On Properties of Compact 4th order Finite-Difference Schemes for the Variable Coefficient Wave Equation

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Abstract

We consider an initial-boundary value problem for the n-dimensional wave equation with the variable sound speed, $n \geqslant 1$. We construct three-level implicit in time and compact in space (three-point in each space direction) 4th order finite-difference schemes on the uniform rectangular meshes including their one-parameter (for $n = 2$) and three-parameter (for $n = 3$) families. We also show that some already known methods can be converted into such schemes. In a unified manner, we prove the conditional stability of schemes in the strong and weak energy norms together with the 4th order error estimate under natural conditions on the time step. We also transform an unconditionally stable 4th order two-level scheme suggested for $n = 2$ to the three-level form, extend it for any $n \geqslant 1$ and prove its stability. We also give an example of a compact scheme for non-uniform in space and time rectangular meshes. We suggest simple fast iterative methods based on FFT to implement the schemes. A new effective initial guess to start iterations is given too. We also present promising results of numerical experiments.

Keywords: wave equation, variable sound speed, compact higher-order scheme, stability, iterative methods

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1 Introduction

Vast literature is devoted to compact higher-order finite-difference schemes for PDEs including elliptic, parabolic, 2nd order hyperbolic and the time-dependent Schrödinger equation, etc. This is due to the fact that the formulas and implementation of compact schemes are not substantially more complex in comparison with the most standard 2nd order schemes but the error of compact schemes is usually several orders of magnitude less on the same mesh leading to significantly less computational work to ensure given accuracy.

In recent years, the case of initial-boundary value problems for the multidimensional wave equation with the variable sound speed $c(x)$ has attracted a lot of attention, see, in particular, [2,4,6,10], where much more relevant references can be found. Among them, in papers [2] for 2D case and [10] for 3D case, some three-term recurrent in time compact higher-order methods on the square spatial mesh have been constructed. In the case $c(x) \equiv \text{const}$, the spectral stability analysis of the methods has been given. The methods are conditionally stable but implicit in time. Therefore, to implement the methods, a direct method (for $n = 2$) and iterative methods of the conjugate gradient and multigrid types (for $n = 2, 3$) have been considered and verified.

In the case $n = 2$, another two-level vector in time 4th order method has been constructed in [4]. Here "the vector method" means that approximations for the solution u and its weighted time derivative $\frac{1}{c^2(x)}\partial_t u$ are constructed jointly. This method is unconditionally stable, but it

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exploits rather cumbersome approximations to the elliptic part of the wave equation involving triple application of a mesh Laplace operator and the inverse operators to the Numerov averages in each spatial coordinate. Consequently, in our opinion, it can hardly be called compact. Note that other two-level vector methods were studied, in particular, in [1, 15].

In the recent paper [14], implicit three-level in time and compact in space (the three-point in each space direction) finite-difference schemes on uniform rectangular meshes have been constructed by other techniques for the initial-boundary value problem (IBVP) with the non-homogeneous Dirichlet boundary condition for the n-dimensional wave equation with constant coefficients, $n \geqslant 1$. The conditional stability together with 4th order error estimates have been rigorously proved for the schemes. Extension of the schemes to the case of non-uniform in space and time rectangular meshes has been also given.

In this paper, we accomplish a generalization of compact schemes from [14] to the case $c(x) \not\equiv \text{const}$ based on a new technique related to averaging the wave equation. Moreover, we present one-parameter (for $n = 2$) and three-parameter (for $n = 3$) families of compact schemes. We also show how the methods from [2, 10] can be rewritten as three-level compact schemes for the wave equation, and they are included into these families of compact approximations of the wave equation in the case of square meshes up to our simpler approximation of the free term in the equation. But notice that we use another (also implicit) approximation of the second initial condition $\partial_t u|_{t=0} = u_1$ similar and closely connected to the approximation of the wave equation itself (going back, in particular, to [15]). We also apply an operator technique that greatly simplifies and shortens derivation, presentation, generalization and analysis of the schemes.

We first consider three-level in time finite-difference schemes with a weight σ and the variable coefficient $c(x)$ in an abstract form and prove a theorem on stability of these schemes in the strong (standard) and weak energy norms with respect to the initial data and free term. The stability is unconditional for $\sigma \geqslant \frac{1}{4}$ and conditional for $\sigma < \frac{1}{4}$. In the latter case, practical stability conditions on the time step of the mesh are often derived by applying the spectral method in the case of the $c(x) \equiv \text{const}$ and then taking the maximal value of $c(x)$ as this constant. The presented theorem justifies that such an approach is correct, in particular, for constructed compact schemes where $\sigma = \frac{1}{12}$. As a corollary of the main theorem, we rigorously prove the 4th order error estimate in the strong energy norm for constructed compact schemes. Notice that the spectral analysis for $c(x) \not\equiv \text{const}$ is impossible, and our analysis is based on the energy method; moreover, namely stability theorems of the mentioned type allow us to prove rigorous error estimates. We emphasize that the rigorous results on the 4th order approximation errors (in the standard sense), stability, error bounds and discrete energy conservation law are new results in the case $c(x) \not\equiv \text{const}$, and they ensure a strong theoretical basis for such compact schemes.

Next we consider the method from [4] mentioned above. Excluding the auxiliary unknown function approximating $\frac{1}{c^2(x)}\partial_t u$, we reduce it to the three-level method with the weight $\sigma = \frac{1}{4}$. We also generalize it to any $n \geqslant 1$ and prove its unconditional stability based on the above general stability theorem, now for $\sigma = \frac{1}{4}$.

We also present an example of extending a three-level compact scheme for any $n \geqslant 1$ to the case of non-uniform in space and time rectangular meshes. Note that compact schemes on non-uniform meshes for other equations were considered, in particular, in [5, 7, 11, 12].

In the case of the uniform rectangular mesh, we construct simple efficient one-step and N-step iterative methods to implement the schemes at each time level, with a preconditioner using FFT. Under the stability condition, they are fast convergent, and the convergence rate is independent both on the meshes and $c(x)$, in particular, on the spread of its values, that is non-trivial and important property for some applications. We also suggest how to select an effective initial guess, which is close to the sought solution at each time level. This choice is based on a simplified scheme for $\sigma = 0$ and also assumes usage of FFT. The one-step iterative method is applied for several numerical experiments.

The paper is organized as follows. In Section 2, we state the IBVP for the wave equation with the variable sound speed and consider three-level in time finite-difference schemes with the weight σ in general form. We adapt one recent theorem to prove the stability in the strong and weak energy norms for such schemes; the obtained stability estimates are unconditional for $\sigma \geqslant \frac{1}{4}$ and conditional for $\sigma < \frac{1}{4}$. The energy conservation law for these schemes is written as well. We also transform methods from [2,10] to the form of considered schemes. In Section 3, we generalize schemes from [14] to the case of the variable sound speed. Moreover, we present one-parameter (for $n = 2$) and three-parameter (for $n = 3$) families of compact schemes and justify the 4th approximation order of the schemes. We also compare the methods from [2, 10] with the constructed schemes. For these schemes, we prove theorems on their conditional stability and 4th order error bound in the strong energy norm. Section 4 presents the three-level form of the two-level method from [4], its extension to any $n \geqslant 1$ and a theorem on their unconditional stability bounds together with the energy conservation law. In Section 5, we also demonsrate how to extend one of the compact schemes suitable for any $n \geqslant 1$ to the case of non-uniform in space and time rectangular meshes.

The last Section 6 is devoted to the fast iterative one-step and N-step methods to implement the constructed compact schemes on the uniform mesh including theorems on their convergence. We also present results of numerical experiments on testing the constructed schemes and the one-step iterative method in 2D case including the wave propagation in a three-layer 2D medium initiated by the Ricker-type wavelet (with discontinuous $c(x)$ and the δ-shaped free term in the wave equation).

2 Symmetric three-level method for second order hyperbolic equations with a variable coefficient and its stability theorem

We consider the following initial-boundary value problem (IBVP) with the Dirichlet boundary condition for the wave equation in a generalized form

$$\rho(x)\partial_t^2 u(x,t) - (a_1^2\partial_1^2 + \ldots + a_n^2\partial_n^2)u(x,t) = f(x,t) \ \text{ in } \ Q_T = \Omega \times (0,T); \tag{2.1}$$

$$u|_{\Gamma_T} = g(x,t); \quad u|_{t=0} = u_0(x), \quad \partial_t u|_{t=0} = u_1(x), \quad x \in \Omega. \tag{2.2}$$

Here $0 < \underline{\rho} \leqslant \rho(x)$ in $\bar{\Omega}$, $a_1 > 0, \ldots, a_n > 0$ are constants (we take them different for uniformity with [14] and to distinct difference operators) and $x = (x_1, \ldots, x_n)$, $n \geqslant 1$. Also Ω is a bounded domain in $\mathbb{R}^n$, $\partial\Omega$ its boundary and $\Gamma_T = \partial\Omega \times (0,T)$ is the lateral surface of Q_T. Note that $c(x) = \frac{1}{\sqrt{\rho(x)}}$ is the variable sound speed in the case $a_1 = \ldots = a_n = 1$.

In this section, we consider a general three-level method with a weight for the IBVP (2.1)-(2.2) with $g = 0$. We present theorem on its stability and give the discrete energy conservation law which are applied below in Sections 3 and 4 for various specific conditionally and unconditionally stable 4th order schemes to ensure their stability and the discrete energy conservation laws. Such an approach is standard in the theory of difference schemes, for example, see [8].

Let H_h be a Euclidean space of functions given on a spatial mesh endowed with an inner product $(\cdot,\cdot)_h$ and the corresponding norm $\|\cdot\|_h$, where h is the parameter related to this mesh. Let B_h and A_h be linear operators in H_h having the properties $B_h = B_h^* > 0$ and $A_h = A_h^* > 0$. As applied to the wave equation (2.1), B_h is an averaging operator and A_h is an approximation to its elliptic part $-(a_1^2\partial_1^2+\ldots+a_n^2\partial_n^2)$. For any operator $C_h=C_h^*>0$ in H_h, one can define the norm $\|w\|_{C_h}=(C_hw,w)_h^{1/2}$ in H_h generated by it.

We introduce the uniform mesh $\overline{\omega}_{h_t}=\{t_m=mh_t\}_{m=0}^M$ on a segment $[0,T]$, with the step $h_t=T/M>0$ and $M\geqslant 2$. Let $\omega_{h_t}=\{t_m\}_{m=1}^{M-1}$ be the internal part of $\overline{\omega}_{h_t}$. We introduce the mesh averages and difference operators

$$\bar{s}_ty=\frac{\check{y}+y}{2},\ \ s_ty=\frac{y+\hat{y}}{2},\ \ \bar{\delta}_ty=\frac{y-\check{y}}{h_t},\ \ \delta_ty=\frac{\hat{y}-y}{h_t},\ \ \mathring{\delta}_ty=\frac{\hat{y}-\check{y}}{2h_t},\ \ \Lambda_ty=\delta_t\bar{\delta}_ty=\frac{\hat{y}-2y+\check{y}}{h_t^2}$$

with $y^m=y(t_m)$, $\check{y}^m=y^{m-1}$ and $\hat{y}^m=y^{m+1}$, as well as the operator of summation with the variable upper limit

$$I_{h_t}^my=h_t\sum_{l=1}^my^l\ \text{ for }\ 1\leqslant m\leqslant M,\ \ I_{h_t}^0y=0.$$

We consider the following symmetric three-level in t method with a weight (parameter) σ for the IBVP (2.1)-(2.2) with $g=0$:

$$B_h(\rho\Lambda_tv)+\sigma h_t^2A_h\Lambda_tv+A_hv=f\ \text{ in }\ H_h\ \text{ on }\ \omega_{h_t}, \tag{2.3}$$

$$B_h(\rho\delta_tv^0)+\sigma h_t^2A_h\delta_tv^0+\tfrac{1}{2}h_tA_hv^0=u_1+\tfrac{1}{2}h_tf^0\ \text{ in }\ H_h, \tag{2.4}$$

where $v\colon\overline{\omega}_{h_t}\to H_h$ is the sought function and the functions $v^0,u_1\in H_h$ and $f\colon\{t_m\}_{m=0}^{M-1}\to H_h$ are given; we omit their dependence on h for brevity. Also σ can depend on $\mathbf{h}:=(h,h_t)$.

Note that the form of equation (2.4) for v^1 goes back to [15] and is essential for several purposes (in particular, it seems most natural in the non-smooth case). It can be rewritten in the form similar to (2.3):

$$\tfrac{1}{0.5h_t}\big[B_h(\rho\delta_tv^0)+\sigma h_t^2A_h\delta_tv^0-u_1\big]+A_hv^0=f^0.$$

Note that clearly $\frac{1}{0.5h_t}(\delta_tu^0-(\partial_tu)_{t=0})\approx(\partial_t^2u)_{t=0}$ for any function $u\in C^2[0,T]$.

Recall that linear algebraic systems in H_h of the form

$$B_h(\rho w^m)+\sigma h_t^2A_hw^m=b^m \tag{2.5}$$

has to be solved at time levels t_m to find the solution v^{m+1} for all $0\leqslant m\leqslant M-1$. One of the possible ways is to find directly $w^0=\delta_tv^0$ from (2.4) and set $v^1=v^0+h_tw^0$, then find $w=\Lambda_tv$ from (2.3) and set $\hat{v}=2v-\check{v}+h_t^2w$. We can define the "diagonal" operator $D_\rho w:=\rho w$ in H_h, then $B_hD_\rho+\sigma h_t^2A_h$ is the operator in the problem (2.5).

