3. Spatial discretization

We start approximating the spatial derivatives in (1) by using finite differences. For the sake of simplicity, we consider the same size step in both directions x and y, that is, for a value of N, $h = \frac{b-a}{N}$ and $M = \frac{d-c}{h}$. Let $x_j = a + (j-1)h$, $j = 1, \dots, N+1$, and $y_l = c + (l-1)h$, $l = 1, \dots, M+1$, be the nodes of the spatial discretization. This produces a uniform grid in the computational domain and a matrix of unknowns $u_{jl}(t) = u(x_j, y_l, t)$.

In general, finite difference approximation involves a stencil of points surrounding u_{jl}. In this section, second order spatial derivatives in the direction x and in the direction y are approximated by second order central finite differences

$$\partial_{xx} u_{jl} \approx \frac{u_{j-1,l} - 2u_{jl} + u_{j+1,l}}{h^2},$$
$$\partial_{yy} u_{jl} \approx \frac{u_{j,l-1} - 2u_{jl} + u_{j,l+1}}{h^2},$$

in stencil form

$$\frac{1}{h^2}\begin{pmatrix} 0 & 0 & 0 \\ 1 & -2 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \frac{1}{h^2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & -2 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

respectively.

Mixed derivative can be approximated by second order finite differences

$$\partial_{xy} u_{jl} \approx \frac{u_{j-1,l-1} - u_{j+1,l-1} + u_{j+1,l+1} - u_{j-1,l+1}}{4h^2},$$

in stencil form

$$\frac{1}{4h^2}\begin{pmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix}. \tag{9}$$

Another alternative stencil forms for second order approximation of second order of mixed derivatives are

$$\frac{1}{2h^2}\begin{pmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{pmatrix}, \quad \frac{1}{2h^2}\begin{pmatrix} 0 & -1 & 1 \\ -1 & 2 & -1 \\ 1 & -1 & 0 \end{pmatrix}. \tag{10}$$

The first stencil form should be used in the case $\alpha_{12} > 0$, whereas the second is suitable when $\alpha_{12} < 0$. If, as it happens in (1), the equation combines ∂_{xx}, ∂_{yy} and ∂_{xy}, choosing (10) instead of (9) for the approximation of mixed derivative, the complete discretization of the differential operator produces an M-matrix [9]. Taking this into account, here mixed derivative is approximated as follows

$$\text{if} \quad \alpha_{12} > 0,$$
$$2\partial_{xy} u_{jl} \approx \frac{u_{j-1,l} + u_{j+1,l} - 2u_{jl} + u_{j,l-1} + u_{j,l+1} - u_{j-1,l+1} - u_{j+1,l-1}}{h^2},$$
$$\text{if} \quad \alpha_{12} < 0,$$
$$2\partial_{xy} u_{jl} \approx \frac{-u_{j-1,l} - u_{j+1,l} + 2u_{jl} - u_{j,l-1} - u_{j,l+1} + u_{j-1,l-1} + u_{j+1,l+1}}{h^2}.$$

Let it be $\mathbf{u}_j$ the approximations to the unknowns $(u(x_j, y_1), \dots, u(x_j, y_{M+1}))^T$, for fixed x_j. Denoting $\mathbf{u}_h = [\mathbf{u}_1^T, \dots, \mathbf{u}_{N+1}^T]^T$, we achieve the second order in time ODEs system

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

where the matrix of the problem is

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$$A = \frac{1}{h^2}B - s^2 I, \tag{12}$$

I is the identity matrix of dimension $(N+1)(M+1)$ and

$$B = \begin{bmatrix} B_1 & B_2 & & & & B_2^T \\ B_2^T & B_1 & B_2 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & B_2^T & B_1 & B_2 \\ B_2 & & & & B_2^T & B_1 \end{bmatrix}. \tag{13}$$

If $\alpha_{12} > 0$,

$$\begin{aligned} B_1 &= (\alpha_{22} + \alpha_{12})C_1 - 2\alpha_{11} I_{M+1}, \\ B_2 &= \alpha_{12} C_2 + \alpha_{11} I_{M+1}, \end{aligned}$$

and, if $\alpha_{12} < 0$,

$$\begin{aligned} B_1 &= (\alpha_{22} - \alpha_{12})C_1 - 2\alpha_{11} I_{M+1}, \\ B_2 &= -\alpha_{12} C_2^T + \alpha_{11} I_{M+1}, \end{aligned}$$

with

$$C_1 = \begin{bmatrix} -2 & 1 & & & & 1 \\ 1 & -2 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 \\ 1 & & & & 1 & -2 \end{bmatrix}, \quad C_2 = \begin{bmatrix} 1 & & & & -1 \\ -1 & 1 & & & \\ & & \ddots & & \\ & & -1 & 1 & \\ 0 & & & -1 & 1 \end{bmatrix}.$$

Notice that B is a block circulant matrix where each block is in turn a circulant matrix.

Lemma 1. *The eigenvalues of matrix B in (13), for the coefficients α_{ij} meeting (2), satisfy*

$$\sigma(B) \subset [-4(\alpha_{11} + \alpha_{22}) - 8|\alpha_{12}|, 0].$$

Proof. We begin considering the case $\alpha_{12} > 0$.

$$\begin{aligned} B &= circ(B_1, B_2, 0, \dots, 0, B_2^T), \\ B_1 &= circ(-2(\alpha_{11} + \alpha_{22} + \alpha_{12}), \alpha_{22} + \alpha_{12}, 0, \dots, 0, \alpha_{22} + \alpha_{12}), \\ B_2 &= circ(\alpha_{11} + \alpha_{12}, 0, \dots, 0, -\alpha_{12}), \\ B_2^T &= circ(\alpha_{11} + \alpha_{12}, -\alpha_{12}, 0, \dots, 0). \end{aligned}$$

We consider the following polynomials associated to the blocks of matrix B

$$\begin{aligned} h_1(z) &= -2(\alpha_{11} + \alpha_{22} + \alpha_{12}) + (\alpha_{22} + \alpha_{12})z + (\alpha_{22} + \alpha_{12})z^M, \\ h_2(z) &= (\alpha_{11} + \alpha_{12}) - \alpha_{12} z^M, \\ h_{N+1}(z) &= (\alpha_{11} + \alpha_{12}) - \alpha_{12} z. \end{aligned}$$

