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On a generalization of the split-step Padé method to the case of unknown vector-functions

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Abstract

The split-step Padé approach is an extremely efficient tool for the integration of pseudodifferential parabolic equations, which are widely used for the modelling of wave propagation. In this study, a generalization of this method to the case of parabolic equations with unknown vector functions is presented. Such generalization requires an algorithm for efficient numerical evaluation of a function of a matrix having differential operators as its elements. After a finite-difference discretization this algorithm reduces to the solution of several Sylvester-like problems. The generalized split-step Padé method presented here can be used in many practical problems of wave propagation modelling.

Keywords: pseudodifferential parabolic equations, coupled Helmholtz equations, split-step Padé, Sylvester equation

1. Introduction

Wide-angle parabolic equations are currently widely used for numerical modelling of wave propagation in many areas of physics, including optics [1, 2], acoustics [3, 4] and radiophysics [5]. Probably, the most advanced tool for their solution is the so-called split-step Padé method, proposed independently by Collins [4] and Avilov [6]. The method consists of a formal factorization of the operator in the scalar Helmholtz equation of the form

$$u_{xx} + u_{yy} + k^2 u = \left(\partial_x + \mathrm{i}\sqrt{k^2 + \partial_y^2}\right)\left(\partial_x - \mathrm{i}\sqrt{k^2 + \partial_y^2}\right)u = 0\,, \tag{1}$$

where $u = u(x, y)$ is an unknown function, $k^2 = k^2(x, y)$ is a variable coefficient playing the role of the wavenumber or the refractive index (subscripts x, y denote partial derivatives with respect to these variables throughout this study). A one-way counterpart of (1), corresponding to wave propagation in the positive direction of the x-axis is called a *pseudodifferential parabolic equation* (PDPE) [6, 7]

$$\left(\partial_x - \mathrm{i}\sqrt{k^2 + \partial_y^2}\right)u = 0\,, \tag{2}$$

since it contains a pseudodifferential operator $\mathrm{i}\sqrt{k^2 + \partial_y^2}$.

The split-step Padé method [4, 7] of solving Eq. (2) consists in formal integration of this equation over the interval $[x, x + h]$, which leads to the equality

$$u(x + h, y) = \exp\left(\mathrm{i}h\sqrt{k^2 + \partial_y^2}\right)u(x, y) \equiv \hat{\mathcal{P}}u(x, y)\,, \tag{3}$$

and in a replacement of the operator $\hat{\mathcal{P}}$ on the right-hand side of this equality (usually called the propagator) by its $[p/p]$ Padé approximant of the form

$$\exp\left(\mathrm{i}h\sqrt{k^2 + \partial_y^2}\right)u \approx \mathrm{e}^{\mathrm{i}k_0 h}\left(d_0 + \sum_{k=1}^{p}\frac{d_k}{1 + b_k\hat{X}}\right)u = \mathrm{e}^{\mathrm{i}k_0 h}\left(d_0 u + \sum_{k=1}^{p} d_k w_k\right), \tag{4}$$

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where k_0 is a reference value of $k(x, y)$, and $\hat{X} = (k^2 - k_0^2 + \partial_y^2)/k_0^2$. The quantities $w_k = w_k(x, y)$ are obtained by solving the following operator equations

$$\left(1 + b_k \hat{X}\right) w_k = u\,,$$

which are actually transformed into e.g. linear systems with tridiagonal matrices by the standard second-order finite difference discretization of the operator $\hat{X}$ [1, 4].

Thus, for a $[p/p]$ Padé approximation of the square root exponential operator, the marching numerical scheme requires p inversions of some sparse (e.g., tridiagonal) matrices for each step along the x-axis.

In this study this method is generalized to the case of a coupled system of equation of the form (1). Such systems naturally arise when the propagation of coupled modes in a 3D waveguide is considered [3, 8]. Although the respective one-way equations were already considered in literature (see, e.g., [3]), the algorithm proposed below is new. It can have application in many areas of science and engineering (e.g., as an alternative to 3D parabolic equation theory [9]).