In [2, 10], for $\sigma\neq 0$, a special trick was applied (here we do not dwell on its motivation). The auxiliary function b is introduced by the recurrent relation

$$\hat{b}=\big(2-\tfrac{1}{\sigma}\big)b-\check{b}-\tfrac{\rho}{\sigma^2h_t^2}v-\tfrac{1}{\sigma}\tilde{f}\ \text{ in }\ H_h\ \text{ on }\ \omega_{h_t}, \tag{2.6}$$

and it is suggested to solve the equation

$$-A_h\hat{v}-\tfrac{1}{\sigma h_t^2}B_h(\rho\hat{v})=B_h\hat{b}\ \text{ in }\ H_h\ \text{ on }\ \omega_{h_t} \tag{2.7}$$

to find $\hat{v}$ (here the notation is slightly changed). Rewriting relation (2.6) as

$$h_t^2\Lambda_tb=-\tfrac{1}{\sigma}b-\tfrac{\rho}{\sigma^2h_t^2}v-\tfrac{1}{\sigma}\tilde{f}$$

and applying $-\sigma B_h$ to it, we get

$$-\sigma h_t^2\Lambda_tB_hb=B_hb+\tfrac{1}{\sigma h_t^2}B_h(\rho v)+B_h\tilde{f}.$$

Applying to it (on both sides) equation (2.7) from right to left (we use it also for $t_0 = 0$ together with $-A_h v^0 - \frac{1}{\sigma h_t^2} B_h(\rho v^0) = B_h b^0$ for the definitions of b^1 and b^0), we obtain

$$B_h(\rho \Lambda_t v) + \sigma h_t^2 A_h \Lambda_t v = -A_h v - \tfrac{1}{\sigma h_t^2} B_h(\rho v) + \tfrac{1}{\sigma h_t^2} B_h(\rho v) + B_h \tilde{f} = -A_h v + B_h \tilde{f}$$

on ω_{h_t}. This is nothing more than equation (2.3) with $f = B_h \tilde{f}$.

For $\sigma < \frac{1}{4}$, we also assume that A_h and B_h are related by the following inequality

$$\|w\|_{A_h} \leqslant \alpha_h \|w\|_{B_h} \quad \forall w \in H_h \quad \Leftrightarrow \quad A_h \leqslant \alpha_h^2 B_h. \tag{2.8}$$

Clearly the minimal value of α_h^2 is the maximal eigenvalue of the generalized eigenvalue problem

$$A_h e = \lambda B_h e, \quad e \in H_h, \quad e \neq 0. \tag{2.9}$$

For method (2.3)-(2.4), we present a theorem on uniform in time stability (unconditional for $\sigma \geqslant \frac{1}{4}$ or conditional for $\sigma < \frac{1}{4}$) in the mesh strong (standard) and weak energy norms with respect to the initial data v^0 and u_1 and the free term f. Let $\|y\|_{L^1_{h_t}(H_h)} := \frac{1}{4} h_t \|y^0\|_h + I_{h_t}^{M-1} \|y\|_h$.

Theorem 2.1. *Let the operators A_h and B_h commute, i.e. $A_h B_h = B_h A_h$. Let either $\sigma \geqslant \frac{1}{4}$ and $\varepsilon_0 = 1$, or*

$$\sigma < \tfrac{1}{4}, \quad (\tfrac{1}{4} - \sigma) h_t^2 \alpha_h^2 \leqslant (1 - \varepsilon_0^2) \underline{\rho} \ \text{ for some } \ 0 < \varepsilon_0 < 1. \tag{2.10}$$

For the solution to method (2.3)-(2.4), the following bounds hold:

(1) in the strong energy norm

$$\max_{1 \leqslant m \leqslant M} \Big[\|\sqrt{\rho}\bar{\delta}_t v^m\|_h^2 + (\sigma - \tfrac{1}{4}) h_t^2 \|\bar{\delta}_t v^m\|^2_{B_h^{-1} A_h} + \|\bar{s}_t v^m\|^2_{B_h^{-1} A_h} \Big]^{1/2}$$
$$\leqslant \Big(\|v^0\|^2_{B_h^{-1} A_h} + \varepsilon_0^{-2} \big\| \tfrac{1}{\sqrt{\rho}} B_h^{-1} u_1 \big\|_h^2 \Big)^{1/2} + 2\varepsilon_0^{-1} \big\| \tfrac{1}{\sqrt{\rho}} B_h^{-1} f \big\|_{L^1_{h_t}(H_h)}, \tag{2.11}$$

where the f-term can be replaced with $2 I_{h_t}^{M-1} \|(A_h B_h)^{-1/2} \bar{\delta}_t f\|_h + 3 \max\limits_{0 \leqslant m \leqslant M-1} \|(A_h B_h)^{-1/2} f^m\|_h$;

(2) in the weak energy norm

$$\max_{0 \leqslant m \leqslant M} \max \Big\{ \Big[\|\sqrt{\rho} v^m\|_h^2 + (\sigma - \tfrac{1}{4}) h_t^2 \|v^m\|^2_{B_h^{-1} A_h} \Big]^{1/2}, \ \|I_{h_t}^m \bar{s}_t v\|_{B_h^{-1} A_h} \Big\}$$
$$\leqslant \Big[\|\sqrt{\rho} v^0\|_h^2 + (\sigma - \tfrac{1}{4}) h_t^2 \|v^0\|^2_{B_h^{-1} A_h} \Big]^{1/2} + 2\|(A_h B_h)^{-1/2} u_1\|_h + 2\|(A_h B_h)^{-1/2} f\|_{L^1_{h_t}(H_h)}, \tag{2.12}$$

where, for $f = \delta_t g$, one can replace the f-term with $2\varepsilon_0^{-1} I_{h_t}^M \big\| \frac{1}{\sqrt{\rho}} B_h^{-1} (g - s_t g^0) \big\|_h$.

Proof. We prove this theorem by applying its non-standard reduction to the recently proved results directly suitable only for $\rho(x) \equiv \text{const}$. Applying B_h^{-1} to equations (2.3)-(2.4), we get

$$(\rho I + \sigma h_t^2 B_h^{-1} A_h) \Lambda_t v + B_h^{-1} A_h v = B_h^{-1} f \ \text{ in } \ H_h \ \text{ on } \ \omega_{h_t}, \tag{2.13}$$
$$(\rho I + \sigma h_t^2 B_h^{-1} A_h) \delta_t v^0 + \tfrac{1}{2} h_t B_h^{-1} A_h v^0 = B_h^{-1} u_1 + \tfrac{1}{2} h_t B_h^{-1} f^0 \ \text{ in } \ H_h. \tag{2.14}$$

We have $D_\rho^* = D_\rho > 0$. The property $A_h B_h = B_h A_h$ implies $A_h B_h^{-1} = B_h^{-1} A_h$ and thus $(B_h^{-1} A_h)^* = B_h^{-1} A_h$. Also the eigenvalue equation in (2.9) can be rewritten as $B_h^{-1} A_h e = \lambda e$ and therefore $B_h^{-1} A_h > 0$; moreover, inequality (2.8) is equivalent to

$$\|w\|_{B_h^{-1} A_h} \leqslant \alpha_h \|w\|_h \ \ \forall w \in H_h. \tag{2.15}$$

Consequently under the imposed conditions on σ and h_t we also have

$$\varepsilon_0^2\|\sqrt{\rho}w\|_h^2 \leqslant \|\sqrt{\rho}w\|_h^2 + (\sigma - \tfrac{1}{4})h_t^2\|w\|_{B_h^{-1}A_h}^2 \quad \forall w \in H_h. \tag{2.16}$$

Now one can apply [14, Theorem 1] (see also [16]) concerning method (2.3)-(2.4) with $\rho(x) \equiv 1$ to method (2.13)-(2.14), with D_ρ, $B_h^{-1}A_h$, $B_h^{-1}f$ and $B_h^{-1}u_1$ in the role of B_h, A_h, f and u_1, respectively, and derive the stated bounds.

We notice that *the discrete energy conservation law*

$$\|\sqrt{\rho}\bar\delta_t v^m\|_h^2 + (\sigma - \tfrac{1}{4})h_t^2\|\bar\delta_t v^m\|_{B_h^{-1}A_h}^2 + \|\bar s_t v^m\|_{B_h^{-1}A_h}^2 = \big(B_h^{-1}A_h v^0, s_t v^0\big)_h$$
$$+\big(B_h^{-1}u_1, \delta_t v^0\big)_h + \tfrac{1}{2}h_t\big(B_h^{-1}f^0, \delta_t v^0\big)_h + 2I_{h_t}^{m-1}(B_h^{-1}f, \mathring{\delta}_t v)_h, 1 \leqslant m \leqslant M, \tag{2.17}$$

see proof of Theorem 1 in [16], not only implies bound (2.11) for the method (2.13)-(2.14) but itself has the independent interest. This natural form is obtained, in particular, due to equation (2.4) for v^1.

Concerning the operators in the second form of the f-term in (2.11) and the last two terms in (2.12), we also take into account the following transformations

$$\|(B_h^{-1}A_h)^{-1/2}B_h^{-1}w\|_h^2 = \big((B_h^{-1}A_h)^{-1}B_h^{-1}w, B_h^{-1}w\big)_h = \big(B_h^{-1}A_h^{-1}w, w\big)_h$$
$$= \big((A_hB_h)^{-1}w, w\big)_h = \|(A_hB_h)^{-1/2}w\|_h \quad \forall w \in H_h.$$

This completes the proof. □

In practice, stability conditions like (2.10) are often obtained by applying the spectral method in the case $\rho(x) \equiv \mathrm{const}$ and then taking in the result $\underline{\rho}$ as this constant. We emphasize that Theorem 2.1 justifies that such an approach is correct in our case. On the other hand, we emphasize that in the case $\rho(x) \equiv \mathrm{const}$ our stability bounds themselves (2.11)-(2.12) *differ* from those in [14].

Recall that each of bounds (2.11) or (2.12) implies existence and uniqueness of the solution to method (2.3)-(2.4) for any given $v^0, u_1 \in H_h$ and f: $\{t_m\}_{m=0}^{M-1} \to H_h$. The same applies to finite-difference schemes below.

Bound (2.12) in the weak energy norm is less standard than (2.11) but namely it contains simple H_h-norm of v^0 most relevant when studying stability with respect to the round-off errors; also bounds in both norms are essential when proving delicate error estimates [15] in dependence with the data smoothness.

3 Construction and properties of compact finite-difference schemes of the 4th order of approximation

Let below $\Omega = (0, X_1) \times \ldots \times (0, X_n)$ and g be general in the boundary condition (2.2) if the opposite is not stated explicitly. Define the uniform rectangular mesh

$$\bar\omega_h = \{x_{\mathbf{k}} = (x_{1k_1}, \ldots, x_{nk_n}) = (k_1h_1, \ldots, k_nh_n);\, 0 \leqslant k_1 \leqslant N_1, \ldots, 0 \leqslant k_n \leqslant N_n\}$$

in $\bar\Omega$ with the steps $h_1 = \frac{X_1}{N_1}, \ldots, h_n = \frac{X_n}{N_n}$, $h = (h_1, \ldots, h_n)$ and $\mathbf{k} = (k_1, \ldots, k_n)$. Let

$$\omega_h = \{x_{\mathbf{k}};\, 1 \leqslant k_1 \leqslant N_1 - 1, \ldots, 1 \leqslant k_n \leqslant N_n - 1\}, \quad \partial\omega_h = \bar\omega_h \backslash \omega_h$$

be the internal part and boundary of $\bar\omega_h$. Define also the meshes $\omega_{\mathbf{h}} := \omega_h \times \omega_{h_t}$ in Q_T and $\partial\omega_{\mathbf{h}} = \partial\omega_h \times \{t_m\}_{m=1}^M$ on $\bar\Gamma_T$.

We introduce the standard difference approximation to $\partial_l^2 w$:

$$(\Lambda_l w)_{\mathbf{k}} = \tfrac{1}{h_l^2}(w_{\mathbf{k}+\mathbf{e}_l} - 2w_{\mathbf{k}} + w_{\mathbf{k}-\mathbf{e}_l}), \quad l = 1, \ldots, n,$$

on ω_h, where $w_{\mathbf{k}} = w(x_{\mathbf{k}})$ and $\mathbf{e}_1, \ldots, \mathbf{e}_n$ is the standard coordinate basis in $\mathbb{R}^n$.

Let below H_h be the space of functions defined on $\bar{\omega}_h$ and equal 0 on $\partial\omega_h$, endowed with the inner product $(v, w)_h = h_1 \ldots h_n \sum_{x_{\mathbf{k}} \in \omega_h} v_{\mathbf{k}} w_{\mathbf{k}}$.

We define the Numerov-type averaging operators and approximation of f

$$s_N := I + \tfrac{1}{12}(h_1^2\Lambda_1 + \ldots + h_n^2\Lambda_n), \quad s_{N\widehat{j}} := I + \tfrac{1}{12} \sum_{1 \leqslant i \leqslant n,\, i \neq j} h_i^2 \Lambda_i, \quad 1 \leqslant j \leqslant n,$$

$$A_N := -(a_1^2 s_{N\widehat{1}}\Lambda_1 + \ldots + a_n^2 s_{N\widehat{n}}\Lambda_n), \quad f_N := s_N f + \tfrac{1}{12} h_t^2 \Lambda_t f,$$

where I is the identity operator; note that $s_{N\widehat{1}} = I$ for $n = 1$. We also set

$$u_{1N} := s_N(\rho u_1) + \tfrac{1}{12} h_t^2 (a_1^2\Lambda_1 + \ldots + a_n^2\Lambda_n) u_1, \tag{3.1}$$

$$f_N^0 := f_{dh_t}^{(0)} + \tfrac{1}{12}(h_1^2\Lambda_1 + \ldots + h_n^2\Lambda_n) f_0, \quad \text{with some} \quad f_{dh_t}^{(0)} = f_d^{(0)} + \mathcal{O}(h_t^3), \tag{3.2}$$

on ω_h, where $f_d^{(0)} := f_0 + \frac{1}{3} h_t (\partial_t f)_0 + \frac{1}{12} h_t^2 (\partial_t^2 f)_0$ and $y_0 := y|_{t=0}$, similarly to [14]. Note the non-trivial form of $u_{1N} \approx \rho u_1$, where the first term contains ρu_1, but the second one does not. Additional details concerning formula (3.2) are given in Remark 3.1 below.

The following basic lemma generalizes [14, Lemmas 1-2] for $\rho(x) \not\equiv \text{const}$.