Then, the eigenvalues of matrix B are (see [16,18])

$$\lambda_{l,k} = \tilde{\varepsilon}_l^0 h_1(\tilde{\omega}_k) + \tilde{\varepsilon}_l h_2(\tilde{\omega}_k) + \tilde{\varepsilon}_l^N h_{N+1}(\tilde{\omega}_k), \; l = 1, \dots, N+1, \; k = 1, \dots, M+1,$$

where,

$$\begin{aligned} \omega_{M+1} &= \exp\left(\frac{2\pi i}{M+1}\right), \quad \tilde{\omega}_k = (\omega_{M+1})^k, \\ \varepsilon_{N+1} &= \exp\left(\frac{2\pi i}{N+1}\right), \quad \tilde{\varepsilon}_l = (\varepsilon_{N+1})^l. \end{aligned}$$

$$\begin{aligned} \lambda_{l,k} = & -2(\alpha_{11} + \alpha_{22} + \alpha_{12}) + (\alpha_{22} + \alpha_{12})\left(\exp\left(\frac{2\pi ik}{M+1}\right) + \exp\left(\frac{2\pi ikM}{M+1}\right)\right) \\ & + \exp\left(\frac{2\pi il}{N+1}\right)\left((\alpha_{11} + \alpha_{12}) - \alpha_{12}\exp\left(\frac{2\pi ikM}{M+1}\right)\right) + \exp\left(\frac{2\pi ilN}{N+1}\right)\left((\alpha_{11} + \alpha_{12}) - \alpha_{12}\exp\left(\frac{2\pi ik}{M+1}\right)\right). \end{aligned}$$

Taking into account that,

$$\exp\left(\frac{2\pi ilN}{N+1}\right)=\exp\left(\frac{-2\pi il}{N+1}\right),$$
$$\exp\left(\frac{2\pi ikM}{M+1}\right)=\exp\left(\frac{-2\pi ik}{M+1}\right),$$
$$\exp\left(\frac{2\pi il}{N+1}\right)\exp\left(\frac{2\pi ikM}{M+1}\right)+\exp\left(\frac{2\pi ilN}{N+1}\right)\exp\left(\frac{2\pi ik}{M+1}\right)$$
$$=2\cos\left(\frac{2\pi l}{N+1}\right)\cos\left(\frac{2\pi k}{M+1}\right)+2\sin\left(\frac{2\pi l}{N+1}\right)\sin\left(\frac{2\pi k}{M+1}\right)$$
$$=2\cos\left(\frac{2\pi l}{N+1}-\frac{2\pi k}{M+1}\right),$$

and then,

$$\lambda_{l,k}=-2(\alpha_{11}+\alpha_{22}+\alpha_{12})+2(\alpha_{11}+\alpha_{12})\cos\left(\frac{2\pi l}{N+1}\right)+2(\alpha_{22}+\alpha_{12})\cos\left(\frac{2\pi k}{M+1}\right)-2\alpha_{12}\cos\left(\frac{2\pi l}{N+1}-\frac{2\pi k}{M+1}\right).$$

Clearly, $\lambda_{l,k}\in D=\{f(x,y):\ (x,y)\in[0,2\pi]\times[0,2\pi]\}$ where

$$f(x,y)=-2(\alpha_{11}+\alpha_{22}+\alpha_{12})+2(\alpha_{11}+\alpha_{12})\cos(x)+2(\alpha_{22}+\alpha_{12})\cos(y)-2\alpha_{12}\cos(x-y).$$

We are going to prove that $D\subset[-4(\alpha_{11}+\alpha_{22})-8|\alpha_{12}|,0]$. For that, we calculate the absolute extrema of function f on the set D. As $f(x, y)$ is a continuous function in the compact domain $[0, 2\pi]\times[0, 2\pi]$, the Weierstrass Theorem guarantees that the absolute maximum and the absolute minimum of $f(x, y)$ are reached in points of $[0, 2\pi]\times[0, 2\pi]$. First, we study the function at the boundary.

If $y\in[0, 2\pi]$,

$$\begin{aligned}f(0,y)&=f(2\pi,y)=-2(\alpha_{11}+\alpha_{22}+\alpha_{12})+2(\alpha_{11}+\alpha_{12})+2(\alpha_{22}+\alpha_{12})\cos(y)-2\alpha_{12}\cos(y)\\&=-2\alpha_{22}(1+\cos(y)).\end{aligned}$$

In that case, $-4\alpha_{22}\le f(0,y)=f(2\pi,y)\le 0$.

If $x\in[0, 2\pi]$,

$$\begin{aligned}f(x,0)&=f(x,2\pi)=-2(\alpha_{11}+\alpha_{22}+\alpha_{12})+2(\alpha_{11}+\alpha_{12})\cos(x)+2(\alpha_{22}+\alpha_{12})-2\alpha_{12}\cos(x)\\&=-2\alpha_{11}(1+\cos(x)).\end{aligned}$$

Thus, $-4\alpha_{11}\le f(x,0)=f(x,2\pi)\le 0$.

Second, we look for the possible extrema of $f(x, y)$ in $(0, 2\pi)\times(0, 2\pi)$, which have to satisfy

$$\frac{\partial f}{\partial x}=-2(\alpha_{11}+\alpha_{12})\sin(x)+2\alpha_{12}\sin(x-y)=0,$$
$$\frac{\partial f}{\partial y}=-2(\alpha_{22}+\alpha_{12})\sin(y)-2\alpha_{12}\sin(x-y)=0,$$

like this,

$$2\alpha_{12}\sin(x-y)=2(\alpha_{11}+\alpha_{12})\sin(x)=-2(\alpha_{22}+\alpha_{12})\sin(y). \tag{14}$$

From (14), it is obtained

$$\sin(y)=-\frac{\alpha_{11}+\alpha_{12}}{\alpha_{22}+\alpha_{12}}\sin(x), \tag{15}$$

and therefore

$$2\alpha_{12}\sin(x-y)=2\alpha_{12}\sin(x)\cos(y)+2\alpha_{12}\frac{\alpha_{11}+\alpha_{12}}{\alpha_{22}+\alpha_{12}}\sin(x)\cos(x), \tag{16}$$

and using another time (14) in (16)

$$2\alpha_{12}\sin(x)\cos(y)+2\alpha_{12}\frac{\alpha_{11}+\alpha_{12}}{\alpha_{22}+\alpha_{12}}\sin(x)\cos(x)=2(\alpha_{11}+\alpha_{12})\sin(x). \tag{17}$$

Eq. (17) is satisfied if $\sin(x)=0$ or

$$\alpha_{12}\cos(y)+\alpha_{12}\frac{\alpha_{11}+\alpha_{12}}{\alpha_{22}+\alpha_{12}}\cos(x)=(\alpha_{11}+\alpha_{12}). \tag{18}$$

From (15), if $\sin(x)=0$, then $\sin(y)=0$, and the only option in $(0, 2\pi)\times(0, 2\pi)$ is (π, π), and $f(\pi,\pi)=-4\alpha_{11}-4\alpha_{22}-8\alpha_{12}<0$.