2. The coupled system of elliptic equations and its one-way counterpart

The main goal of this study is to generalize the SSP algorithm outlined in the previous section to the case of a coupled system of J elliptic equations [3, 10]

$$u_{m,xx} + u_{m,yy} + k_m^2 u_m + \sum_{j=1}^{J} V_{jm} u_j + \sum_{j=1}^{J} W_{jm} u_{j,y} = 0\,, \tag{5}$$

where $\mathbf{V}(y) = (V_{jm}(y))$ and $\mathbf{W}(y) = (W_{jm}(y))$ are y-dependent $J \times J$ matrices (typically full). In fact, the equations (5) can also contain the terms with $u_{j,x}$, but without any loss of generality they can be eliminated by a change of variables. Note also that in practical problems of wave propagation the equations (5) are solved on the unbounded domain $\mathbb{R}^2$ with the radiation boundary conditions imposed at $\sqrt{x^2 + y^2} \to \infty$. They also usually have an input term (e.g., $\delta(x)\delta(y)$) representing the source of the waves on the right-hand side, but in the one-way counterparts of (5) or (2) the sources are modelled by the Cauchy data (loosely connected to the above input terms by a form of the Duhamel's principle) as described in [11].

Let us first introduce a vector-matrix form of the coupled equations (5), which is essential for further discussion. First, we define a vector function $\mathbf{u}(x, y) = (u_1, u_2, \ldots, u_J)$ consisting of the unknown functions (we emphasize that it is a row vector). The system of scalar equations (5) can now be rewritten in vectorized form as

$$\mathbf{u}_{xx} + \mathbf{u}_{yy} + \mathbf{u}\mathbf{K}^2 + \mathbf{u}_y\mathbf{W} + \mathbf{u}\mathbf{V} = 0\,, \tag{6}$$

where $\mathbf{W}(x, y)$, $\mathbf{V}(x, y)$ are the coupling matrices, and $\mathbf{K} = \mathrm{diag}(k_1, k_2, \ldots, k_M)$ is a diagonal matrix with the quantities $k_m(x, y)$ along the main diagonal, i.e., such that $\mathbf{K}_{mn} = \delta_{mn} k_m$).

Introducing the operator $\hat{R}_M$ of right multiplication by any matrix $\mathbf{M}$, we rewrite the equation (6) as

$$\mathbf{u}_{xx} = -\partial_y^2 \mathbf{u} - \hat{R}_W \partial_y \mathbf{u} - \hat{R}_V \mathbf{u}\,. \tag{7}$$

Next, we can perform the formal factorization of (7) and obtain the following one-way equation along the x direction

$$\mathbf{u}_x = \mathrm{i}\sqrt{\partial_y^2 + \hat{R}_W \partial_y + \hat{R}_V}\,\mathbf{u}, \quad x > 0\,. \tag{8}$$

This equation contains the square root of a matrix with differential operators as elements. In principle, it is a pseudodifferential parabolic equation for an unknown vector function. In the following it will be called vectorized PDPE (VPDPE).

We can formally integrate (8) over the interval $[x, x + h]$ to get

$$\mathbf{u}(x + h, y) = \exp\left(\mathrm{i}k_0 h\sqrt{1 + \hat{X}}\right)\mathbf{u}(x, y)\,,$$

where k_0 is a reference value of k_j (it can be the same for all j), and the operator $\hat{X}$ is defined by the formula

$$\partial_y^2 + R_Q \partial_y + R_S = k_0^2(1 + \hat{X})\,.$$

3. Generalized split-step Padé approach for solving VPDPE

As in the adiabatic (uncoupled) case, the propagator allows an approximation by an exponential of the form

$$\mathbf{u}(x+h,y) = \mathrm{e}^{ik_0 h}\left(d_0 + \sum_{k=1}^{p} \frac{d_k}{1+c_k\hat{X}}\right)\mathbf{u}(x,y) = \mathrm{e}^{ik_0 h}\left(d_0\mathbf{u}(x,y) + \sum_{k=1}^{p} d_k\mathbf{f}_k\right). \tag{9}$$

The terms $\mathbf{f}_k(x,y)$ in this case are obtained by solving the following operator equations

$$(1+c_k\hat{X})\,\mathbf{f}_k(x,y) = \mathbf{u}(x,y)\,. \tag{10}$$

In the following, we consider the solution of an equation (10) for one step of the marching scheme separately, i.e., we fix the value of x and omit the subscript k for the moment

$$(1+c\hat{X})\,\mathbf{f} = \mathbf{u}\,.$$

To perform a finite-difference discretization of Eq. (10) in y, we replace the vector function $\mathbf{u}(y)$ by a matrix $\mathbf{U} = (U_{\ell j})$ with N rows (number of grid points in y) and J columns (number of modes). Then the matrices $\mathbf{f}_k(y) \sim \mathbf{F}_k(y)$ can be found by solving the following matrix equation (where we drop the subscript as explained above)

$$k_0^2\left(\frac{1}{c}-1\right)\mathbf{F} + \mathbf{D}_2\mathbf{F} + \hat{\mathcal{L}}(\mathbf{F}) + \mathbf{F}\mathbf{S} = \mathbf{B}_n\,, \tag{11}$$

where the linear operator $\hat{\mathcal{L}}$ acting on $N\times J$ matrices is defined as

$$(\hat{\mathcal{L}}(\mathbf{F}))_{k\ell} = \sum_{n=1}^{N}\sum_{j=1}^{J}(\mathbf{D}_1)_{kn}\,\mathbf{F}_{nj}\,\mathbf{Q}_{j\ell n}\,, \tag{12}$$