Lemma 3.1. *Let the coefficient ρ and solution u to the IBVP* (2.1)-(2.2) *be sufficiently smooth respectively in $\bar{\Omega}$ and $\bar{Q}_T$. Then the following formulas hold*

$$s_N(\rho \Lambda_t u) - \tfrac{1}{12} h_t^2 (h_1^2 a_1^2 \Lambda_1 + \ldots + a_n^2 h_n^2 \Lambda_n) \Lambda_t u - A_N u - f_N = \mathcal{O}(|\mathbf{h}|^4) \ \text{ on } \omega_{\mathbf{h}}, \tag{3.3}$$

$$s_N(\rho \delta_t u)^0 - \tfrac{h_t^2}{12}(h_1^2 a_1^2 \Lambda_1 + \ldots + a_n^2 h_n^2 \Lambda_n)(\delta_t u)^0 - \tfrac{h_t}{2} A_N u_0 - u_{1N} - \tfrac{h_t}{2} f_N^0 = \mathcal{O}(|\mathbf{h}|^4) \ \text{on } \omega_h. \tag{3.4}$$

Proof. We apply a new technique based on averaging of equation (2.1) related to the polylinear finite elements like in [14]; the more standard Numerov-type technique could be also used. An advantage of the averaging technique is that approximations of f and u_1 in the non-smooth case (important in practice) become clear from the right-hand sides of formulas (3.10) and (3.12) below (we use this in Section 6) but remain obscure in the frame of the Numerov-type technique.

1. We define the well-known average in the variable x_k related to the linear finite elements

$$(q_k w)(x_k) = \tfrac{1}{h_k} \int_{-h_k}^{h_k} w(x_k + \xi)\big(1 - \tfrac{|\xi|}{h_k}\big)\, d\xi.$$

For a function $w(x_k)$ smooth on $[0, X_k]$, the following relations hold

$$q_k \partial_k^2 w = \Lambda_k w, \tag{3.5}$$

$$q_k w = w + q_k \rho_{k2}(\partial_k^2 w), \tag{3.6}$$

$$q_k w = w + \tfrac{1}{12} h_k^2 \partial_k^2 w + q_k \rho_{k4}(\partial_k^4 w) = w + \tfrac{1}{12} h_k^2 \Lambda_k w + \tilde{\rho}_{k4}(\partial_k^4 w), \tag{3.7}$$

$$|q_k \rho_{ks}(\partial_k^s w)| \leqslant c_s h_k^s \|\partial_k^s w\|_{C(I_{kl})}, \ s = 2, 4, \ \ |\tilde{\rho}_{k4}(\partial_k^4 w)| \leqslant \tilde{c}_4 h_k^4 \|\partial_k^4 w\|_{C(I_{kl})} \tag{3.8}$$

at the nodes $x_k = x_{kl}$, $1 \leqslant l \leqslant N_k - 1$, with the constants c_s and $\tilde{c}_4$ independent on the mesh and $I_{kl} := [x_{k(l-1)}, x_{k(l+1)}]$. Formula (3.5) is well-known and is checked by integrating by parts. Other relations hold due to Taylor's formula at $x_k = x_{kl}$ with the residual in the integral form

$$\rho_{ks}(w)(x_k) = \frac{1}{(s-1)!} \int_{x_{kl}}^{x_k} w(\xi)(x_k - \xi)^{s-1}\, d\xi, \tag{3.9}$$

for $s = 2, 4$, together with the elementary formula

$$\tfrac{1}{h_k} \int_{-h_k}^{h_k} \tfrac{1}{2}\xi^2 \big(1 - \tfrac{|\xi|}{h_k}\big)\, d\xi = \tfrac{1}{12} h_k^2.$$

The respective formulas hold for the averaging operator q_t in the variable $t = x_{n+1}$ as well since one can set $X_{n+1} = T$ and $h_{n+1} = h_t$.

We apply the operator $\bar{q} q_t$ with $\bar{q} := q_1 \dots q_n$ to the wave equation (2.1) at the nodes of $\omega_{\mathbf{h}}$, use formula (3.5) and get:

$$\bar{q}(\rho \Lambda_t u) - (a_1^2 \bar{q}_{\widehat{1}} \Lambda_1 u + \ldots + a_n^2 \bar{q}_{\widehat{n}} \Lambda_n u) = \bar{q} q_t f, \quad \text{with } \ \bar{q}_{\widehat{i}} := \prod_{1 \leqslant k \leqslant n,\, k \neq i} q_k; \tag{3.10}$$

here $\bar{q}_{\widehat{1}} = I$ for $n = 1$. The above expansions for $q_1, \dots, q_n, q_{n+1} = q_t$ lead to the formula

$$\rho \Lambda_t u + \sum_{i=1}^n \tfrac{1}{12} h_i^2 \Lambda_i (\rho \Lambda_t u) - \sum_{i=1}^n a_i^2 \Big[\Lambda_i u + \Big(\sum_{1 \leqslant j \leqslant n,\, j \neq i} \tfrac{1}{12} h_j^2 \Lambda_j\Big) \Lambda_i u + \tfrac{1}{12} h_t^2 \Lambda_t \Lambda_i u\Big]$$
$$= f + \tfrac{1}{12} \sum_{i=1}^n h_i^2 \Lambda_i f + \tfrac{1}{12} h_t^2 \Lambda_t f + O(|\mathbf{h}|^4),$$

and thus, using the above defined operators s_N and A_N as well as f_N, to formula (3.3) as well.

2. In addition, we define the one-sided average in t over $(0, h_t)$:

$$q_t y^0 = \tfrac{2}{h_t} \int_0^{h_t} y(t) \big(1 - \tfrac{t}{h_t}\big)\, dt. \tag{3.11}$$

We apply $\frac{h_t}{2} \bar{q} q_t (\cdot)^0$ to the wave equation (2.1) and, since $\frac{h_t}{2}(q_t \partial_t u)^0 = (\delta_t u)^0 - (\partial_t u)_0$, obtain

$$\bar{q}(\rho \delta_t u)^0 - \tfrac{h_t}{2}(a_1^2 \bar{q}_{\widehat{1}} \Lambda_1 u + \ldots + a_n^2 \bar{q}_{\widehat{n}} \Lambda_n u) q_t u^0 = \bar{q}(\rho u_1) + \tfrac{h_t}{2} \bar{q} q_t f^0. \tag{3.12}$$

Using Taylor's formula at $t = 0$ and calculating the arising integrals in t over $(0, h_t)$, we get

$$\tfrac{h_t}{2} q_t f^0 = \tfrac{h_t}{2} f_0 + \tfrac{h_t^2}{6} (\partial_t f)_0 + \tfrac{h_t^3}{24} (\partial_t^2 f)_0 + O(h_t^4) = \tfrac{h_t}{2} f_d^{(0)} + O(h_t^4), \tag{3.13}$$

with $f_d^{(0)}$ defined above. Here we omit the integral representations for $O(h_t^4)$-terms for brevity. Similarly to the previous Item 1 and due to expansion (3.13), we find

$$\bar{q}(\rho \delta_t u)^0 = s_N (\rho \delta_t u)^0 + O(|h|^4), \quad \bar{q}(\rho u_1) = s_N(\rho u_1) + O(|h|^4), \tag{3.14}$$

$$\tfrac{h_t}{2} q_t \bar{q} f^0 = \tfrac{h_t}{2} f_d^{(0)} + \tfrac{1}{12} h_i^2 \Lambda_i f_0 + O(|\mathbf{h}|^4). \tag{3.15}$$

Also due to Taylor's formula in t at $t = 0$ one can write down

$$u(\cdot, t) = u_0 + t u_1 + \tfrac{t^2}{h_t}((\delta_t u)^0 - u_1) + O(t^3).$$

Thus similarly first to (3.13) and second to (3.14) as well as according to formula (3.6) and the first bound (3.8) we obtain

$$\frac{h_t}{2}a_k^2\bar{q}_{\widehat{k}}\Lambda_k q_t u^0 = a_k^2\big[\frac{h_t}{2}\bar{q}_{\widehat{k}}\Lambda_k u_0 + \frac{h_t^2}{6}\bar{q}_{\widehat{k}}\Lambda_k u_1 + \frac{h_t^2}{12}\bar{q}_{\widehat{\imath}}\Lambda_k((\delta_t u)^0 - u_1)\big] + O(h_t^4)$$
$$= \frac{h_t}{2}a_k^2 s_{N\widehat{k}}\Lambda_k u_0 + \frac{h_t^2}{12}a_k^2\Lambda_k u_1 + \frac{h_t^2}{12}a_k^2 s_{N\widehat{k}}\Lambda_k(\delta_t u)^0 + O(|\mathbf{h}|^4), \quad 1 \leqslant k \leqslant n. \tag{3.16}$$

We insert all the derived expansions (3.13)-(3.16) into formula (3.12), rearrange the summands and obtain formula (3.4) with u_{1N} and f_N^0 defined above. □

Remark 3.1. *Let* $0 < h_t \leqslant \bar{h}_t \leqslant T$. *If* f *is sufficiently smooth in* t *in* $\bar{Q}_{\bar{h}_t}$ *(or* $\bar{\Omega}\times[-\bar{h}_t,\bar{h}_t]$*), then* $f_{dh_t}^{(0)} = f_d^{(0)} + \mathcal{O}(h_t^3)$ *(see (3.2)) for the following three- and two-level approximations*

$$f_{dh_t}^{(0)} = \tfrac{7}{12}f^0 + \tfrac{1}{2}f^1 - \tfrac{1}{12}f^2, \quad f_{dh_t}^{(0)} = \tfrac{1}{3}f^0 + \tfrac{2}{3}f^{1/2} \quad \textit{with} \quad f^{1/2} := f|_{t=h_t/2} \tag{3.17}$$

(or $f_{dh_t}^{(0)} = f^0 + \frac{1}{3}h_t\mathring{\delta}_t f^0 + \frac{1}{12}h_t^2\Lambda_t f^0 = -\frac{1}{12}f^{-1} + \frac{5}{6}f^0 + \frac{1}{4}f^1$ *with* $f^{-1} := f|_{t=-h_t}$*). These formulas are easily checked using Taylor's formula at* $t = 0$.

In our construction of compact schemes for the IBVP (2.1)-(2.2), in general we will follow [14]. Preliminarily we consider the scheme of the form

$$s_N(\rho\Lambda_t v) - \tfrac{1}{12}h_t^2(a_1^2\Lambda_1 + \ldots + a_n^2\Lambda_n)\Lambda_t v + A_N v = f_N \ \text{ on } \ \omega_{\mathbf{h}}, \tag{3.18}$$

$$v|_{\partial\omega_{\mathbf{h}}} = g, \quad s_N(\rho\delta_t v^0) - \tfrac{1}{12}h_t^2(a_1^2\Lambda_1 + \ldots + a_n^2\Lambda_n)v^0 + \tfrac{1}{2}h_t A_N v^0 = u_{1N} + \tfrac{1}{2}h_t f_N^0 \ \text{ on } \ \omega_h. \tag{3.19}$$

On the left in formulas (3.3)-(3.4) in Lemma 3.1, the approximation errors of the equations for this scheme stand, and thus these formulas mean here that the scheme has the approximation order $\mathcal{O}(|\mathbf{h}|^4)$. For $n = 1$, the scheme takes the simplest form

$$s_N(\rho\Lambda_t v) - \tfrac{1}{12}h_t^2 a_1^2\Lambda_1\Lambda_t v - a_1^2\Lambda_1 v = f_N \ \text{ on } \ \omega_{\mathbf{h}}, \tag{3.20}$$

$$v|_{\partial\omega_{\mathbf{h}}} = g, \quad s_N(\rho\delta_t v^0) - \tfrac{1}{12}h_t^2 a_1^2\Lambda_1\delta_t v^0 - \tfrac{1}{2}h_t a_1^2\Lambda_1 v^0 = u_{1N} + \tfrac{1}{2}h_t f_N^0 \ \text{ on } \ \omega_h, \tag{3.21}$$

that is a particular case (for $g = 0$) of the general method (2.3)-(2.4) for $B_h = s_N$, $A_h = -a_1^2\Lambda_1$ and $\sigma = \frac{1}{12}$.

But for $n \geqslant 2$ scheme (3.18)-(3.19) is no more of type (2.3)-(2.4). Therefore we first replace it with the following scheme

$$s_N(\rho\Lambda_t v) + \tfrac{1}{12}h_t^2 A_N\Lambda_t v + A_N v = f_N \ \text{ on } \ \omega_{\mathbf{h}}, \tag{3.22}$$

$$v|_{\partial\omega_{\mathbf{h}}} = g, \quad s_N(\rho\delta_t v^0) + \tfrac{1}{12}h_t^2 A_N\delta_t v^0 + \tfrac{1}{2}h_t A_N v^0 = u_{1N} + \tfrac{1}{2}h_t f_N^0 \ \text{ on } \ \omega_h, \tag{3.23}$$

that corresponds to the case $B_h = s_N$, $A_h = A_N$ and $\sigma = \frac{1}{12}$. Since

$$A_N + a_1^2\Lambda_1 + \ldots + a_n^2\Lambda_n = a_1^2(I - s_{N\widehat{1}})\Lambda_1 + \ldots + a_n^2(I - s_{N\widehat{n}})\Lambda_n,$$

the approximation error of this scheme is also of the order $\mathcal{O}(|\mathbf{h}|^4)$.

For $n = 2$, one can easily generalize this scheme by the extension

$$s_N = I + \tfrac{1}{12}h_1^2\Lambda_1 + \tfrac{1}{12}h_2^2\Lambda_2 \mapsto s_{N\beta} := s_N + \beta\tfrac{h_1^2}{12}\tfrac{h_2^2}{12}\Lambda_1\Lambda_2, \tag{3.24}$$

with the parameter β, keeping its approximation order. Note that $\Lambda_1\Lambda_2 > 0$ in H_h.