Next, we are going to prove that (18) does not have any solution. From (18), we have

$$\cos(y) = -\frac{\alpha_{11}+\alpha_{12}}{\alpha_{22}+\alpha_{12}}\cos(x) + \frac{\alpha_{11}+\alpha_{12}}{\alpha_{12}}. \tag{19}$$

Using that $\sin^2(y)+\cos^2(y)=1$ and (15) and (19) we achieve

$$\cos(x) = -\frac{\alpha_{12}(\alpha_{22}+\alpha_{12})}{2(\alpha_{11}+\alpha_{12})^2} + \frac{\alpha_{12}}{2(\alpha_{22}+\alpha_{12})} + \frac{\alpha_{22}+\alpha_{12}}{2\alpha_{12}}. \tag{20}$$

We are going to prove that the right term in (20) is greater than 1, which can not be. The second part of the Eq. (20) is equivalent to

$$\frac{\alpha_{22}^2\alpha_{11}^2 + 2\alpha_{11}^2\alpha_{12}^2 + 2\alpha_{22}^2\alpha_{11}\alpha_{12} + 2\alpha_{11}^2\alpha_{22}\alpha_{12} + 4\alpha_{11}\alpha_{22}\alpha_{12}^2 + 4\alpha_{11}\alpha_{12}^3 + \alpha_{12}^4}{2\alpha_{11}^2\alpha_{22}\alpha_{12} + 2\alpha_{11}^2\alpha_{12}^2 + 4\alpha_{11}\alpha_{22}\alpha_{12}^2 + 4\alpha_{11}\alpha_{12}^3 + 2\alpha_{22}\alpha_{12}^3 + 2\alpha_{12}^4}. \tag{21}$$

To prove that (21) is greater than 1 it suffices that

$$\begin{aligned}&\alpha_{22}^2\alpha_{11}^2 + 2\alpha_{11}^2\alpha_{12}^2 + 2\alpha_{22}^2\alpha_{11}\alpha_{12} + 2\alpha_{11}^2\alpha_{22}\alpha_{12} + 4\alpha_{11}\alpha_{22}\alpha_{12}^2 + 4\alpha_{11}\alpha_{12}^3 + \alpha_{12}^4\\ &\quad > 2\alpha_{11}^2\alpha_{22}\alpha_{12} + 2\alpha_{11}^2\alpha_{12}^2 + 4\alpha_{11}\alpha_{22}\alpha_{12}^2 + 4\alpha_{11}\alpha_{12}^3 + 2\alpha_{22}\alpha_{12}^3 + 2\alpha_{12}^4,\end{aligned}$$

or equivalently

$$2\alpha_{22}^2\alpha_{11}\alpha_{12} - 2\alpha_{22}\alpha_{12}^3 + \alpha_{22}^2\alpha_{11}^2 - \alpha_{12}^4 = 2\alpha_{22}\alpha_{12}(\alpha_{11}\alpha_{22} - \alpha_{12}^2) + \alpha_{11}^2\alpha_{22}^2 - \alpha_{12}^4 > 0,$$

which is true thanks to (2).

Then, summarizing the absolute minimum of $f(x, y)$ in $[0, 2\pi]\times[0, 2\pi]$ is $-4\alpha_{11} - 4\alpha_{22} - 8\alpha_{12}$ and the absolute maximum is 0.

Now, we consider the case $\alpha_{12} < 0$.

$$\begin{aligned}B &= circ(B_1, B_2, 0, \ldots, 0, B_2^T),\\ B_1 &= circ(-2(\alpha_{11}+\alpha_{22}-\alpha_{12}), \alpha_{22}-\alpha_{12}, 0, \ldots, 0, \alpha_{22}-\alpha_{12}),\\ B_2 &= circ(\alpha_{11}-\alpha_{12}, \alpha_{12}, 0, \ldots, 0),\\ B_2^T &= circ(\alpha_{11}-\alpha_{12}, 0, \ldots, 0, \alpha_{12}).\end{aligned}$$

We consider the following polynomials associated to the blocks of matrix B

$$\begin{aligned}h_1(z) &= -2(\alpha_{11}+\alpha_{22}-\alpha_{12}) + (\alpha_{22}-\alpha_{12})z + (\alpha_{22}-\alpha_{12}))z^M,\\ h_2(z) &= (\alpha_{11}-\alpha_{12}) + \alpha_{12}z,\\ h_{N+1}(z) &= (\alpha_{11}-\alpha_{12}) + \alpha_{12}z^M.\end{aligned}$$

In a similar way as in the previous case we achieve

$$\lambda_{l,k} = -2(\alpha_{11}+\alpha_{22}-\alpha_{12}) + 2(\alpha_{11}-\alpha_{12})\cos\left(\frac{2\pi l}{N+1}\right) + 2(\alpha_{22}-\alpha_{12})\cos\left(\frac{2\pi k}{M+1}\right) + 2\alpha_{12}\cos\left(\frac{2\pi l}{N+1} + \frac{2\pi k}{M+1}\right).$$

In this case we consider the function

$$\begin{aligned}f(x,y) &= -2(\alpha_{11}+\alpha_{22}+|\alpha_{12}|) + 2(\alpha_{11}+|\alpha_{12}|)\cos(x) + 2(\alpha_{22}+|\alpha_{12}|)\cos(y) - 2|\alpha_{12}|\cos(x+y),\\ &\qquad (x,y)\in[0,2\pi]\times[0,2\pi].\end{aligned}$$

Following a similar reasoning than in the case $\alpha_{12} > 0$, we reach an equation similar to (17) but in this case with $|\alpha_{12}|$.

Consequently, we conclude

$$\sigma(B) \subset [-4(\alpha_{11}+\alpha_{22}) - 8|\alpha_{12}|, 0]. \qquad \square$$

Lemma 2. *The matrix*

$$A = \frac{1}{h^2}B - s^2 I$$

is symmetric negative definite.

Proof. As the matrix B in (13) is symmetric, this is also true for the matrix A.

Since the eigenvalues of the matrix A are

$$\sigma(A) = \left\{\frac{1}{h^2}\mu - s^2, \quad \mu\in\sigma(B)\right\},$$

from Lemma 1 we deduce the result. □

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Theorem 3. *The discrete energy*

$$E_h(t)(\mathbf{u},\mathbf{v}) = \frac{h^2}{2}(\mathbf{v}^T\mathbf{v} - \mathbf{u}^T A\mathbf{u}), \tag{22}$$

is conserved for $(\mathbf{u}_h, d\mathbf{u}_h/dt)$*, being* $\mathbf{u}_h$ *the solution of (11).*

Proof. From Lemma 2, (22) is a norm. If $\mathbf{u}_h$ is a solution of (11),

$$\begin{aligned}\frac{dE_h}{dt}(t)(\mathbf{u}_h, d\mathbf{u}_h/dt) &= h^2 \frac{d\mathbf{u}_h}{dt}^T \frac{d^2\mathbf{u}_h}{dt^2} - h^2 \frac{d\mathbf{u}_h}{dt}^T A\mathbf{u}_h \\ &= h^2 \frac{d\mathbf{u}_h}{dt}^T \left(\frac{d^2\mathbf{u}_h}{dt^2} - A\mathbf{u}_h\right) = 0.\end{aligned}$$

□

Then the discrete energy norm is conserved and the problem (11) is well posed.