$\mathbf{D}_2$ and $\mathbf{D}_1$ are square $N\times N$ matrices corresponding to finite-difference approximations of the second and the first derivatives with respect to the transverse variable y, respectively, and, by definition, $\mathbf{F}_{nj} = (\mathbf{f})_j(y_n)$.

Note that the p matrix equations (11) to be solved at each step of the marching scheme are similar to the so-called *generalized Sylvester problem*. The only difference is that after the finite difference discretization in y, the functions $\mathbf{Q}(y)$ and $\mathbf{S}(y)$ become tensors $J\times J\times N$. Despite this difference, the equations (10) can be solved by exactly the same vectorization procedure and construction similar to the tensor product of matrices. Let us replace the matrix $\mathbf{F}$ by a column vector vec($\mathbf{F}$) obtained by stacking columns of the matrix $\mathbf{F}$ (this is called 'vectorizing' a matrix). Then the operator $\hat{\mathcal{L}}$ can be replaced by multiplication by a block matrix vec($\hat{\mathcal{L}}$) of size $NJ\times NJ$ defined as

$$\mathrm{vec}(\hat{\mathcal{L}}(\mathbf{F})) = \mathrm{vec}(\hat{\mathcal{L}})\ \mathrm{vec}(\mathbf{F}) = \left[\begin{array}{c|c|c} \bar{Q}_{11}D_1 & \dots & \bar{Q}_{1J}D_1 \\ \hline \vdots & \ddots & \vdots \\ \hline \bar{Q}_{J1}D_1 & \dots & \bar{Q}_{JJ}D_1 \end{array}\right]\mathrm{vec}(\mathbf{F})\,, \tag{13}$$

where

$$\bar{Q}_{j\ell} = \mathrm{diag}(Q_{j\ell 1},\dots,Q_{j\ell N}) = \begin{bmatrix} Q_{j\ell 1} & & \\ & \ddots & \\ & & Q_{j\ell N}\end{bmatrix}$$

is a diagonal matrix $N\times N$ consisting of the values of the function $Q_{j\ell}(y)$ at the grid points in y.

Note that the computations reported below were performed using MATLAB routines for constructing the Kronecker product of matrices and for matrix inversion. The code was surprisingly efficient despite the fact that we had $J = 30$ and $N = 4000$, which is already suitable for handling practical products. Apparently, MATLAB is able to exploit the block structure of the matrices involved (by using an appropriate permutation of the columns). The same procedure can be used to implement the algorithm in industrial-grade software similar to AMPLE (see `https://www.poi.dvo.ru/en/AMPLE`.

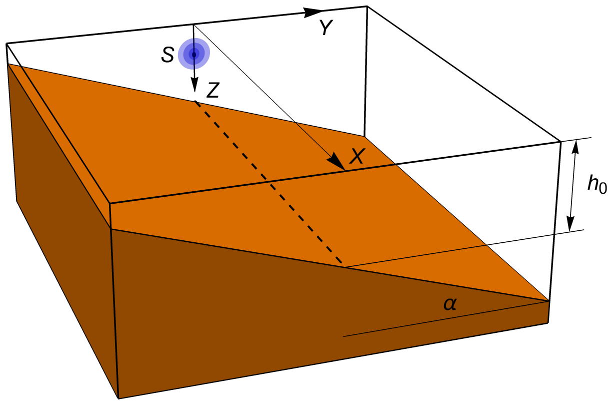

Figure 1: The coastal wedge: an acoustic waveguide where mode amplitudes are governed by the system (5).

4. An example: propagation in the wedge

In this section, we consider the solution of an equation of the form (6) that naturally arises in shallow water acoustics. Consider a typical area of shallow water near the coast, as shown in Fig. 1. We do not give an exact description of the test case parameters, as they are provided in numerous papers using this benchmark (see, e.g., [8, 9, 11, 12]).