But the last scheme fails for $n \geqslant 3$ similarly to [3, 14]. Recall that the point is that the minimal eigenvalue of s_N as the operator in H_h is such that

$$\lambda_{\min}(s_N) > 1 - \tfrac{n}{3}, \quad \lambda_{\min}(s_N) = 1 - \tfrac{n}{3} + O\big(\tfrac{1}{N_1^2} + \ldots + \tfrac{1}{N_n^2}\big)$$

that is suitable only for $n = 1, 2$, since s_N becomes almost singular for $n = 3$ and even $\lambda_{\min}(s_N) < 0$ for $n \geqslant 4$, for small $|h|$ (and a crucial property $s_N > 0$ is not valid any more). Thus for $n = 3$ it is of sense to replace s_N with $\bar{s}_N$ and pass to the scheme

$$\bar{s}_N(\rho\Lambda_t v) + \tfrac{1}{12}h_t^2 A_N\Lambda_t v + A_N v = f_N \ \text{ on } \ \omega_{\mathbf{h}}, \tag{3.25}$$

$$v|_{\partial\omega_{\mathbf{h}}} = g, \quad \bar{s}_N(\rho\delta_t v^0) + \tfrac{1}{12}h_t^2 A_N\delta_t v^0 + \tfrac{1}{2}h_t A_N v^0 = u_{1N} + \tfrac{1}{2}h_t f_N^0 \ \text{ on } \ \omega_h. \tag{3.26}$$

Next, for any $n \geqslant 1$, one can further replace A_N with $\bar{A}_N$ and get the following unified scheme

$$\bar{s}_N(\rho\Lambda_t v) + \tfrac{1}{12}h_t^2 \bar{A}_N\Lambda_t v + \bar{A}_N v = f_N \ \text{ on } \ \omega_{\mathbf{h}}, \tag{3.27}$$

$$v|_{\partial\omega_{\mathbf{h}}} = g, \quad \bar{s}_N(\rho\delta_t v^0) + \tfrac{1}{12}h_t^2 \bar{A}_N\delta_t v^0 + \tfrac{1}{2}h_t \bar{A}_N v^0 = u_{1N} + \tfrac{1}{2}h_t f_N^0 \ \text{ on } \ \omega_h \tag{3.28}$$

(for $\rho(x) \equiv 1$, it goes back to [3] in the case of the time-dependent Schrödinger equation). In the last two schemes, we use the operators

$$\bar{s}_N := \prod_{k=1}^{n} s_{kN}, \quad \bar{s}_{N\hat{l}} := \prod_{1\leqslant k\leqslant n,\, k\neq l} s_{kN}, \quad s_{kN} := I + \tfrac{1}{12}h_k^2\Lambda_k, \tag{3.29}$$

$$\bar{A}_N := -(a_1^2\bar{s}_{N\hat{1}}\Lambda_1 + \ldots + a_n^2\bar{s}_{N\hat{n}}\Lambda_n), \tag{3.30}$$

where $\bar{s}_N$ is the splitting version of s_N, and $\bar{s}_{N\hat{l}}$ is similar to $\bar{s}_N$ excluding the direction x_l, with $\bar{s}_{N\hat{1}} = I$ for $n = 1$. All of them are symmetric positive definite as the operators in H_h.

We also have $(\frac{2}{3})^n I < \bar{s}_N < I$ in H_h. The following formula connects $\bar{s}_N$ and s_N

$$\bar{s}_N = s_N + \sum_{k=2}^{n} \bar{s}_N^{(k)}, \quad \bar{s}_N^{(k)} := (\tfrac{1}{12})^k \sum_{1\leqslant i_1<\ldots<i_k\leqslant n} h_{i_1}^2\ldots h_{i_k}^2\Lambda_{i_1}\ldots\Lambda_{i_k}. \tag{3.31}$$

Notice that $(-1)^k\bar{s}_N^{(k)} > 0$ in H_h, $2 \leqslant k \leqslant n$.

Here $\bar{A}_N = A_N$ for $n = 1, 2$, and for $n = 1$ the last scheme coincides with (3.20)-(3.21) but

$$\bar{A}_N = A_N + \bar{A}_N^{(3)} = -(a_1^2\Lambda_1 + a_2^2\Lambda_2 + a_3^2\Lambda_3) + \bar{A}_N^{(2)} + \bar{A}_N^{(3)},$$

$$\bar{A}_N^{(2)} := -\tfrac{1}{12}\big[(a_1^2h_2^2 + a_2^2h_1^2)\Lambda_1\Lambda_2 + (a_1^2h_3^2 + a_3^2h_1^2)\Lambda_1\Lambda_3 + (a_2^2h_3^2 + a_3^2h_2^2)\Lambda_2\Lambda_3\big],$$

$$\bar{A}_N^{(3)} := -\tfrac{1}{12^2}(a_1^2h_2^2h_3^2 + a_2^2h_1^2h_3^2 + a_3^2h_1^2h_2^2)\Lambda_1\Lambda_2\Lambda_3 \tag{3.32}$$

for $n = 3$, with $\bar{A}_N^{(2)} < 0$ and $\bar{A}_N^{(3)} > 0$ in H_h.

Due to the formulas

$$\bar{A}_N - A_N = -a_1^2(\bar{s}_{N\hat{1}} - s_{N\hat{1}})\Lambda_1 - \ldots - a_n^2(\bar{s}_{N\hat{n}} - s_{N\hat{n}})\Lambda_n$$

and (3.31), the approximation errors of schemes (3.25)-(3.26) and (3.27)-(3.28) have the same order $\mathcal{O}(|\mathbf{h}|^4)$ as the preceding scheme (3.22)-(3.23).

For $n = 3$, one can easily generalize scheme (3.25)-(3.26) by the extensions

$$\bar{s}_N = s_{1N}s_{2N}s_{3N} \mapsto s_{N\beta\gamma} := s_N + \beta\bar{s}_N^{(2)} + \gamma\bar{s}_N^{(3)}, \quad A_N \mapsto A_{N\theta} := A_N + \theta\bar{A}_N^{(3)}, \tag{3.33}$$

with the three parameters β,γ and θ, keeping its approximation order. Here we have explicitly

$$\bar{s}_N^{(2)}=\tfrac{1}{12^2}(h_1^2h_2^2\Lambda_1\Lambda_2+h_1^2h_3^2\Lambda_1\Lambda_3+h_2^2h_3^2\Lambda_2\Lambda_3),\ \ \bar{s}_N^{(3)}=\tfrac{1}{12^3}h_1^2h_2^2h_3^2\Lambda_1\Lambda_2\Lambda_3\ \text{ for }\ n=3 \tag{3.34}$$

as well as

$$s_{N\beta}=(1-\beta)s_N+\beta\bar{s}_N \text{ for } n=2;\ \ s_{N\beta\beta}=(1-\beta)s_N+\beta\bar{s}_N,\ A_{N\theta}:=(1-\theta)A_N+\theta\bar{A}_N \text{ for } n=3.$$

The following explicit expansions in Λ_k for the operators at the upper time level in (3.22) for $n=2$ and (3.25) for $n=3$ hold

$$s_N(\rho w)+\tfrac{1}{12}h_t^2A_Nw=\rho w+\tfrac{1}{12}\big[(h_1^2\Lambda_1+h_2^2\Lambda_2)(\rho w)-h_t^2(a_1^2\Lambda_1+a_2^2\Lambda_2)w\big]$$
$$-(\tfrac{1}{12})^2h_t^2\big(a_1^2h_2^2+a_2^2h_1^2\big)\Lambda_1\Lambda_2w\ \text{ for }\ n=2,$$
$$\bar{s}_N(\rho w)+\tfrac{1}{12}h_t^2\bar{A}_Nw=\rho w+\tfrac{1}{12}\big[(h_1^2\Lambda_1+h_2^2\Lambda_2+h_3^2\Lambda_3)(\rho w)-h_t^2(a_1^2\Lambda_1+a_2^2\Lambda_2+a_3^2\Lambda_3)w\big],$$
$$+\bar{s}_N^{(2)}(\rho w)-\tfrac{1}{12^2}h_t^2\big[(a_1^2h_2^2+a_2^2h_1^2)\Lambda_1\Lambda_2+(a_1^2h_3^2+a_3^2h_1^2)\Lambda_1\Lambda_3+(a_2^2h_3^2+a_3^2h_2^2)\Lambda_2\Lambda_3\big]w$$
$$+\bar{s}_N^{(3)}(\rho w)-\tfrac{1}{12}h_t^2\bar{A}_N^{(3)}w\ \text{ for }\ n=3,$$

see also formulas in (3.34) and (3.32) for the last two terms. In the particular case of a_i and h_i independent on i (i.e., for the square spatial mesh), the formulas are simplified, and the operators on the left in them differ only up to factors from those given in the related formulas (21)-(22) in [2] and (11) in [10]. Moreover, turning to formulas (2.6)-(2.7), one can show that in this case equations (3.22) for $n=2$ and (3.27) for $n=3$ are equivalent to respective methods from [2, 10] up to our simpler approximations of f. But it should be emphasized that we prefer to supplement them by other than in [2, 10] similar equations (3.23) and (3.28) for v^1.

Also, in the same particular case, the family of methods with the operators

$$s_{N\beta\gamma}(\rho w)+\tfrac{1}{12}h_t^2A_{N\theta},\ \ \text{with }\ \beta=2,\ \ \gamma=12(1-\varkappa),\ \theta=4(\varkappa-1),\ -\tfrac{1}{2}<\varkappa<3 \tag{3.35}$$

at the upper level was also studied in [10, Section 3.2.2], though according to the above analysis, the values $\varkappa\leqslant 1$ (including the so-called canonical based scheme for $\varkappa=1$ in [10]) can hardly be recommended for exploiting. These methods are related to equation (3.25) with the extended operators (3.33) in the same way (actually for any β, γ and θ).

Now we prove the conditional stability theorem for all the above constructed schemes.

Theorem 3.1. *Let $g=0$ in (2.2). Let us consider:*

1. *scheme (3.22)-(3.24) for $n=2$,*
2. *scheme (3.25)-(3.26) and (3.33) for $n=3$,*
3. *scheme (3.27)-(3.28) for $n\geqslant 1$ (for $n=1$, the scheme (3.20)-(3.21) is the same)*

and set respectively $(B_h,A_h)=(s_{N\beta},A_N)$, $(B_h,A_h)=(s_{N\beta\gamma},A_{N\theta})$ and $(\bar{s}_N,\bar{A}_N)$.

Let the parameters β,γ and θ be chosen such that $B_h>0$ and $A_h>0$ in H_h, and $A_h\leqslant\alpha_h^2B_h$ with some α_h (see (2.8)) for the first and second schemes. Let also $0<\varepsilon_0<1$, and the condition

$$\tfrac{1}{6}h_t^2\alpha_h^2\leqslant(1-\varepsilon_0^2)\underline{\rho}, \tag{3.36}$$

for the first and second schemes, or the explicit condition

$$h_t^2\big(\tfrac{a_1^2}{h_1^2}+\ldots+\tfrac{a_n^2}{h_n^2}\big)\leqslant(1-\varepsilon_0^2)\underline{\rho} \tag{3.37}$$

for the third scheme, be valid (see also Remark 3.2 below). Then, for any free terms f_N: $\{t_m\}_{m=0}^{M-1} \to H_h$ and $u_{1N} \in H_h$ (not only for those specific defined above), the solutions to all three schemes satisfy the following two stability bounds:

$$\max_{1\leqslant m\leqslant M} \Big(\varepsilon_0^2\|\sqrt{\rho}\bar{\delta}_t v^m\|_h^2 + \|\bar{s}_t v^m\|^2_{B_h^{-1}A_h}\Big)^{1/2}$$
$$\leqslant \Big(\|v^0\|^2_{B_h^{-1}A_h} + \varepsilon_0^{-2}\big\|\tfrac{1}{\sqrt{\rho}}B_h^{-1}u_{1N}\big\|_h^2\Big)^{1/2} + 2\varepsilon_0^{-1}\big\|\tfrac{1}{\sqrt{\rho}}B_h^{-1}f_N\big\|_{L^1_{h_t}(H_h)}, \tag{3.38}$$

where the f_N-term can be taken also as $2I_{h_t}^{M-1}\|B_h^{-1/2}A_h^{-1/2}\bar{\delta}_t f_N\|_h + 3\max\limits_{0\leqslant m\leqslant M-1}\|B_h^{-1/2}A_h^{-1/2}f_N^m\|_h$;

$$\max_{0\leqslant m\leqslant M}\max\big\{\varepsilon_0\|\sqrt{\rho}v^m\|_h,\ \|I_{h_t}^m\bar{s}_t v\|_{B_h^{-1}A_h}\big\}$$
$$\leqslant \|\sqrt{\rho}v^0\|_h + 2\|B_h^{-1/2}A_h^{-1/2}u_{1N}\|_h + 2\|B_h^{-1/2}A_h^{-1/2}f_N\|_{L^1_{h_t}(H_h)}, \tag{3.39}$$

where, for $f_N = \delta_t g$, one can replace the f_N-term with $2\varepsilon_0^{-1}I_{h_t}^M\big\|\frac{1}{\sqrt{\rho}}B_h^{-1}(g - s_t g^0)\big\|_h$.

Remark 3.2. *Let us comment on the stability condition* (3.36)*. For $(B_h, A_h) = (s_{N\beta}, A_N)$ with $\beta \geqslant 0$ for $n = 2$,*

$$(B_h, A_h) = (s_{N\beta\gamma}, A_{N\theta}) \ \text{ with } \ \beta \geqslant \varepsilon_1,\ \gamma \leqslant \varepsilon_1 \ \text{ with some } \ 0 < \varepsilon_1 \leqslant 1,\ 0 \leqslant \theta \leqslant 1 \ \text{ for } \ n = 3$$

and $(B_h, A_h) = (\bar{s}_N, \bar{A}_N)$ for $n \geqslant 1$, conditions $B_h > 0$ and $A_h > 0$ in H_h hold, as well as condition (2.8) *has recently been studied in [14, Lemma 3] (for $\beta = 0$ and $\theta = 0, 1$ that is enough here). Consequently condition* (3.36) *is valid under the assumption*

$$C_1 h_t^2\big(\tfrac{a_1^2}{h_1^2} + \ldots + \tfrac{a_n^2}{h_n^2}\big) \leqslant (1 - \varepsilon_0^2)\underline{\rho}$$

where $C_1 = \frac{4}{3}, \varepsilon_1^{-1}$ or 1 respectively for the first, second or third scheme. The reason is that, under the assumptions made on β, γ and θ, the following operator inequalities in H_h hold

$$s_N \leqslant s_{N\beta} \ \text{ for } \ n = 2, \quad \varepsilon_1\bar{s}_N \leqslant s_{N\beta\gamma} \text{ and } A_{N\theta} \leqslant \bar{A}_N \ \text{ for } \ n = 3. \tag{3.40}$$

This is an example, and we do not intend here to study condition (2.8) *for general β, γ and θ.*

Proof. The theorem follows directly from the general stability Theorem 2.1, for B_h and A_h listed in the statement, in the particular case $\sigma = \frac{1}{12}$, specifying assumption (2.10) and inequality (2.15). Here B_h and A_h commute since they have the same system of eigenvectors in H_h.