4. Time discretization

We rewrite problem (11) as a first order system, naming $\mathbf{v}_h = [\frac{d}{dt}\mathbf{u}_1^T, \ldots, \frac{d}{dt}\mathbf{u}_{N+1}^T]^T$,

$$\frac{d}{dt}\begin{bmatrix}\mathbf{u_h}\\ \mathbf{v}_h\end{bmatrix} = \begin{bmatrix}0 & I\\ A & 0\end{bmatrix}\begin{bmatrix}\mathbf{u_h}\\ \mathbf{v}_h\end{bmatrix}, \tag{23}$$

where I is the identity matrix of dimension $(N+1)(M+1)$. We notice system (23) is a Hamiltonian problem.

4.1. Exponential splitting method

Denoting k the time step, we propose to approximate the exact solution of (23),

$$\begin{bmatrix}\mathbf{u(t+k)}\\ \mathbf{v}(t+k)\end{bmatrix} = \exp\left(k\begin{bmatrix}0 & I\\ A & 0\end{bmatrix}\right)\begin{bmatrix}\mathbf{u(t)}\\ \mathbf{v}(t)\end{bmatrix}, \ t \geq 0,$$

by using an exponential splitting method as time integrator. We split the matrix of the problem (23) in two parts

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

The intermediate problems

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

can be solved exactly using that $M_i^2 = 0$ for $i = 1, 2$ and,

$$\exp(kM_1) = \begin{bmatrix}I & kI\\ 0 & I\end{bmatrix}, \quad \exp(kM_2) = \begin{bmatrix}I & 0\\ kA & I\end{bmatrix}.$$

Then, the flows of these intermediate problems applied to $[\mathbf{u}, \mathbf{v}]^T$ are

$$\begin{aligned}\psi_k^{[1]} &: \exp(kM_1)\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix} = \begin{bmatrix}\mathbf{u+kv}\\ \mathbf{v}\end{bmatrix},\\ \psi_k^{[2]} &: \exp(kM_2)\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix} = \begin{bmatrix}\mathbf{u}\\ \mathbf{v}+kA\mathbf{u}\end{bmatrix}.\end{aligned}$$

To advance a step of size k in time, once we have solved exactly each intermediate step, it is necessary combining these solutions to obtain an approximation of the solution of (23). To do this, first we use the symmetric second order Strang splitting $\mathcal{S}^{[2]}$

$$\mathcal{S}_k^{[2]} = \psi_{k/2}^{[1]} \circ \psi_k^{[2]} \circ \psi_{k/2}^{[1]}, \tag{24}$$

and then, by composition of $\mathcal{S}^{[2]}$, we consider the fourth order integrator $\mathcal{S}^{[4]}$ [23,25]

$$\mathcal{S}_k^{[4]} = \mathcal{S}_{\alpha k}^{[2]} \circ \mathcal{S}_{\beta k}^{[2]} \circ \mathcal{S}_{\alpha k}^{[2]}, \quad \text{with} \quad \alpha = \frac{1}{2 - 2^{1/3}}, \quad \beta = 1 - 2\alpha. \tag{25}$$

The advantage of composing exact solutions in this way is that geometric properties of the true flow are preserved. Symplectic time integrators [10,22] not only provides better qualitative properties of the numerical solution, but also better accuracy when a long time computation is made.

It is possible to save some computational cost in (25) by join together the last step in the composition of $\mathcal{S}^{[2]}_{\alpha k}$ and the first one in $\mathcal{S}^{[2]}_{\beta k}$ and similarly, the last one in the composition of $\mathcal{S}^{[2]}_{\beta k}$ and the first one in $\mathcal{S}^{[2]}_{\alpha k}$. That is,

$$\begin{aligned}\mathcal{S}^{[4]}_k &= \psi^{[1]}_{\alpha k/2}\circ\psi^{[2]}_{\alpha k}\circ\psi^{[1]}_{\alpha k/2}\circ\psi^{[1]}_{\beta k/2}\circ\psi^{[2]}_{\beta k}\circ\psi^{[1]}_{\beta k/2}\circ\psi^{[1]}_{\alpha k/2}\circ\psi^{[2]}_{\alpha k}\circ\psi^{[1]}_{\alpha k/2},\\ &= \psi^{[1]}_{\alpha k/2}\circ\psi^{[2]}_{\alpha k}\circ\psi^{[1]}_{(\alpha+\beta)k/2}\circ\psi^{[2]}_{\beta k}\circ\psi^{[1]}_{(\alpha+\beta)k/2}\circ\psi^{[2]}_{\alpha k}\circ\psi^{[1]}_{\alpha k/2}.\end{aligned} \tag{26}$$

Notice that, if many steps are performed without output, only three evaluation of $\psi^{[1]}$ and $\psi^{[2]}$ are required per time step.

This splitting method is explicit and it is easy to implement. However, it is not unconditionally stable and the stability has to be studied.

4.2. Stability discussion

To study the stability of the numerical solution obtained with the scheme proposed in the previous subsection, we consider the stability matrix and the stability interval associated to the method. Since A is symmetric negative definite, the matrix $(-A)^{1/2}$ is well defined. Considering

$$Q = \begin{bmatrix}(-A)^{1/2} & 0\\ 0 & I\end{bmatrix},$$

the matrix $M(k,-A)$ with which the method $\mathcal{S}^{[4]}_k$ proceeds,

$$\mathcal{S}^{[\triangle]}_{\|}:\quad M(k,-A)\begin{bmatrix}\mathbf{u}\\ \mathbf{v}\end{bmatrix},$$

can be expressed as $M(k,-A) = Q^{-1}R(k(-A)^{1/2})Q$, where $R(\omega)$ is the stability matrix of the method. Following [7], $R(\omega)$ can be computed as

$$\begin{bmatrix}1 & \frac{\alpha}{2}\omega\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\ -\alpha\omega & 1\end{bmatrix}\begin{bmatrix}1 & \frac{\alpha+\beta}{2}\omega\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\ -\beta\omega & 1\end{bmatrix}\begin{bmatrix}1 & \frac{\alpha+\beta}{2}\omega\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\ -\alpha\omega & 1\end{bmatrix}\begin{bmatrix}1 & \frac{\alpha}{2}\omega\\ 0 & 1\end{bmatrix}. \tag{27}$$

Then,

$$R(\omega) = \begin{bmatrix}R_1(\omega) & R_2(\omega)\\ R_3(\omega) & R_4(\omega)\end{bmatrix}$$

where

$$R_1(\omega) = R_4(\omega) = 1 - \frac{\omega^2}{2} + \frac{\omega^4}{24} + \frac{1}{36}(6 + 5\cdot 2^{1/3} + 4\cdot 2^{2/3})\omega^6, \tag{28}$$

$$R_2(\omega) = \omega - \frac{\omega^3}{6} - \frac{1+2^{1/3}}{72\cdot 2^{2/3}}\omega^5 + \frac{25 + 20\cdot 2^{1/3} + 16\cdot 2^{2/3}}{1728}\omega^7, \tag{29}$$

$$R_3(\omega) = -\omega + \frac{\omega^3}{6} + \frac{4 + 4\cdot 2^{1/3} + 3\cdot 2^{2/3}}{144}\omega^5. \tag{30}$$