The acoustic field $P(x, y, z)$ due to a point source in such problems can be represented as a superposition of normal modes $\phi_j(z, x, y)$

$$P(x, y, z) = \sum_{j=1}^{J} U_j(x, y)\phi_j(z, x, y)\,, \tag{14}$$

where $U_j(x, y)$ are called mode amplitudes (see e.g. [10, 11] for details). It is known that these amplitudes satisfy the equations (5), where $k_m = k_m(y)$ is the propagation constant of the m-th mode (in this particular case the media parameters do not depend on x), and V_{jm}, W_{jm} are coupling coefficients that can be easily found after computing ϕ_j (the computation of ϕ_j is done by solving a Sturm-Liouville problem, and numerous methods are available to do this in a very efficient way, see [10]).

Although sufficiently far from the source the field can be calculated by the adiabatic counterpart of (5) (i.e. the uncoupled system where all V_{jm}, W_{jm} are set to zero and we have an equation of the type (2) for each mode amplitude), at close range, where upslope/downslope propagation plays an important role, this simplification does not work. Similarly, simpler parabolic equations with mode coupling (see, e.g., [8]) cannot be used in this case due to the limitations of their aperture in the horizontal plane.

In order to achieve high accuracy of the solution in this case, we set $p = 11$ and $J = 30$. Our goal is to compute the acoustic field along the line $z = 30$ m, $x = 1000$ m and to compare the results with the benchmark solution obtained by the source image method [13]. Note that we used starters (the Cauchy data modelling the point source) proposed in [11] and truncated the computational domain by using the same PML as in [7].

The plot of the acoustic field $P(x, y, z)$ (in dB re $P(1\text{ m})$) obtained by solving VPDPE (8) using the SSP method is shown in Fig. 2. It can be clearly seen that our solution (red solid line) shows an excellent agreement with the reference (black dashed line). It can be observed that the adiabatic solution obtained using the equations (2) for each mode amplitude is very inaccurate in the considered region (although it can be used in the far field as shown in [11]).

5. Conclusion

In this study, a generalization of the SSP algorithm to the case of a one-way wave equation for an unknown vector function is presented. This algorithm can be applied to many practical problems in underwater acoustics and optics. On the one hand, the coupled mode parabolic wave equation (8) is a generalization of its scalar counterpart, while

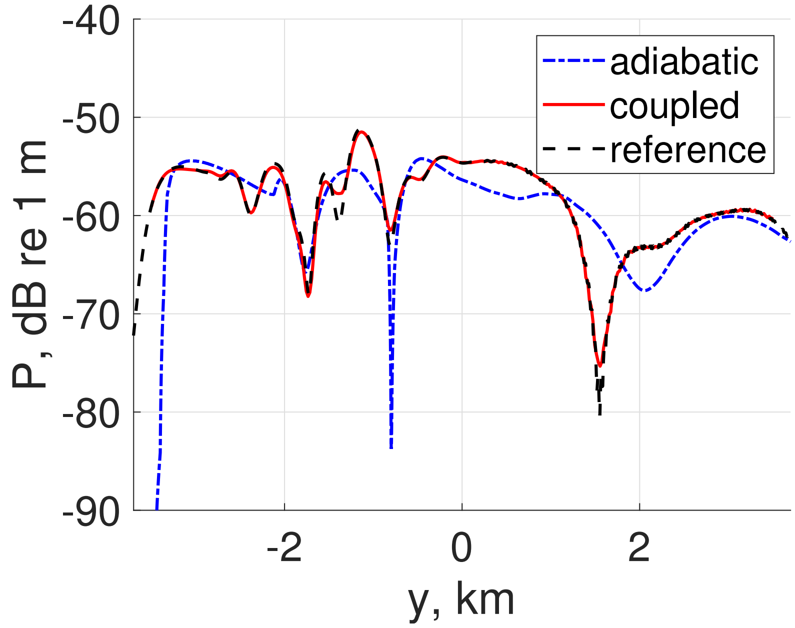

Figure 2: Acoustic field in the wedge along the line $z = 30$ m, $x = 1000$ m as a function of y, computed by solving VPDPE (8) using the generalized SSP algorithm (red line) and by its adiabatic counterpart (2) for each mode (blue line). Reference solution is represented by the black dashed line.

on the other hand it can be considered as a generalization of the vectorized WKBJ method [14] to the case of 3D problems.

The reported method presents a mathematical framework for handling the problems of guided wave propagation in the case of three-dimensional waveguides where the modes are trapped in one spatial direction. It allows to describe and study the energy coupling between such modes. In addition, it can be used as a theoretical basis for new general-purpose computational tools for many areas of physics.

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