In the second form of the f_N-term in (3.38) and in the last two terms on the right in (3.39), we also take into account that $(A_h B_h)^{-1/2} = B_h^{-1/2}A_h^{-1/2}$ due to the last mentioned property. □

Remark 3.3. *Usually $\nu_0 I \leqslant B_h \leqslant \nu I$ in H_h with some $\nu \geqslant \nu_0 > 0$ both independent of $\mathbf{h}$; in particular, under the assumptions on β and γ from Remark 3.2 one has*

$$\tfrac{1}{3}I < s_{N\beta} < \big(1 + \tfrac{1}{9}\beta\big)I \ \text{ for } \ n = 2, \quad \varepsilon_1(\tfrac{2}{3})^3 I < s_{N\beta\gamma} < \big(1 + \tfrac{1}{3}\beta + \tfrac{1}{27}\max\{-\gamma, 0\}\big)I \ \text{ for } \ n = 3$$

due to the inequalities $-\frac{1}{4}h_k^2\Lambda_k < I$, (3.40) *and $(\frac{2}{3})^n I < \bar{s}_N < I$ in H_h. Then one can simplify the above stability bounds replacing the operator B_h^{-1} with the constant ν^{-1} on the left and/or replacing B_h^{-1} with ν_0^{-1} and $B_h^{-1/2}$ with $\nu_0^{-1/2}$ on the right.*

Next, based on Theorem 3.1, we prove the 4th order error bound for the same schemes.

Theorem 3.2. *Let the coefficient ρ and solution u to the IBVP* (2.1)-(2.2) *be sufficiently smooth respectively in $\bar\Omega$ and $\bar Q_T$. Then under the hypotheses of Theorem 3.1 but excluding $g=0$ and for $\nu_0 I\leqslant B_h\leqslant \nu I$ with some $\nu\geqslant\nu_0>0$ (see Remark 3.3) as well as $v^0=u_0$ on $\bar\omega_h$, for all three schemes listed in it, the following 4th order error bound in the strong energy norm holds*

$$\max_{1\leqslant m\leqslant M}\big[\varepsilon_0\|\sqrt{\rho}\bar\delta_t(u-v)^m\|_h+\|\bar s_t(u-v)^m\|_{A_h}\big]=\mathcal{O}(|\mathbf{h}|^4).$$

Let $a_{\min}=\min_{1\leqslant i\leqslant n}a_i$, $\Delta_h=\Lambda_1+\ldots+\Lambda_n$ be the simplest approximation of the Laplace operator, and $\varepsilon_2=1$ for the first and third schemes or $0<\varepsilon_2\leqslant\theta\leqslant 1$ for the second one. Then

$$\sqrt{\varepsilon_2}a_{\min}\big(\tfrac{2}{3}\big)^{(n-1)/2}\|w\|_{-\Delta_h}\leqslant\|w\|_{A_h}\quad\forall w\in H_h. \tag{3.41}$$

Proof. Recall that the approximation errors of the equations for all the schemes are defined as

$$\psi:=B_h(\rho\Lambda_t u)+\tfrac{1}{12}h_t^2A_h\Lambda_t u+A_hu-f_N\ \text{ on }\ \omega_{\mathbf{h}},$$
$$\psi^0:=B_h(\rho\delta_t u^0)+\tfrac{1}{12}h_t^2A_h\Lambda_t\delta_t u^0+\tfrac12 h_tA_hu_0-u_{1N}-\tfrac12 h_tf_N^0\ \text{ on }\ \omega_h,$$

cf. formulas (3.3)-(3.4) for scheme (3.18)-(3.19). For all the schemes, it was checked above that

$$\max_{\omega_{\mathbf{h}}}|\psi|+\max_{\omega_h}|\psi^0|=\mathcal{O}(|\mathbf{h}|^4). \tag{3.42}$$

Due to equations for v as well as the definitions of ψ and ψ^0, the error $r:=u-v$ satisfies the following equations

$$B_h(\rho\Lambda_t r)+\tfrac{1}{12}h_t^2A_h\Lambda_t r+A_hr=\psi\ \text{ on }\ \omega_{\mathbf{h}},$$
$$r|_{\partial\omega_{\mathbf{h}}}=0,\quad B_h(\rho\delta_t r^0)+\tfrac{1}{12}h_t^2A_h\Lambda_t\delta_t r^0+\tfrac12 h_tA_hr_0=\psi^0\ \text{ on }\ \omega_h,$$

with the approximation errors on the right, and $r^0=0$. The stability bound (3.38), Remark 3.3 and estimate (3.42) imply the error bound

$$\max_{1\leqslant m\leqslant M}\big(\varepsilon_0\|\sqrt{\rho}\bar\delta_t r^m\|_h+\nu^{-1/2}\|\bar s_t r^m\|_{A_h}\big)\leqslant\frac{1}{\varepsilon_0\sqrt{\nu_0\underline{\rho}}}\big(\|\psi^0\|_h+2I_{h_t}^{M-1}\|\psi\|_h\big)=\mathcal{O}(|\mathbf{h}|^4).$$

Inequality (3.41) follows from the simple operator inequalities

$$a_{\min}^2\tfrac23(-\Delta_h)\leqslant A_N,\quad \varepsilon_2a_{\min}^2\big(\tfrac23\big)^2(-\Delta_h)\leqslant\varepsilon_2\bar A_N\leqslant A_{N\theta},\quad a_{\min}^2\big(\tfrac23\big)^{n-1}(-\Delta_h)\leqslant\bar A_N$$

in H_h respectively for the operators in the first, second and third schemes in Theorem 3.1. □

Inequality (3.41) shows that the error norm in Theorem 3.2 is stronger than the standard mesh energy norm not related to the specific operators in the schemes.

Usually $h_t=\mathcal{O}(|h|)$ according to conditions (3.36) and (3.37), then $\mathcal{O}(|\mathbf{h}|^4)=\mathcal{O}(|h|^4)$.

Clearly under the hypotheses of Theorem 3.1, for example, for scheme (3.22)-(3.24) for $n=2$, the general energy conservation law (2.17) takes the non-trivial form

$$\|\sqrt{\rho}\bar\delta_t v^m\|_h^2-\tfrac16 h_t^2\|\bar\delta_t v^m\|^2_{s_{N\beta}^{-1}A_N}+\|\bar s_t v^m\|^2_{s_{N\beta}^{-1}A_N}=\big(s_{N\beta}^{-1}A_Nv^0,s_tv^0\big)_h$$
$$+\big(s_{N\beta}^{-1}u_{1N},\delta_t v^0\big)_h+\tfrac12 h_t\big(s_{N\beta}^{-1}f_N^0,\delta_t v^0\big)_h+2I_{h_t}^{m-1}(s_{N\beta}^{-1}f,\mathring{\delta}_t v)_h,\ 1\leqslant m\leqslant M.$$

The energy conservation laws for the second and third schemes in Theorem 3.1 are similar.

4 An unconditionally stable finite-difference scheme of the 4th order of approximation

Now we discuss the two-level method from [4, formulas (14), (26)] constructed for $n=2$. For $g=0$, in our notation it can be rewritten as a system of two operator equations

$$\bar{\delta}_t v = c^2\big[I-\tfrac{1}{12}h_t^2 L_h(c^2 I)\big]\bar{s}_t w + d \ \text{ in } \ H_h, \tag{4.1}$$

$$\bar{\delta}_t w = \big[L_h-\tfrac{1}{12}h_t^2 L_h(c^2 L_h)\big]\bar{s}_t v + \tilde{f} \ \text{ in } \ H_h \tag{4.2}$$

on $\overline{\omega}_{h_t}\backslash\{0\}$, where the additional sought function w approximates $\frac{1}{c^2}\partial_t u$ and originally

$$L_h := s_{1N}^{-1}\Lambda_1 + s_{2N}^{-1}\Lambda_2 = -\bar{s}_N^{-1}A_N \ \text{ for } \ n=2.$$

The given free terms d and $\tilde{f}$ on the right in (4.1)-(4.2) are zero in [4], and we have inserted them to cover the case of the non-homogeneous wave equation and for more detailed stability analysis (in practice, d and $\tilde{f}$ are never zero due to the round-off errors). It is well-known that such type methods are closely related to more standard three-level methods like (2.3)-(2.4) with $\sigma=\frac{1}{4}$, for example, see [15, Section 8].

To demonstrate that, we exclude w from this system. Applying the operators $\frac{1}{c^2}\delta_t$ to (4.1) and s_t to (4.2), we find respectively

$$\rho\Lambda_t v = \big[I-\tfrac{1}{12}h_t^2 L_h(c^2 I)\big]\delta_t\bar{s}_t w + \rho\delta_t d,$$

$$s_t\bar{\delta}_t w = L_h\big(I-\tfrac{1}{12}h_t^2 c^2 L_h\big)s_t\bar{s}_t v + s_t\tilde{f}.$$

Inserting $s_t\bar{\delta}_t w$ from the second equation into the first one and using the formulas

$$\delta_t\bar{s}_t w = s_t\bar{\delta}_t w = \tfrac{\hat{w}-\check{w}}{2h_t}, \quad s_t\bar{s}_t v = v^{(1/4)} \equiv \tfrac{1}{4}(\hat{v}+2v+\check{v}),$$

we obtain the following closed equation for v

$$\rho\Lambda_t v + A_h v^{(1/4)} = f_h \ \text{ on } \ \omega_{h_t}, \tag{4.3}$$

where we have set

$$A_h := \big[I-\tfrac{1}{12}h_t^2 L_h(c^2 I)\big](-L_h)\big(I-\tfrac{1}{12}h_t^2 c^2 L_h\big), \quad f_h := \big[I-\tfrac{1}{12}h_t^2 L_h(c^2 I)\big]s_t\tilde{f} + \rho\delta_t d. \tag{4.4}$$

Notice that $A_h^* = A_h > 0$ in H_h since $(-L_h)^* = -L_h > 0$ and

$$(A_h y, y)_h = (-L_h z, z)_h, \quad \text{with } \ z := \big(I-\tfrac{1}{12}h_t^2 c^2 L_h\big)y, \quad \forall y\in H_h. \tag{4.5}$$

Next, we use the formula $\bar{s}_t w = \check{w} + \frac{1}{2}h_t\bar{\delta}_t w$ in equation (4.1) and divide it by c^2. We also use the same formula for v in (4.2) and apply the operator $\frac{1}{2}h_t\big[I-\frac{1}{12}h_t^2 L_h(c^2 I)\big]$ to it:

$$\rho\bar{\delta}_t v = \big[I-\tfrac{1}{12}h_t^2 L_h(c^2 I)\big](\check{w}+\tfrac{1}{2}h_t\bar{\delta}_t w) + \rho d$$

$$= \big[I-\tfrac{1}{12}h_t^2 L_h(c^2 I)\big]\check{w} + \tfrac{1}{2}h_t\big[I-\tfrac{1}{12}h_t^2 L_h(c^2 I)\big]\big\{\big[L_h-\tfrac{1}{12}h_t^2 L_h(c^2 L_h)\big](\check{v}+\tfrac{1}{2}h_t\bar{\delta}_t v)+\tilde{f}\big\} + \rho d.$$

Considering the first time level $t_1 = h_t$, we find

$$\big(\rho I + \tfrac{1}{4}h_t^2 A_h\big)\delta_t v^0 + \tfrac{1}{2}h_t A_h v^0 = u_{1h} + \rho d^1 + \tfrac{1}{2}h_t f_h^0, \tag{4.6}$$

where we have set

$$u_{1h} := \big[I - \tfrac{1}{12}h_t^2 L_h(c^2 I)\big]w^0, \quad f_h^0 := \big[I - \tfrac{1}{12}h_t^2 L_h(c^2 I)\big]\tilde{f}^1 + \rho\delta_t d^0, \tag{4.7}$$

with $d^0 := -d^1$ (thus $\frac{1}{2}h_t\rho\delta_t d^0 = \rho d^1$), and it is natural to take $w^0 = \rho u_1$ on $\bar{\omega}_h$.

Since $v^{(1/4)} = v + \frac{1}{4}h_t^2\Lambda_t v$, equations (4.3) and (4.6) form the particular case of method (2.3)-(2.4) for $B_h = I$ and $\sigma = \frac{1}{4}$, with A_h, f_h, u_{1h} and f_h^0 given in (4.4) and (4.7).

We emphasize that the derived three-level method (4.3) and (4.6) is straightforwardly generalized to any $n \geqslant 1$ by taking

$$L_h = s_{1N}^{-1}\Lambda_1 + \ldots + s_{nN}^{-1}\Lambda_n = -\bar{s}_N^{-1}\bar{A}_N, \tag{4.8}$$

see formulas (3.29)-(3.30). Clearly its two-level operator form are the same equations (4.1)-(4.2) with this generalized L_h.

Let us derive the *unconditional stability* of the generalized method for any $n \geqslant 1$.