The splitting method is stable if the size of the powers of $M(k,-A)$ are bounded in the matrix norm associated to the discrete energy norm. In a similar way than in [2], we rewrite the discrete energy (22) as

$$\begin{aligned}E_h(t)(\mathbf{u},\mathbf{v}) &= \frac{h^2}{2}\left(\mathbf{v}^T\cdot\mathbf{v} + ((-A)^{1/2}\mathbf{u})^T((-A)^{1/2}\mathbf{u})\right)\\ &= \|[(-A)^{1/2}\mathbf{u},\mathbf{v}]\|_2 = \|Q[\mathbf{u},\mathbf{v}]^T\|_2 := \|[\mathbf{u},\mathbf{v}]\|_Q.\end{aligned}$$

Therefore,

$$\begin{aligned}\|M^n(k,-A)\|_Q &= \|QM^n(k,-A)Q^{-1}\|_2\\ &= \|\left(QM(k,-A)Q^{-1}\right)^n\|_2\\ &= \|R^n(k(-A)^{1/2})\|_2.\end{aligned} \tag{31}$$

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The study of the boundedness of the powers (31) is not easy in general (cf. [1]) but, in order to do this, it is necessary to consider the *stability interval* of the method.

Definition 4. The stability interval of a method with stability matrix $R(\omega)$ is $[0, \omega_*]$ if ω_* is the largest nonnegative value such that

$$\rho(R(\omega)) \le 1, \quad \omega \in [0, \omega_*],$$

where $\rho(R(\omega))$ is the spectral radius of $R(\omega)$.

Theorem 5. *The value of ω_* in the stability interval of (26) is*

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

Proof. From (27), $\det(R(\omega)) = 1$. Then the eigenvalues $\lambda_1(\omega)$, $\lambda_2(\omega)$ of $R(\omega)$ are the solutions of

$$\lambda^2 - 2R_1(\omega)\lambda + 1 = 0.$$

If $R_1(\omega)^2 - 1 > 0$ the eigenvalues of $R(\omega)$ are real numbers and, since $\lambda_1(\omega)\lambda_2(\omega) = 1$, we deduce that $\rho(R(\omega)) > 1$.
If $R_1(\omega)^2 - 1 < 0$ the eigenvalues of $R(\omega)$ are complex numbers satisfying $|\lambda_j(\omega)| = 1$ for $j = 1, 2$ and then $\rho(R(\omega)) = 1$.
If $R_1(\omega)^2 - 1 = 0$ the eigenvalues of $R(\omega)$ are real numbers with modulus 1 and then $\rho(R(\omega)) = 1$.
Let it be ω_* the real nonnegative solution of $R_1(\omega) - 1 = 0$. From (28) ω_* is the only real nonnegative solution of

$$\omega^2\left(-\frac{1}{2} + \frac{1}{24}\omega^2 + \gamma\omega^4\right) = 0,$$

whose expression is

$$\omega_* = \sqrt{\frac{-1+\sqrt{1+1152\gamma}}{48\gamma}} \approx 0.9711.$$

As

$$-\frac{1}{2} + \frac{1}{24}\omega^2 + \gamma\omega^4 \le 0, \quad \omega \in [0, \omega^*],$$

thus

$$R_1(\omega) - 1 \le 0, \quad \omega \in [0, \omega_*].$$

Moreover,

$$R_1(\omega) + 1 = 2 - \frac{1}{2}\omega^2 + \frac{1}{24}\omega^4 + \gamma\omega^6 > 2 - \frac{1}{2}\omega^2 \ge \frac{3}{2}, \quad \omega \in [0, 1].$$

We conclude that

$$R_1(\omega)^2 - 1 = (R_1(\omega) - 1)(R_1(\omega) + 1) \le 0, \quad \omega \in [0, \omega_*],$$

and we achieve the result. □

Since the eigenvalues of $k(-A)^{1/2} = \frac{k}{h}(-B + s^2h^2I)^{1/2}$ must be in the *stability interval*, we obtain the stability condition

$$\frac{k}{h}\sqrt{4(\alpha_{11}+\alpha_{22}) + 8|\alpha_{12}| + s^2h^2} < \sqrt{\frac{-1+\sqrt{1+1152\gamma}}{48\gamma}}.$$

This will be reached, for sh small enough, when

$$\frac{k}{h} < \frac{0.9711}{\sqrt{4(\alpha_{11}+\alpha_{22}) + 8|\alpha_{12}|}}. \tag{32}$$

Our numerical experiments corroborate that stability is achieved when the time step k is chosen to meet (32).

5. Fourth order spatial discretization

Computational cost becomes especially important when the number of equations in the system increases. In order to approach Eq. (1) with periodic boundary conditions (3)–(6) and initial conditions (7), with higher accuracy, it is convenient to introduce finite differences with order greater than two. Like this, higher computational efficiency can be achieved. In this section we consider fourth order approximation of the spatial derivatives in a similar way as in Section 1.3.1 of [8] and in Section 3.1 of [12].

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

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

in stencil form

$$\frac{1}{12h^2}\begin{pmatrix} 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ -1 & 16 & -30 & 16 & -1\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \frac{1}{12h^2}\begin{pmatrix} 0 & 0 & -1 & 0 & 0\\ 0 & 0 & 16 & 0 & 0\\ 0 & 0 & -30 & 0 & 0\\ 0 & 0 & 16 & 0 & 0\\ 0 & 0 & -1 & 0 & 0 \end{pmatrix},$$

respectively.

Mixed derivative are approximated by the following fourth order finite differences

$$\partial_{xy} u_{jl} \approx \frac{1}{144h^2}(u_{j-2,l-2}-8u_{j-2,l-1}+8u_{j-2,l+1}-u_{j-2,l+2}-8u_{j-1,l-2}+64u_{j-1,l-1}-64u_{j-1,l+1}+8u_{j-1,l+2}8u_{j+1,l-2}$$
$$-64u_{j+1,l-1}+64u_{j+1,l+1}-8u_{j+1,l+2}-u_{j+2,l-2}+8u_{j+2,l-1}-8u_{j+2,l+1}+u_{j+2,l+2}),$$

in stencil form

$$\frac{1}{144h^2}\begin{pmatrix} -1 & 8 & 0 & -8 & 1\\ 8 & -64 & 0 & 64 & -8\\ 0 & 0 & 0 & 0 & 0\\ -8 & 64 & 0 & -64 & 8\\ 1 & -8 & 0 & 8 & -1 \end{pmatrix}.$$

As in Section 3, we consider $\mathbf{u}_j$ the approximations to the unknowns $(u(x_j,y_1),\dots,u(x_j,y_{M+1}))^T$, for fixed x_j. We consider $\mathbf{u}_h=[\mathbf{u}_1^T,\dots,\mathbf{u}_{N+1}^T]^T$, and $\mathbf{v}_h=[\frac{d}{dt}\mathbf{u}_1^T,\dots,\frac{d}{dt}\mathbf{u}_{N+1}^T]^T$. We rewrite this problem as a first order ordinary differential system,

$$\frac{d}{dt}\begin{bmatrix}\mathbf{u_h}\\ \mathbf{v}_h\end{bmatrix}=\begin{bmatrix}0 & I\\ A & 0\end{bmatrix}\begin{bmatrix}\mathbf{u_h}\\ \mathbf{v}_h\end{bmatrix}, \tag{33}$$

where I is the identity matrix of dimension $(N+1)(M+1)$, $A=\frac{1}{h^2}B-s^2I$,

$$B=\frac{1}{72}\begin{bmatrix} B_1 & B_2 & B_3 & & & & B_3^T & B_2^T\\ B_2^T & B_1 & B_2 & B_3 & & & & B_3^T\\ B_3^T & B_2^T & B_1 & B_2 & B_3 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & B_3^T & B_2^T & B_1 & B_2 & B_3\\ B_3 & & & & B_3^T & B_2^T & B_1 & B_2\\ B_2 & B_3 & & & & B_3^T & B_2^T & B_1 \end{bmatrix}, \tag{34}$$

$$C_1=\begin{bmatrix} -180 & 96 & -6 & & & & -6 & 96\\ 96 & -180 & 96 & -6 & & & & -6\\ -6 & 96 & -180 & 96 & -6 & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & -6 & 96 & -180 & 96 & -6\\ -6 & & & & -6 & 96 & -180 & 96\\ 96 & -6 & & & & -6 & 96 & -180 \end{bmatrix},$$

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Table 1
The three cases of α_{ij} considered.

Run	α_{11}	α_{22}	α_{12}
1.2	0.875	0.625	−0.217
2.2	0.160	0.940	0.225
2.4	0.472	0.628	0.443

Table 2
Minimum eigenvalue of matrix B.

Run	Second order FD	Fourth order FD
1.2	−7.7360	−7.9981
2.2	−6.2000	−5.8663
2.4	−7.9440	−5.9727

$$C_2 = \begin{bmatrix} 0 & 64 & -8 & & & & 8 & -64 \\ -64 & 0 & 64 & -8 & & & & 8 \\ 8 & -64 & 0 & 64 & -8 & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & 8 & -64 & 0 & 64 & -8 \\ -8 & & & & 8 & -64 & 0 & 64 \\ 64 & -8 & & & & 8 & -64 & 0 \end{bmatrix},$$

$$C_3 = \begin{bmatrix} 0 & -8 & 1 & & & & -1 & 8 \\ 8 & 0 & -8 & 1 & & & & -1 \\ -1 & 8 & 0 & -8 & 1 & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & -1 & 8 & 0 & -8 & 1 \\ 1 & & & & -1 & 8 & 0 & -8 \\ -8 & 1 & & & & -1 & 8 & 0 \end{bmatrix},$$

$$\begin{aligned} B_1 &= \alpha_{22}C_1 - 180\alpha_{11}I_{M+1}, \\ B_2 &= \alpha_{12}C_2 + 96\alpha_{11}I_{M+1}, \\ B_3 &= \alpha_{12}C_3 - 6\alpha_{11}I_{M+1}. \end{aligned}$$

Notice that A is a symmetric matrix which is five block circulant matrix and, in turn, each block is a circulant matrix with five elements non zero in each row.

Combining this spatial discretization with the time splitting (26), we obtain a high order scheme whose order of consistency is four in space and four in time. In this case, as in the second order case studied in Section 2, to get the numerical solution computed with method (26) is stable, the eigenvalues of $k(-A)^{1/2}$ must be in the *stability interval* of the method.

6. Numerical experiments

In this Section we consider the problem described in Section 1 with initial conditions

$$u_0(x,y) = \begin{cases} \dfrac{(x+0.2)^3(0.2-x)^3(y+0.2)^3(0.2-y)^3}{(0.2)^{12}}, & -0.2 < x, y < 0.2, \\ 0, & \text{otherwise}, \end{cases}$$

and $v_0(x,y) = 0$, with compact support contained in the computational domain $[-1/4, 1/4] \times [-1/4, 1/4]$. The polynomial in u_0 is chosen so that $u_0 \in C^1([-1/4, 1/4] \times [-1/4, 1/4])$. These initial conditions are the same used in the numerical experiments in previous paper [2].

We set the dispersion coefficient $s^2 = 1$. For the numerical experiments we have selected three cases of coefficients α_{ij} from [5]. Table 1 displays these coefficients with the same notation used in [5].

We have numerically computed the eigenvalues of matrix B (34) from Section 5, for the α_{ij} considered, and we can conclude that they are non positive real numbers. Table 2 displays $-4\alpha_{11} - 4\alpha_{22} - 8\alpha_{12}$, the lower boundary of the minimum eigenvalue of matrix B of Section 3 and λ_{min} the minimum eigenvalue of matrix B of Section 5 computed numerically for $N = 80$, for the three cases of coefficients α_{ij}.

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Table 3
Ratio of stability.

Run	Second order FD	Fourth order FD
1.2	0.3491	0.3434
2.2	0.3900	0.4009
2.4	0.3445	0.3974

Table 4
Energy of second order and fourth order finite differences for run 1.2.

$E(0)$=1.369728648529847		
[illegible]	$E_{h,\,2}$	$E_{h,\,4}$
[illegible]	1.367571822518154	1.369706858644256
100	1.369189187080928	1.369727238677717
200	1.369593766456254	1.369728558830660
400	1.369694926954860	1.369728642872906

Table 5
Energy of second order and fourth order finite differences for run 2.2.

$E(0)$=1.006948225489684		
[illegible]	$E_{h,\,2}$	$E_{h,\,4}$
[illegible]	1.005656444288419	1.006932246239829
100	1.006625342563159	1.006947191598221
200	1.006867508130111	1.006948159710693
400	1.006928046352305	1.006948221342952

From Section 4, to ensure stability when the exponential splitting method is used, k/h has to satisfy

$$\frac{k}{h} < \frac{0.9711}{\sqrt{|\lambda_{min}|}}.$$

Table 3 displays the ratio of stability $\dfrac{0.9711}{\sqrt{|\lambda_{min}|}}$.

It can be seen in Table 3 that the stability condition for the splitting method is acceptable.

Now, we are going to compare the continuous energy (8) for the test problem with the discrete energy

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

of the semi-discrete problems. We denote by $E_{h,\,2}(t)$ the discrete energy where matrix A is the matrix obtained in Section 3, when second order finite differences are used, and $E_{h,\,4}(t)$ the discrete energy where matrix A is the matrix obtained in Section 5, when fourth order finite differences are considered.

Taking into account that the function to integrate in (8) for the test problem is separable and using integration by parts, it can be seen that

$$E(0) = \frac{1}{2}((\alpha_{11}+\alpha_{22})I_1 + s^2 I_2),$$

where

$$I_1 = \frac{4!\,5!\,2^{24}\,18}{(7\ldots11)(7\ldots13)},$$

$$I_2 = \frac{(6!)^2\,2^{28}}{100\,(7\ldots13)^2}.$$

Tables 4–6 display the continuous energy and the discrete energies for several values of N and the three cases of coefficients α_{ij} selected. Likewise, energy error for the second order finite differences and the fourth-order finite differences are shown in Fig. 1. It can be appreciated, from these results, the second and fourth order of the discretization of Sections 3 and 5, respectively.