Theorem 4.1. *For the solution to method* (4.3)-(4.6) *and* (4.8) *for any* $n \geqslant 1$*, the following stability bounds hold:*

$$\max_{1\leqslant m\leqslant M}\big(\|\sqrt{\rho}\bar{\delta}_t v^m\|_h^2 + \|\bar{s}_t v^m\|_{A_h}^2\big)^{1/2} \leqslant \Big(\|v^0\|_{A_h}^2 + \varepsilon_0^{-2}\big\|\tfrac{1}{\sqrt{\rho}}u_{1h}\big\|_h^2\Big)^{1/2} + 2\big\|\tfrac{1}{\sqrt{\rho}}f_h\big\|_{L^1_{h_t}(H_h)},$$

for any free terms f_h: $\{t_m\}_{m=0}^{M-1} \to H_h$ *and* $u_{1h} \in H_h$*, where the* f_h*-term can be replaced with* $2I_{h_t}^{M-1}\|A_h^{-1/2}\bar{\delta}_t f_h\|_h + 3\max_{0\leqslant m\leqslant M-1}\|A_h^{-1/2}f_h^m\|_h$*;*

$$\max_{0\leqslant m\leqslant M}\max\big\{\|\sqrt{\rho}v^m\|_h,\, \|I_{h_t}^m\bar{s}_t v\|_{A_h}\big\} \leqslant \|\sqrt{\rho}v^0\|_h$$

$$+2\|(-L_h)^{-1/2}w^0\|_h + \tfrac{h_t}{2}\|(-L_h)^{-1/2}\tilde{f}^1\|_h + 2I_{h_t}^{M-1}\|(-L_h)^{-1/2}s_t\tilde{f}\|_h + 2I_{h_t}^M\|\sqrt{\rho}g\|_h, \tag{4.9}$$

for any d, $\tilde{f}$: $\{t_m\}_{m=1}^M \to H_h$ *and* $w^0 \in H_h$*, together with the energy conservation law*

$$\|\sqrt{\rho}\bar{\delta}_t v^m\|_h^2 + \|\bar{s}_t v^m\|_{A_h}^2 = \big(A_h v^0, s_t v^0\big)_h + \big(u_{1h} + \tfrac{1}{2}h_t f_h^0, \delta_t v^0\big)_h + 2I_{h_t}^{m-1}(f_h, \mathring{\delta}_t v)_h,\ 1 \leqslant m \leqslant M.$$

Proof. The first stability bound, the second stability bound in the form

$$\max_{0\leqslant m\leqslant M}\max\big\{\|\sqrt{\rho}v^m\|_h,\, \|I_{h_t}^m\bar{s}_t v\|_{A_h}\big\} \leqslant \|\sqrt{\rho}v^0\|_h + 2\|A_h^{-1/2}u_{1h}\|_h + 2\|A_h^{-1/2}f_h\|_{L^1_{h_t}(H_h)} \tag{4.10}$$

and the stated energy conservation law directly follow from general Theorem 2.1 and law (2.17) in the case $B_h = I$ and $\sigma = \frac{1}{4}$ (recall that then $\varepsilon_0 = 1$). In addition, the term $\rho\delta_t d$ can be extracted from f_h in (4.10) and added as $2I_{h_t}^M\|\sqrt{\rho}g\|_h$ (since $s_t g^0 = 0$) on the right like it stands in (4.9). Notice that the bounds and the law are especially simplified in this particular case.

Moreover, the following chain of transformations hold

$$\|A_h^{-1/2}w\|_h^2 = (A_h^{-1}w, w)_h = \Big(\big(I - \tfrac{1}{12}h_t^2 c^2 L_h\big)^{-1}(-L_h)^{-1}\big[I - \tfrac{1}{12}h_t^2 L_h(c^2 I)\big]^{-1}w, w\Big)_h$$

$$= \|(-L_h)^{-1/2}\big[I - \tfrac{1}{12}h_t^2 L_h(c^2 I)\big]^{-1}w\|_h^2 \quad \forall w \in H_h,$$

cf. (4.5). This result allows us to pass from the norms of u_{1h} and f_h given in (4.10) to norms of w^0 and $\tilde{f}$ standing in bound (4.9). □

Note that here the norms $\|\cdot\|_{A_h}$ can be rewritten in terms of $\|\cdot\|_{-L_h}$ and L_h according to formula (4.5) that remains valid for any $n \geqslant 1$.

We finally emphasize that clearly the operator A_h and the right-hand terms f_h and u_{1h}, see (4.4) and (4.7), with L_h given in (4.8), and consequently the implementation of the method are much more complicated than the corresponding operators and the right-hand terms in the schemes constructed in Section 3 since the latter ones do not contain neither non-explicit (inverse) operators nor powers of the mesh operators.

5 The case of non-uniform meshes in space and time

In this Section, we briefly dwell on the case of non-uniform rectangular meshes in x and t when the schemes can be extended following [14]. Note that this is necessary, in particular, for extending the schemes to more general domains including those composed from rectangular parallelepipeds or for implementing a dynamic choice of the time step. We confine ourselves only by the scheme like (3.27)-(3.28) for any $n \geqslant 1$ and emphasize that the scheme now will be constructed directly, *without* considering intermediate schemes like above in Section 3.

Define the general non-uniform meshes $\overline{\omega}_{h_t}$ in t and $\bar{\omega}_{hk}$ in x_k with the nodes

$$0 = t_0 < t_1 < \ldots < t_M = T, \quad 0 = x_{k0} < x_{k1} < \ldots < x_{kN_k} = X_k$$

and the steps $h_{tm} = t_m - t_{m-1}$ and $h_{kl} = x_{kl} - x_{k(l-1)}$, $1 \leqslant k \leqslant n$. Let $\omega_{hk} = \{x_{kl}\}_{l=1}^{N_k-1}$. We set

$$h_{t+,m} = h_{t(m+1)}, \quad h_{*t} = \tfrac{1}{2}(h_t + h_{t+}), \quad h_{k+,l} = h_{k(l+1)}, \quad h_{*k} = \tfrac{1}{2}(h_k + h_{k+})$$

and define also the maximal mesh steps

$$h_{t\max} = \max_{1\leqslant m\leqslant M} h_{tm}, \quad h_{\max} = \max_{1\leqslant k\leqslant n}\max_{1\leqslant l\leqslant N_k} h_{kl}, \quad \mathbf{h}_{\max} = \max\{h_{\max}, h_{t\max}\}.$$

Let now $\bar{\omega}_h = \bar{\omega}_{h1} \times \ldots \times \bar{\omega}_{hn}$, $\omega_h = \omega_{h1} \times \ldots \times \omega_{hn}$ and $\partial\omega_h = \bar{\omega}_h \backslash \omega_h$.

We generalize the above defined difference operators in t and x_k as

$$\delta_t y = \tfrac{1}{h_{t+}}(\hat{y} - y), \quad \bar{\delta}_t y = \tfrac{1}{h_t}(y - \check{y}), \quad \Lambda_t y = \tfrac{1}{h_{*t}}(\delta_t y - \bar{\delta}_t y),$$
$$\Lambda_k w_l = \tfrac{1}{h_{*k}}\big[\tfrac{1}{h_{k(l+1)}}(w_{l+1} - w_l) - \tfrac{1}{h_{kl}}(w_l - w_{l-1})\big], \quad \text{with} \quad w_l = w(x_{kl}).$$

Next we generalize the above averaging technique including the following average in x_k:

$$q_k w(x_{kl}) = \frac{1}{h_{*k,l}} \int_{I_{kl}} w(x_k) e_{kl}(x_k)\, dx_k,$$
$$\text{with} \quad e_{kl}(x_k) = \tfrac{x_k - x_{k(l-1)}}{h_{kl}} \quad \text{on} \quad [x_{k(l-1)}, x_{kl}], \;\; e_{kl}(x_k) = \tfrac{x_{k(l+1)} - x_k}{h_{k(l+1)}} \quad \text{on} \quad [x_{kl}, x_{k(l+1)}].$$

For a function $w(x_k)$ smooth on $[0, X_k]$, formula (3.5) remains valid. Also now we have

$$q_k w = w + q_k \rho_{k1}(\partial_k w),$$
$$q_k w = w + \tfrac{1}{3}(h_{k+} - h_k)\partial_k w + \tfrac{1}{12}\big[(h_{k+})^2 - h_{k+}h_k + h_k^2\big]\partial_k^2 w + q_k \rho_{k3}(\partial_k^3 w) \qquad (5.1)$$

on ω_{hk}. The first bound (3.8) is now valid for $s = 1, 3$, with h_k replaced with h_{*k}, that follows from Taylor's formula after calculating the arising integrals of polynomials over I_{kl} and using residual (3.9). Next, once again due to Taylor's formula, we derive

$$\partial_k w = \tfrac{1}{2}(\bar{\delta}_k w + \delta_k w) - \tfrac{1}{4}(h_{k+} - h_k)\partial_k^2 w + \rho_k^{(1)}(\partial_k^3 w), \quad \partial_k^2 w = \Lambda_k w + \rho_{k3}^{(2)}(\partial_k^3 w), \qquad (5.2)$$
$$|\rho_k^{(s)}(\partial_k^3 w)| \leqslant c^{(s)} h_{*k}^{3-s} \|\partial_k^3 w\|_{C(I_{kl})}, \quad s = 1, 2, \qquad (5.3)$$

on ω_{hk}. Inserting expansions (5.2) into expansion (5.1) and using (5.3) lead to the formulas

$$q_k w = s_{kN} w + \tilde{\rho}_{k3}(\partial_k^3 w), \quad |\tilde{\rho}_{k3}(\partial_k^3 w)| \leqslant \tilde{c}_3 h_{*k}^3 \|\partial_k^3 w\|_{C(I_{kl})}, \qquad (5.4)$$

on ω_{hk}, with the generalized Numerov-type averaging operator in x_k

$$s_{kN} := I + \tfrac{1}{3}(h_{k+} - h_k)\big[\tfrac{1}{2}(\bar\delta_k + \delta_k) - \tfrac{1}{4}(h_{k+} - h_k)\Lambda_k\big] + \tfrac{1}{12}\big[(h_{k+})^2 - h_{k+}h_k + h_k^2\big]\Lambda_k$$
$$= I + \tfrac{1}{6}(h_{k+} - h_k)(\bar\delta_k + \delta_k) + \tfrac{1}{12}h_k h_{k+}\Lambda_k.$$

Consequently the following two more forms for s_{kN} also hold

$$s_{kN}w_l = w_l + \tfrac{1}{12}[(h_{k+}\beta_k\delta_k - h_k\alpha_k\bar\delta_k)w]_l = \tfrac{1}{12}(\alpha_{kl}w_{l-1} + 10\gamma_{kl}w_l + \beta_{kl}w_{l+1}),$$
$$\text{with}\ \ \alpha_k = 2 - \tfrac{h_{k+}^2}{h_k h_{*k}},\ \beta_k = 2 - \tfrac{h_k^2}{h_{k+}h_{*k}},\ \gamma_k = 1 + \tfrac{(h_{k+}-h_k)^2}{5h_k h_{k+}},\ \alpha_k + 10\gamma_k + \beta_k = 12$$

on ω_{hk}. Note that other derivations and forms for s_{kN} can be found in [5, 7, 11].

Quite similarly the following formulas with the generalized average $q_t w = q_{n+1}w$ and the Numerov-type operator s_{tN} in t hold on ω_{h_t}:

$$q_t w = s_{tN}w + \tilde\rho_{t3}(\partial_t^3 w),\ \ |\tilde\rho_{t3}(\partial_t^3 w)| \leqslant \tilde c_3 h_{*t}^3\|\partial_t^3 w\|_{C[t_{m-1},t_{m+1}]}, \tag{5.5}$$
$$s_{tN}y = y + \tfrac{1}{12}(h_{t+}\beta_t\delta_t - h_t\alpha_t\bar\delta_t)y = \tfrac{1}{12}(\alpha_t\check y + 10\gamma_t y + \beta_t\hat y),$$
$$\text{with}\ \ \alpha_t = 2 - \tfrac{h_{t+}^2}{h_t h_{*t}},\ \beta_t = 2 - \tfrac{h_t^2}{h_{t+}h_{*t}},\ \gamma_t = 1 + \tfrac{(h_{t+}-h_t)^2}{5h_t h_{t+}}.$$

Let the operators $\bar s_N$, $\bar s_{N\hat l}$ and $\bar A_N$ be defined as in (3.29)-(3.30) but with the generalized terms s_{kN} and Λ_k. Formula (3.10) for u remains valid and due to expansions (5.4)-(5.5) implies

$$\bar s_N(\rho\Lambda_t u) - (a_1^2\bar s_{N\hat 1}\Lambda_1 + \ldots + a_n^2\bar s_{N\hat n}\Lambda_n)s_{tN}u = \bar q q_t f + O(\mathbf{h}_{\max}^3)\ \ \text{on}\ \ \omega_{\mathbf{h}}.$$

Formula (3.12) for u remains valid as well, where $q_t y^0$ is given by formula (3.11) with h_{t1} instead of h_t. It concerns only time levels $t_0 = 0$ and $t_1 = h_{t1}$ thus easily covers the case of the non-uniform mesh in t and implies now

$$\bar s_N(\rho\delta_t u)^0 = \bar q(\rho u_1) + (a_1^2\bar s_{N\hat 1}\Lambda_1 + \ldots + a_n^2\bar s_{N\hat n}\Lambda_n)\big[\tfrac{h_{t1}}{2}u_0 + \tfrac{h_{t1}^2}{12}u_1 + \tfrac{h_{t1}^2}{12}(\delta_t u)^0\big] + \bar q q_t f^0 + O(\mathbf{h}_{\max}^3)$$

on ω_h, cf. (3.16).

Due to the above formulas for Λ_t and s_{tN} as well as expansions (5.4)-(5.5), the last two expansions for u with omitted $O(\mathbf{h}_{\max}^3)$-terms imply the generalized scheme (3.27)-(3.28) on the non-uniform mesh

$$\tfrac{1}{h_{*t}}\big\{\bar s_N(\rho\delta_t v) + \tfrac{h_{*t}h_{t+}}{12}\beta_t\bar A_N\delta_t v - \big[\bar s_N(\rho\bar\delta_t v) + \tfrac{h_{*t}h_t}{12}\alpha_t\bar A_N\bar\delta_t v\big]\big\} + \bar A_N v = \bar s_N s_{tN}f\ \ \text{on}\ \ \omega_{\mathbf{h}}, \tag{5.6}$$

$$v|_{\partial\omega_{\mathbf{h}}} = g,\ \bar s_N(\rho\delta_t v)^0 + \tfrac{h_{t1}^2}{12}\bar A_N(\delta_t v)^0 + \tfrac{h_{t1}}{2}\bar A_N v_0 = \bar s_N(\rho u_1) - \tfrac{h_{t1}^2}{12}\bar A_N u_1 + \tfrac{h_{t1}}{2}f_N^0\ \ \text{on}\ \ \omega_h, \tag{5.7}$$

with $f_N^0 = \bar s_N f_0 + \frac{h_{t1}}{3}(\delta_t f)^0$. Its equations have the approximation errors of the order $O(\mathbf{h}_{\max}^3)$.