Finally, in the following experiments we compare the behavior of the splitting scheme and the fourth-order four-stage Runge–Kutta method when fourth order finite differences introduced in Section 5 and the energy norm $E_{h,\,4}(t)$ are considered. We measure the relative energy error $|E_{h,4}(t) - E_{h,4}(0)|/|E_{h,4}(0)|$. We set $N = M = 200$ and $k = 10^{-3}$. Fig. 2 displays relative energy error for the exponential splitting integrator and the fourth-order four-stage Runge–Kutta method, for times from 0 to 100, for the three selected runs.

Table 6
Energy of second order and fourth order finite differences for run 2.4.

$E(0)$=1.006948225489684		
[illegible]	$E_{h,\,2}$	$E_{h,\,4}$
[illegible]	1.006615902030712	1.006932246239829
100	1.006866032223891	1.006947191598225
200	1.006927732266519	1.006948159710716
400	1.006943105621258	1.006948221342970

Table 7
$N = 100$, final time $T = 100$, run 2.2.

	$k = 2 \times 10^{-3}$		$k = 2 \times 10^{-4}$	
	Error	CPU	Error	CPU
Splitting	7.4541×10^{-8}	2.9122×10^{2}	7.2273×10^{-12}	2.8812×10^{3}
rk4	1.1375×10^{-5}	4.1804×10^{2}	2.6421×10^{-10}	4.1067×10^{3}

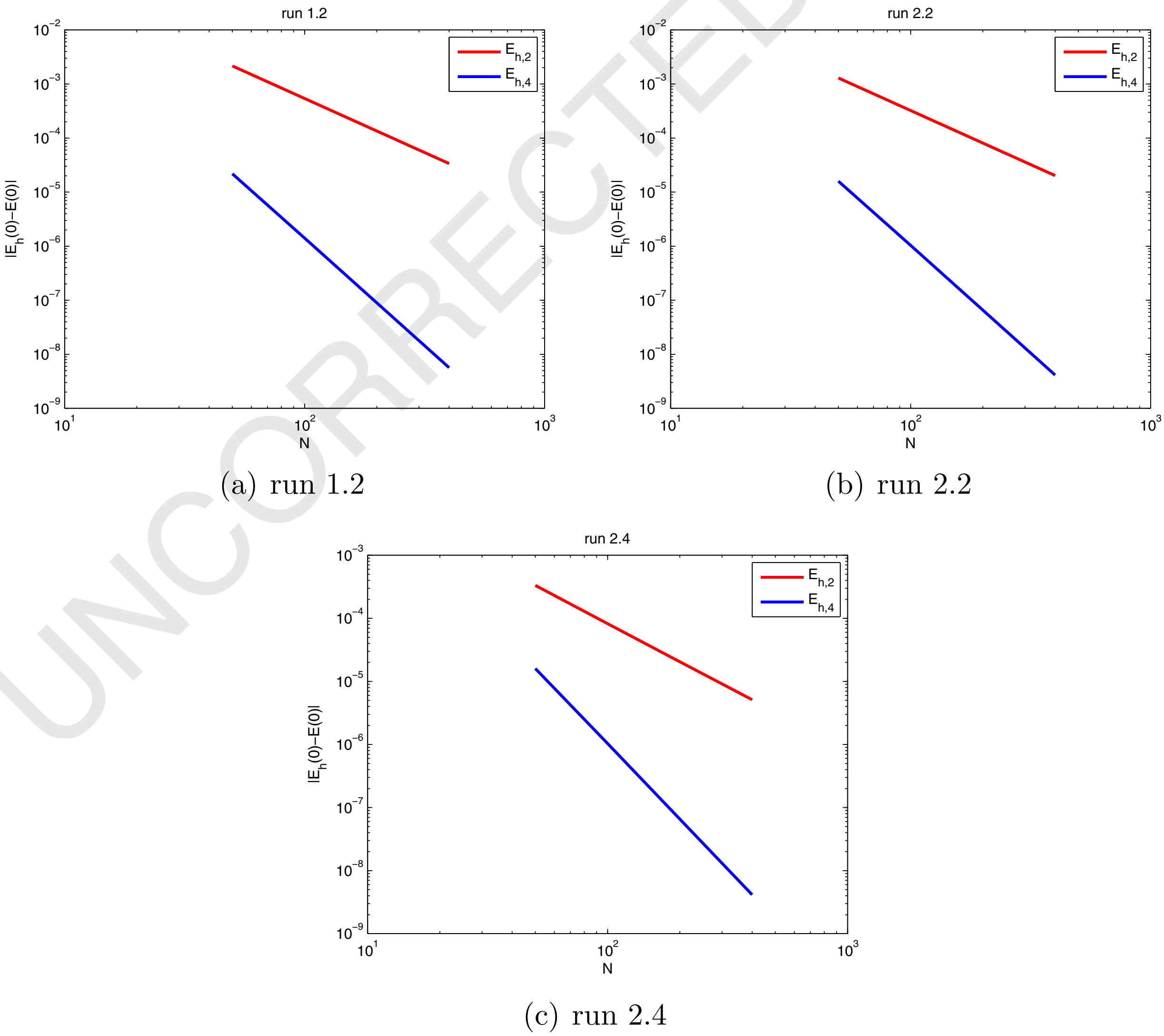


Fig. 1. Energy error for the second order finite differences and the fourth-order finite differences, for run 1.2, run 2.2 and run 2.4.

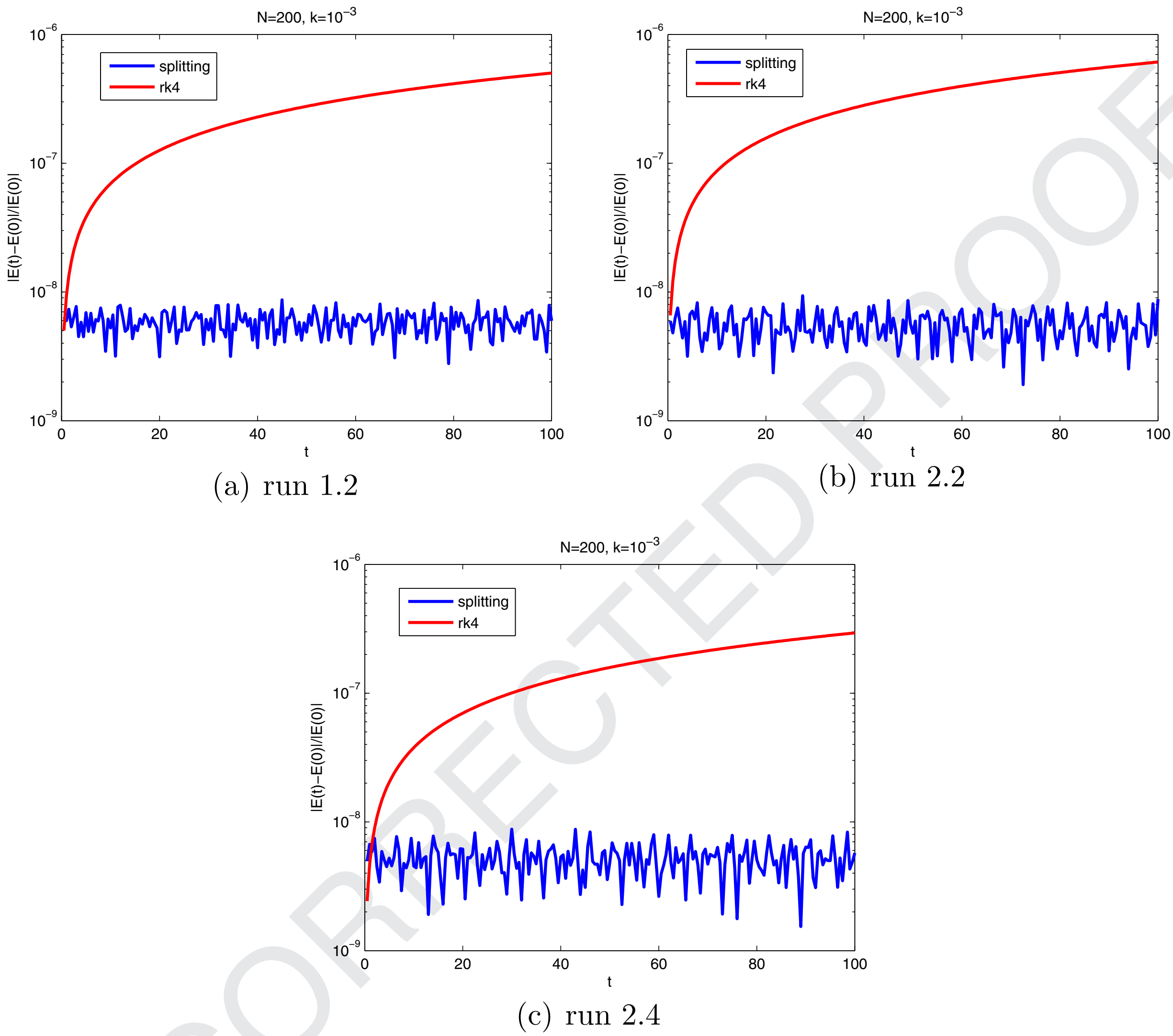


Fig. 2. Relative energy error for the exponential splitting integrator and the fourth-order four-stage Runge–Kutta method, for run 1.2, run 2.2 and run 2.4.

In the three cases, the splitting method maintains the same size error throughout the interval of time [0, 100]. This agrees with the fact that scheme (26) is a geometric integrator. Whereas for the Runge–Kutta method the size of the error grows when the time increases.

Lastly, we study the efficiency of the splitting scheme by comparing with the fourth-order four-stage Runge–Kutta method measuring the computational cost in terms of CPU time. For the exponential splitting integrator, if the last step in the composition (26) of $\mathcal{S}_k^{[4]}$ for one step and the first one in $\mathcal{S}_k^{[4]}$ for the next step are joined together, that is, $\psi^{[1]}_{\alpha k/2} \circ \psi^{[1]}_{\alpha k/2} = \psi^{[1]}_{\alpha k}$, only three times of step 1 are needed for each step in time. A similar analysis of the efficiency of the algorithms to the one done in [2] can be done here. Then, regarding the products required, for the Runge–Kutta method and the splitting method, the relation is four to three.

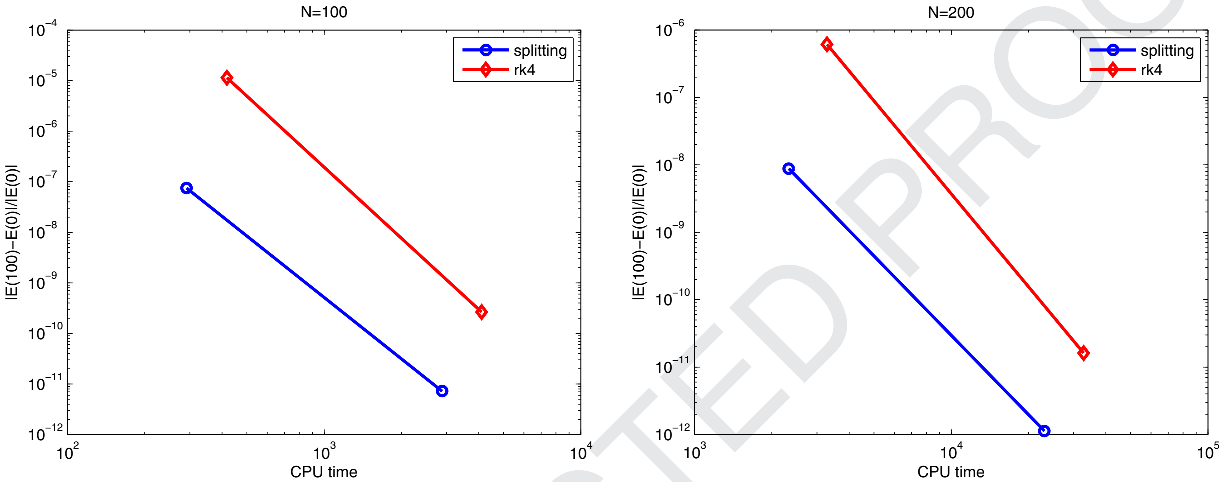
We have ran both algorithms for $N = 100$, with $k = 2 \times 10^{-3}, 2 \times 10^{-4}$ and for $N = 200$, with $k = 10^{-3}, 10^{-4}$ and we have measured the relative energy error and the computational cost in terms of CPU time, for final time $T = 100$.

Table 8 shows the relative energy error and the CPU for the splitting method and the Runge–Kutta method. Fixed the time step k the ratio between the CPU for the Runge–Kutta method and the splitting method is 1.4081 for $k = 10^{-3}$ and 1.3929 for $k = 10^{-4}$, near to the expected value 4/3. It can be seen in Fig. 3 that the splitting method is better than the Runge–Kutta method. For the same error the computational cost is smaller.

The numerical experiments confirm the good behavior in the long time integration and the efficiency of the splitting method considered.

Table 8
$N = 200$, final time $T = 100$, run 2.2.

	$k = 10^{-3}$		$k = 10^{-4}$	
	Error	CPU	Error	CPU
Splitting	8.7994×10^{-9}	2.3291×10^{3}	1.1304×10^{-12}	2.3056×10^{4}
rk4	6.1077×10^{-7}	3.2796×10^{3}	1.6152×10^{-11}	3.2817×10^{4}



(a) $N = 100$ (b) $N = 200$

Fig. 3. Relative energy error at $T = 100$ versus CPU time for the exponential splitting integrator and the fourth-order four-stage Runge–Kutta method for run 2.2, for $N = 100$ and $N = 200$.

Uncited references

[19].

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