For the uniform mesh in t, the left-hand side of (5.6) takes the form like above in (3.27):

$$\bar s_N(\rho\Lambda_t v) + \tfrac{1}{12}h_t^2\bar A_N\Lambda_t v + \bar A_N v = \bar s_N s_{tN}f,$$

and the equation has the higher approximation order $O(h_{\max}^3 + h_{t\max}^4)$ due to relations (3.7)-(3.8) for $k = n+1$.

Other above constructed schemes can be also generalized to the case of non-uniform meshes in the similar manner. In addition, one can check also that the approximation errors still has the 4th order $O(\mathbf{h}_{\max}^4)$ for non-uniform meshes with slowly varying mesh steps, cf. [12], provided that, for example, $f_N^0 = \bar s_N f^0 - f^0 + f_{dh_t}^{(0)}$.

Here we do not intend to study the stability issue in the case of the non-uniform mesh (even only in space) which is essentially more cumbersome since the operators s_{kN} are not self-adjoint as well as s_{kN} and Λ_k do not commute any more. Moreover, this can lead to much stronger conditions on h_t, especially in the case when the corresponding eigenvalue problem (2.9) has complex eigenvalues, see [12, 13]. On the other hand, for smoothly varying mesh steps and not only, results of 1D numerical experiments are positive, see [12, 14].

6 Iterative methods and numerical experiments

6.1. We go back to equation (2.5) at the upper time level, or omitting the superscript m and taking $\sigma = \frac{1}{12}$, to the equation

$$B_h(\rho w) + \tfrac{1}{12}h_t^2 A_h w = b \ \text{ in } \ H_h, \tag{6.1}$$

with any commuting operators $B_h^* = B_h > 0$ and $A_h^* = A_h > 0$, in particular, for all pairs of operators (B_h, A_h) considered in Section 3. Thus we assume that the non-homogeneous boundary condition $v|_{\partial\omega_\mathbf{h}} = g$ is reduced to the homogeneous one $v|_{\partial\omega_\mathbf{h}} = 0$ by respective change in f_N and u_{1N} at the mesh nodes of ω_h closest to $\partial\omega_h$.

We first consider the one-step iterative method with a constant parameter $\theta > 0$:

$$B_h\big(\rho\tfrac{w^{(l+1)}-w^{(l)}}{\theta}\big) + B_h(\rho w^{(l)}) + \tfrac{1}{12}h_t^2 A_h w^{(l)} = b, \quad l \geqslant 0, \tag{6.2}$$

where B_h serves as a preconditioner. Its equivalent practical form is

$$w^{(l+1)} = w^{(l+1)}(\theta) := (1-\theta)w^{(l)} - \tfrac{\theta}{\rho}B_h^{-1}\big(\tfrac{1}{12}h_t^2 A_h w^{(l)} - b\big), \quad l \geqslant 0. \tag{6.3}$$

For schemes from Section 3, application of B_h^{-1} can be effectively implemented by FFT.

Theorem 6.1. *Let the stability condition* (3.36) *on h_t be valid for some $0 < \varepsilon_0 < 1$.*

For the one-step iterative method (6.2) *with the parameter $\theta := \theta_{opt} = 2/(1 + \bar{\lambda}(\varepsilon_0^2))$, where $\bar{\lambda}(\varepsilon_0^2) := 1 + \frac{1}{2}(1-\varepsilon_0^2)$, the convergence rate estimate holds*

$$\|w - w^{(l)}\| \leqslant q_0^l \|w - w^{(0)}\|, \quad l \geqslant 0, \quad \forall w^{(0)} \in H_h, \tag{6.4}$$

in two norms $\|\cdot\| = \|\sqrt{\rho}\cdot\|_h$ and $\|\cdot\|_{\mathcal{A}_\mathbf{h}}$, with $\mathcal{A}_\mathbf{h} := D_\rho + \frac{1}{12}h_t^2 B_h^{-1}A_h$ and

$$q_0 = q_0(\varepsilon_0^2) := \frac{\bar{\lambda}(\varepsilon_0^2) - 1}{\bar{\lambda}(\varepsilon_0^2) + 1} = \frac{1-\varepsilon_0^2}{5-\varepsilon_0^2} \leqslant 0.2 \quad \text{on} \quad [0,1).$$

Proof. We rewrite equation (6.1) and the iterative method (6.2) in the canonical forms

$$\mathcal{A}_\mathbf{h} w = \tilde{b} := B_h^{-1}b, \quad D_\rho w^{(l+1)} = D_\rho w^{(l)} - \theta(\mathcal{A}_\mathbf{h} w^{(l)} - \tilde{b}), \quad l \geqslant 0, \tag{6.5}$$

with the preconditioner D_ρ. Recall that $D_\rho^* = D_\rho > 0$ and $\mathcal{A}_\mathbf{h}^* = \mathcal{A}_\mathbf{h} > 0$. Moreover, under condition (3.36), the following spectral equivalence inequalities hold

$$D_\rho \leqslant \mathcal{A}_\mathbf{h} = D_\rho + \tfrac{1}{12}h_t^2 B_h^{-1}A_h \leqslant \bar{\lambda}(\varepsilon_0^2)D_\rho \ \text{ in } \ H_h, \quad \text{with} \ \ \bar{\lambda}(\varepsilon_0^2) = 1 + \tfrac{1}{2}(1-\varepsilon_0^2). \tag{6.6}$$

Thus according to the theory of iterative methods in the form (6.5), for example, see [9], the optimal vaue of the parameter θ is θ_{opt}, and the convergence rate estimate (6.4) is valid. □

We also can consider the N-step iterative method with the Chebyshev parameters

$$w^{(l+1)} = (1-\theta^{(l)})w^{(l)} - \tfrac{\theta^{(l)}}{\rho}B_h^{-1}\big(\tfrac{1}{12}h_t^2 A_h w^{(l)} - b\big), \tag{6.7}$$

$$\theta^{(l)} := \frac{\theta_{opt}}{1 + q_0 \cos\frac{\pi(l+1/2)}{N}}, \quad l = 0, \dots, N-1, \tag{6.8}$$

see much more details in [9].

Theorem 6.2. *Let condition* (3.36) *on* h_t *be valid for some* $0<\varepsilon_0<1$. *For the* N*-step iterative method* (6.7)-(6.8)*, the convergence rate estimate holds*

$$\|w-w^{(N)}\| \leqslant \tfrac{2q_1^N}{1+2q_1^N}\|w-w^{(0)}\| \quad \forall w^{(0)}\in H_h,$$

in two norms $\|\cdot\|=\|\sqrt{\rho}\cdot\|_h$ *and* $\|\cdot\|_{\mathcal{A}_\mathbf{h}}$*, with*

$$q_1=q_1(\varepsilon_0^2):=\frac{\bar{\lambda}^{1/2}(\varepsilon_0^2)-1}{\bar{\lambda}^{1/2}(\varepsilon_0^2)+1}=\frac{1-\varepsilon_0^2}{5-\varepsilon_0^2+4\sqrt{1+\frac{1}{2}(1-\varepsilon_0^2)}}\leqslant\frac{1}{5+4\sqrt{1.5}}\approx 0.1010 \quad on \quad [0,1).$$

Proof. The result is valid due to the theory of the N-step iterative methods, for example, see [9], taking into account the spectral equivalence inequalities (6.6). □

Let us discuss the convergence rates of the suggested iterative methods. Importantly, q_0 and q_1 are *independent of both the meshes and* ρ, in particular, the spread of its values $\hat{\rho}=\overline{\rho}/\underline{\rho}$ with $\underline{\rho}\leqslant\rho(x)\leqslant\overline{\rho}$ on $\bar{\Omega}$. The last point is essential for some applications. In the typical case $\varepsilon_0^2=\frac{1}{2}$, one has $q_0(\frac{1}{2})=\frac{1}{9}\approx 0.1111$. For the $\sqrt{2}$ times stronger condition (3.36) on h_t with $\varepsilon_0^2=\frac{3}{4}$, one has already $q_0(\frac{3}{4})\approx 0.05882$. Recall that often the much higher common ratio $q_0=0.5$ is considered as good.

One has also, in particular, $q_1(\frac{1}{2})\approx 0.05573$ and $q_1(\frac{3}{4})\approx 0.02944$. It is easy to see that

$$0.5<\frac{q_1(\varepsilon_0^2)}{q_0(\varepsilon_0^2)}\leqslant\frac{5}{5+4\sqrt{1.5}}\approx 0.5051 \quad \text{on} \quad [0,1),$$

thus the iterative method (6.7)-(6.8) is much faster than (6.2), as well as q_0, q_1 and $\frac{q_1}{q_0}$ decrease on $[0,1)$. Moreover, $q_l(\varepsilon_0^2)\to 0$ as $\varepsilon_0\to 1-0$, $l=0,1$, i.e., the common ratios become *arbitrarily small* as condition (3.36) on h_t turns more and more stronger.

It is well-known that often the variational counterparts of the above iterative methods, namely, the steepest descent and conjugate gradient methods are more preferable. Here we do not come into details and mention only that in the former method the parameter $\theta=\theta_l$ is defined such that

$$\|w-w^{(l+1)}(\theta_l)\|_{\mathcal{A}_\mathbf{h}}=\min_{\theta>0}\|w-w^{(l+1)}(\theta)\|_{\mathcal{A}_\mathbf{h}}.$$

The explicit formula for θ_l (for example, see [9]) is given by the formula

$$\theta_l=\frac{(D_\rho y^{(l)},y^{(l)})_h}{(\mathcal{A}_\mathbf{h}y^{(l)},y^{(l)})_h}=\frac{\|\sqrt{\rho}y^{(l)}\|_h^2}{\|\sqrt{\rho}y^{(l)}\|_h^2+\frac{1}{12}h_t^2\big(B_h^{-1}A_hy^{(l)},y^{(l)}\big)_h},\quad y^{(l)}:=w^{(l)}+\tfrac{1}{\rho}B_h^{-1}\big(\tfrac{1}{12}h_t^2A_hw^{(l)}-b\big).$$

The above iterative methods can be generalized for equation (6.1) with any $\sigma\neq 0$ instead of $\frac{1}{12}$ that is essential, in particular, for implementation of the scheme from Section 4 (no methods to this end were described in [4]).

Concerning the initial guess for methods (6.2) and (6.7)-(6.8), one can base simply on the formula $v^{m+1,(0)}=v^m$, for $0\leqslant m\leqslant M-1$, or $v^{m+1,(0)}=2v^m-v^{m-1}$, for $1\leqslant m\leqslant M-1$. But it seems much better to use closely related equations (2.3)-(2.4) for $\sigma=0$ in the form:

$$(\Lambda_t v)^{m,(0)}=-\tfrac{1}{\rho}B_h^{-1}(A_hv^m-f^m) \quad \text{in} \quad H_h, \quad 1\leqslant m\leqslant M-1, \tag{6.9}$$
$$(\delta_t v^0)^{(0)}=-\tfrac{1}{\rho}B_h^{-1}\big(\tfrac{1}{2}h_tA_hv^0-u_1-\tfrac{1}{2}h_tf^0\big) \quad \text{in} \quad H_h,$$

and this expectation is confirmed in numerical experiments. Here applying B_h^{-1} can be again effectively implemented by FFT. Note that a discussion on the choice of the initial guess can be found in [2].

6.2. Now we describe results of our numerical experiments. To be definite, we take $n = 2$ and use mainly scheme (3.22)-(3.23) that below we call *scheme* S_0; we also apply the second formula (3.17) to compute f_N^0. In order to compare the results with those presented in literature, we solve two test problems from [4] including the wave propagation in a the three-layer medium for the square spatial mesh and also take one more problem for the rectangular one. Our numerical tests have been performed on the computer with Intel® Xeon® processor E5-2670, 8GB RAM, and the algorithm has been implemented using C++ language.

We rewrite the IBVP (2.1)-(2.2) for $n = 2$ and $g = 0$ as

$$\partial_t^2 u - c^2(x,y)(\partial_x^2 u + \partial_y^2 u) = \varphi(x,y,t) \ \text{ for } \ (x,y) \in [0,X] \times [0,X], \ 0 < t \leqslant T,$$

$$u|_{\Gamma_T} = 0, \quad u(x,y,0) = u_0(x,y), \quad \partial_t u(x,y,0) = u_1(x,y) \ \text{ for } \ (x,y) \in [0,X] \times [0,X].$$

Example 1. First we take $X = T = 2$, $c^2(x,y) = 1 + \left(\frac{\pi x}{8}\right)^2 + \left(\frac{\pi y}{8}\right)^2$. The data $u_0(x)$, $u_1 = 0$ and $\varphi(x,y,t)$ are chosen so that the solution is the simple standing wave $u(x,y,t) = \sin(\pi x)\sin(\pi y)\cos(\pi t)$ as in [4].

Table 1 contains the errors $e_{L^2}(N)$ and $e_{L^\infty}(N)$ in the mesh L_2 and L_∞ norms (i.e., in H_h and the mesh uniform norms) at $t = T$ together with the corresponding experimental convergence rates:

$$p_{L^q}(N) = \log \frac{e_{L^q}(N)}{e_{L^q}(N/2)} \Big/ \log 2, \quad q = 2, \infty.$$

Here we take $h_x = h_y = h = \frac{X}{N}$. Also hereafter N_{iter} denotes the maximal number of iterations (6.2) required to solve the systems of equations with the given tolerance 10^{-10}. CPU time is also included. Several spatial steps h are used, and due to the stability condition the time step is restricted to $h_t = 0.25h$.

Table 1: Example 1: errors $e_{L^q}(N)$, convergence rates $p_{L^q}(N)$, numbers of iterations N_{iter} and CPU times for a sequence of meshes

N	$h_x = h_y$	$e_{L^2}(N)$	$p_{L_2}(N)$	$e_{L^\infty}(N)$	$p_{L_\infty}(N)$	N_{iter}	CPU time
8	1/4	3.3660e-3	—	3.5483e-3	—	6	0.001 s
16	1/8	2.0104e-4	4.065	2.2719e-4	3.965	6	0.012 s
32	1/16	1.2128e-5	4.051	1.4623e-5	3.958	5	0.085 s
64	1/32	7.4564e-7	4.023	9.1493e-7	3.998	5	0.608 s

Clearly scheme S_0 demonstrates the 4th order accuracy in both norms. The obtained L^2 errors are about 5 times more accurate than those in [4, Table 12]. Also it can be seen that N_{iter} is small, and the CPU time is approximately proportional to the size of the discrete problem.

Next we investigate in more details the convergence of the proposed iterative method (6.2) with the initial guess defined by (6.9). The given problem is solved for different values of ε_0^2 and the number M defining the time step $h_t = \frac{T}{M}$. Table 2 contains the values of N_{iter} for $h_x = \frac{1}{32}$. For comparison, in brackets we also present its values when a simple guess $w^{(0)} = w$ is used. We observe that the convergence of the iterative method (6.2) with the initial guess defined by (6.9) is very fast requiring no more than 5 iterations to reach the high tolerance

10^{-10}, and its rate is only slightly sensitive to the value of the parameter θ. The role of this initial guess is essential since it reduces N_{iter} at least twice. Still this dependence can become more pronounced for not so smooth solutions when errors in high modes are more important.

Table 2: Example 1: N_{iter} for different M and parameters θ in (6.2).

M	$\theta = \frac{8}{9}$ ($\varepsilon_0^2 = \frac{1}{2}$)	$\theta = \frac{16}{17}$ ($\varepsilon_0^2 = \frac{3}{4}$)	$\theta = \frac{32}{33}$ ($\varepsilon_0^2 = \frac{7}{8}$)
256	5 (10)	5 (9)	5 (9)
512	5 (10)	4 (9)	4 (8)
1024	4 (10)	4 (9)	3 (8)
2048	4 (9)	3 (8)	3 (8)

Example 2. Next we take $X = T = 1$, $c^2(x,y) = (1 + x^2 + 4y^2)^{-1}$. The data u_0, u_1 and φ are chosen so that the solution is the simple standing wave $u(x,y,t) = \sin(\pi x)\sin(4\pi y)\exp(t)$. In this example, the wave propagation in x and y directions is different, thus the mesh steps $h_x = \frac{1}{N} \neq h_y = \frac{1}{4N}$ are taken.

Table 3 contains the errors $e_{L^2}(N)$ and $e_{L^\infty}(N)$ at $t = 1$ together with the corresponding experimental convergence rates for scheme S_0. Clearly the scheme is robust for $h_x \neq h_y$ as well.

Table 3: Example 2: errors $e_{L^q}(N)$ and convergence rates $p_{L^q}(N)$ of the solution to scheme S_0, i.e., (3.22)-(3.23), for a sequence of meshes

N	h_x	h_y	h_t	$e_{L^2}(N)$	$p_{L_2}(N)$	$e_{L^\infty}(N)$	$p_{L_\infty}(N)$
4	1/4	1/16	1/32	3.3710e-3	—	3.6410e-3	—
8	1/8	1/32	1/64	1.9822e-4	4.088	2.3470e-4	3.955
16	1/16	1/64	1/128	1.1960e-5	4.051	1.4849e-5	3.982
32	1/32	1/128	1/256	7.2937e-7	4.035	9.2547e-7	4.004

For comparison, we solve the same problem by using the modified 4th order scheme (3.25)-(3.26) (suitable for any n) and put the same type results in Table 4. The results for both schemes are very close thus for other tests we apply only the former one. Nevertheless we note carefully that all the errors are (very) slightly larger for the latter scheme; this is since it exploits the more dissipative in space operator $\bar{s}_N = s_N + \frac{h_x^2}{12}\frac{h_y^2}{12}\Lambda_x\Lambda_y$ rather than s_N in the former scheme.

Example 3. Finally, the wave propagation is studied in the three-layer medium with the sound speeds s_1, s_2 and $s_3 = s_1$ (unless otherwise stated) respectively in its left, middle and right layers of the same thickness. Here we take $X = Y = 3000\ m = 3\ km$. The source is defined as the Ricker-type wavelet known in geophysics and given by

$$\varphi(x,y,t) = \delta(x - x_0, y - y_0)\sin(50t)e^{-200t^2},$$

where $\delta(x - x_0, y - y_0)$ is the Dirac distribution located at the center of domain $(x_0, y_0) = (1500\,m, 1500\,m)$. Also we take $u_0 = u_1 = 0$. It was shown in [4] that the wave dynamics is complicated. The computational challenges arise due to discontinuous coefficient c^2 and the very non-smooth distributional source function φ.

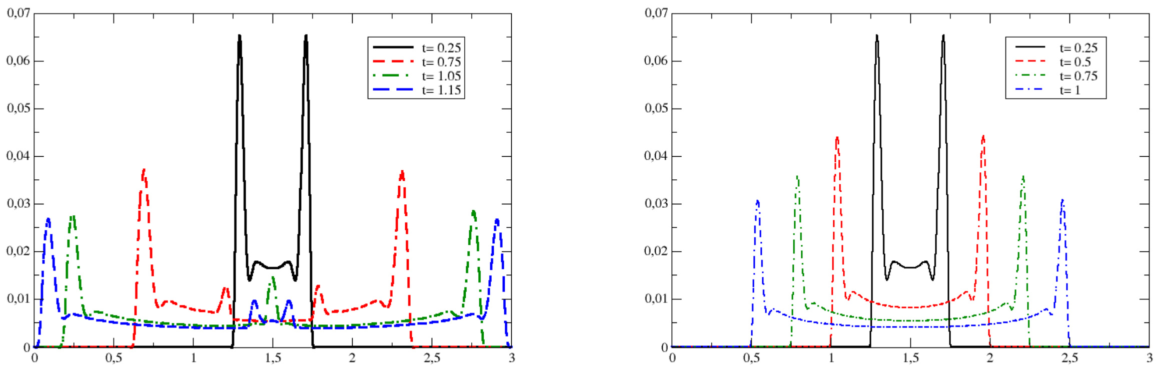
Table 4: Example 2: errors $e_{L^q}(N)$ and convergence rates $p_{L^q}(N)$ of the solution to scheme (3.25)-(3.26) for a sequence of meshes

N	h_x	h_y	h_t	$e_{L^2}(N)$	$p_{L_2}(N)$	$e_{L^\infty}(N)$	$p_{L_\infty}(N)$
4	1/4	1/16	1/32	3.4940e-3	—	3.7327e-3	—
8	1/8	1/32	1/64	2.0533e-4	4.089	2.4078e-4	3.956
16	1/16	1/64	1/128	1.2386e-5	4.051	1.5246e-5	3.981
32	1/32	1/128	1/256	7.5548e-7	4.035	9.5043e-7	4.004

We take $h_x = h_y = h = \frac{X}{N}$ with even N and approximate $\delta(x - x_0, y - y_0)$ as the mesh delta-function that equals h^{-2} at the node (x_0, y_0) and 0 at other nodes according to (3.10).

Let first $s_1 = 1500$ and $s_2 = 1000$ m/s as in [4]. Figure 1(a) shows 1D profiles of waves at $y = 1.5$ km for various times in the three-layer medium. At $t = 0.25$, the wave moves still inside the middle layer only. At $t = 0.75$, the wave fronts have already passed the interfaces of layers, have decreased their amplitude and move through the left and right layers towards the boundary; simultaneously, the reflected waves of much smaller amplitude move back inside the middle layer. At $t = 1.05$, both reflected waves collide and acquire larger amplitude. Then they continue their movement as shown at $t = 1.15$.

For comparison, Figure 1(b) shows 1D profiles of waves at $y = 1.5$ km in the homogeneous medium for $s_1 = s_2 = 1000$ m/s. Now only the refraction wave exists and moves towards the boundary with a constant velocity; the graphs on the both figures are the same at $t = 0.25$.



(a) (b)

Figure 1: Dynamics of the waves at different times for: (a) the three-layer medium; (b) the homogeneous medium for $s_1 = s_2 = 1000$ m/s

Next, in Figure 2 we present the dynamics of the waves at $y = 1.5$ km in the case of three different sound speeds $s_1 = 1500$, $s_2 = 1000$ and $s_3 = 3000$. At $t = 0.25$, the graph is the same once again. At $t = 0.6$ and $t = 0.7$, the wave fronts have already passed the interfaces of layers. In contrast to Figure 1, the amplitudes and speeds of the right refracted and reflected waves are higher than of the left ones.

In addition, we investigate experimentally the robustness of our iterative method with respect to jumps in the sound speed and the convergence order of scheme S_0. Such an analysis

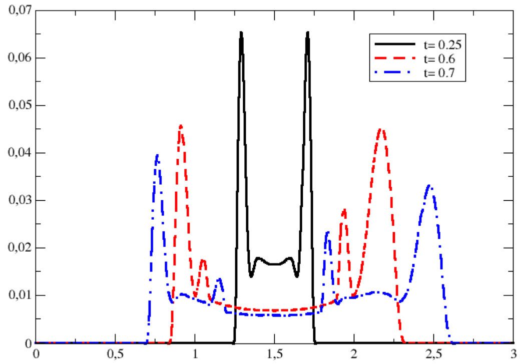


Figure 2: Dynamics of the waves at different times for the three-layer medium with $s_1 = 1500$, $s_2 = 1000$ and $s_3 = 3000$ m/s

was not done in [4]. Table 5 contains the values of N_{iter} for different speeds s_1 together with $s_2 = 1000$ m/s. In computations, the space steps are $h = 15$ and 7.5 m; the time steps h_t are respectively selected from the stability requirement. The presented results confirm that the iterative method (6.2) with the initial guess defined by (6.9) is both robust and fast.

Table 5: Example 3: N_{iter} for different speeds s_1 in the left and right layers

s_1	T	h	h_t	N_{iter}	h	h_t	N_{iter}
1000	1.0	15	0.005	9	7.5	0.0025	9
1500	0.8	15	0.004	9	7.5	0.002	9
3000	0.6	15	0.002	9	7.5	0.001	9
6000	0.6	15	0.0012	9	7.5	0.0006	9

Table 6 contains the errors $\bar{e}_{L^2}(N)$ and $e_{L^\infty}(N)$ in the mesh scaled L_2 and L_∞ norms at $t = 0.8$, for $h = \frac{X}{N}$, with $N = 100, 200, 400$, and $h_t = \frac{0.8}{N}$. The approximations to these errors are computed as

$$\bar{e}_{L^2}(N) = \frac{1}{X}\|v_h - v_{h/2}\|_{L^2}, \quad e_{L^\infty}(N) = \|v_h - v_{h/2}\|_{L^\infty},$$

where X equals the square root of the domain area, and v_h is the solution to the scheme S_0 for $h = \frac{X}{N}$. The computations are accomplished for the homogeneous case $s_1 = s_2 = 1000$ m/s and three-layer one with $s_1 = 1500$ and $s_2 = 1000$ m/s. We see that since the exact solution is a non-smooth function, the convergence rates are essentially reduced, and they are visibly higher in a simpler case of the constant sound speed. The results in L^2 norm are much better than in L^∞ one. Both of these last details are natural.

For comparison, we also investigate the accuracy of the standard explicit 2nd order scheme $\Lambda_t z - c^2(\Lambda_x + \Lambda_y)z = \varphi$ for the same tests as given in Table 6. Table 7 contains the errors $\bar{e}_{L^2}(N)$ and $e_{L^\infty}(N)$ in the mesh scaled L_2 and L_∞ norms at $t = 0.8$, for $h = \frac{X}{N}$, $N = 100, 200, 400$, and $h_t = \frac{0.8}{N}$. Here the errors are computed as

$$\bar{e}_{L^2}(N) = \frac{1}{X}\|z_h - v_{h_0}\|_{L^2}, \quad \bar{e}_{L^\infty}(N) = \|z_h - v_{h_0}\|_{L^\infty},$$

Table 6: Example 3: errors $\bar{e}_{L^2}(N)$ and $e_{L^\infty}(N)$ and convergence rates $p_{L^q}(N)$ of for a sequence of meshes and two speeds $s_1 = 1000$ and 1500 in the left and right layers

s_1	N	h	h_t	$\bar{e}_{L^2}(N)$	$p_{L_2}(N)$	$e_{L^\infty}(N)$	$p_{L_\infty}(N)$
1000	100	30	0.008	1.78919e-3	—	0.012093	—
1000	200	15	0.004	4.04097e-4	2.146	0.004069	1.571
1000	400	7.5	0.002	9.88333e-5	2.032	0.001387	1.553
1500	100	30	0.008	2.01559e-3	—	0.012093	—
1500	200	15	0.004	6.18800e-4	1.704	0.005448	1.150
1500	400	7.5	0.002	2.11363e-4	1.550	0.002736	0.994

where v_{h_0} is the solution of scheme S_0 for $h_0 = \frac{X}{800}$ and $h_t = 0.001$ and z_h is the solution of the explicit 2nd order scheme. Clearly, for the 2nd order scheme, the errors are larger and the convergence rates are worse than for scheme S_0, thus the latter scheme is better in the non-smooth case as well (the same practical conclusion for $n = 1$ is done in [14]).

Table 7: Example 3: errors $\bar{e}_{L^2}(N)$ and $\bar{e}_{L^\infty}(N)$ and convergence rates $p_{L^q}(N)$ for the standard explicit 2nd order scheme for a sequence of meshes and $s_1 = 1000$

s_1	N	h	h_t	$\bar{e}_{L^2}(N)$	$p_{L_2}(N)$	$\bar{e}_{L^\infty}(N)$	$p_{L_\infty}(N)$
1000	200	15	0.004	2.57470e-3	—	0.015435	—
1000	400	7.5	0.002	9.75537e-4	1.400	0.008072	0.935
1000	800	3.75	0.001	3.18427e-4	1.615	0.004047	0.996

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Availability of Data and Materials The datasets generated during the current study are available from the corresponding author on reasonable request. They support our published claims and comply with field standards.

Compliance with Ethical Standards

Conflict of interest There is no any conflict of interests/competing interests to declare that are relevant to the content of this article.

Code Availability (software application or custom code) Our custom codes are not publicly available. They support our published claims and comply with field standards.

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