Numerical approximation of the one-way Helmholtz equation using the differential evolution method

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Abstract This paper is devoted to increasing the computational efficiency of the finite-difference methods for solving the one-way Helmholtz equation in unbounded domains. The higher-order rational approximation of the propagation operator was taken as a basis. Computation of appropriate approximation coefficients and grid sizes is formulated as the problem of minimizing the discrete dispersion relation error. Keeping in mind the complexity of the developed optimization problem, the differential evolution method was used to tackle it. The proposed method does not require manual selection of the artificial parameters of the numerical scheme. The stability of the scheme is provided by an additional constraint of the optimization problem. A comparison with the Padé approximation method and rational interpolation is carried out. The effectiveness of the proposed approach is shown.

Keywords: wave propagation · Helmholtz equation · differential evolution · optimization · rational approximation

1 Introduction

Despite the constant increase in the computing power, the numerical solution of many mathematical physics equations remains a very resource-intensive operation. Fast and efficient numerical schemes usually use complex approximations and require quite sophisticated software implementation. Even more nontrivial is the question of the stability of complex numerical schemes and the determination of the limits of their applicability. Despite the existence of general-purpose numerical schemes, such as the finite element method, the construction and detailed study of a new numerical scheme is required in each specific case.

This study is aimed at improving the efficiency of the computer simulation methods for wave propagation in large integration domains without boundaries. Such kind of problems arise in computational hydroacoustics [5,18], tropospheric radio wave propagation [12,22,16], geophysics [21], optics and quantum mechanics [6]. Despite the different nature of the physical phenomena occurring in these scientific domains, the underlying mathematical models are to a certain extent universal [20].

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DOI: 10.1007/978-3-031-08751-6_15

The existing numerical methods for solving this class of problems have two significant disadvantages, which are fully manifested when trying to implement them as part of complex software systems. Firstly, they depend on several artificial computational parameters, which are usually selected manually by experts. The expert does not have reliable mechanisms for verifying the adequacy of the selected parameters, which can lead to errors. Secondly, they usually do not take into account the specific parameters of the propagation environment in an optimal way, which leads to significant overspending of computing resources and a decrease in the relevance of the results obtained.

To answer these questions, in this paper it is proposed to use stochastic methods [8] to optimize numerical schemes. The use of stochastic methods for constructing numerical schemes has been an actively developing scientific direction over the past few years. In particular, the physics-informed neural networks (PINN) method is actively developing [10,13]. In the PINN method, the solution of the equation is sought in the form of a deep neural network. The method proposed in this paper assumes the preservation of the numerical scheme structure, only its coefficients and parameters are upgraded.

This article is a continuation of the work on improving the numerical schemes for solving the Helmholtz equation. Previously, a method for finding optimal computation parameters for the Padé approximation was proposed [14]. Works [16,15] discovered the possibility of increasing the performance of existing schemes by using more suitable rational approximations.

The paper is organized as follows. The next section briefly describes the problem statement and numerical scheme based on rational approximation. Section 3 provides a discrete dispersion analysis of the numerical scheme under consideration. Section 4 is devoted to the optimization of coefficients and parameters of the scheme using the differential evolution method. Section 5 shows the application of the proposed method to the wedge diffraction problem and comparison with other rational approximation methods.

2 Rational approximation of the one-way Helmholtz equation

We are seeking the solution to the two-dimensional scalar Helmholtz equation

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial z^2} + k^2 n^2 (x, z) \psi = 0, \tag{1}$$

where $\psi(x, z)$ is the wave field, $k = 2\pi/\lambda$ is the wavenumber, λ is the wave length, $n(x, z)$ is the refractive index. It is assumed that the length in x of the propagation medium is much larger than the height in z.

The wave field is generated by an initial condition of the form

$$\psi(0, z) = \psi_0(z),$$

where $\psi_0(z)$ is a known function.

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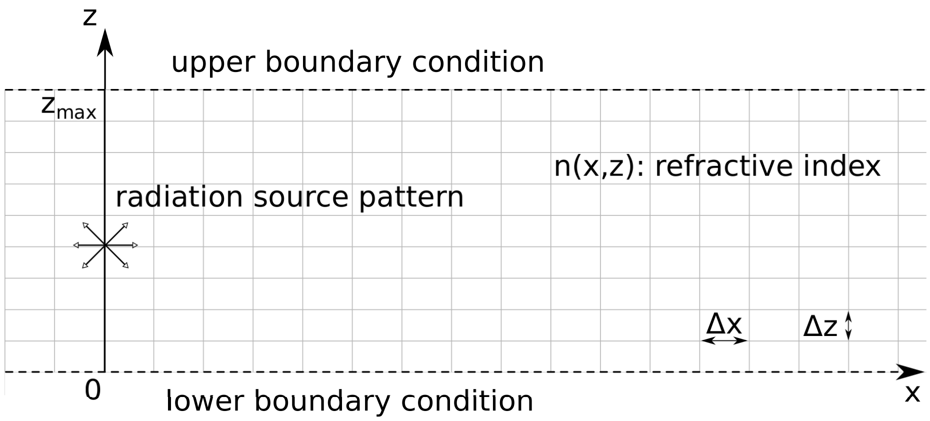

Figure 1. Schematic description of the considered problem [16].

The considered problem is schematically shown in Fig. 1.

Following [16,9] and neglecting to backscatter, we obtain the so-called one-way Helmholtz equation, written as a step-by-step solution along x-axis

$$u^{n+1} = \exp\left(ik\Delta x\left(\sqrt{1+L}-1\right)\right)u^n \tag{2}$$

$$u(x,z) = e^{-ikx}\psi(x,z),$$

$$u^n(z) = u(n\Delta x, z).$$

As suggested in [4], we apply a rational approximation of order $[n/m]$ the propagation operator (2)

$$\exp\left(ik\Delta x\left(\sqrt{1+L}-1\right)\right) \approx \frac{\prod_{l=1}^{n} 1+a_l L}{\prod_{l=1}^{m} 1+b_l L} = \prod_{l=1}^{p}\frac{1+a_l L}{1+b_l L}, \tag{3}$$

$$Lu = \frac{1}{k^2}\frac{\partial^2 u}{\partial z^2} + \left(n^2(x,z)-1\right)u,$$

meaning of coefficients $a_1 \dots a_p, b_1 \dots b_p$ will be clarified in the following sections.

Rational approximation (3) makes it possible to represent the action of the propagation operator (2) as a sequence of one-dimensional differential equations

$$\begin{cases} (1+b_1 L)\, v_1^n = (1+a_1 L)\, u^{n-1} \\ (1+b_l L)\, v_l^n = (1+a_l L)\, v_{l-1}^n \qquad l = 2,\dots,p-1, \\ \dots \\ (1+b_p L)\, u^n = (1+a_p L)\, v_{p-1}^n. \end{cases}$$

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where $v_1 \dots v_{p-1}$ are some auxiliary functions.

Operator L can be approximated by the following 2nd order finite-difference schema

$$Lu \approx \frac{1}{k^2 \Delta z^2} \left[u_{j-1} - 2u_j + u_{j+1} \right] + \left(n_j^2 - 1 \right) u_j,$$

where

$$u_j = u(j \Delta z).$$

Thus, we obtain a finite-difference step-by-step numerical scheme for solving the Helmholtz equation in elongated domain.

3 Dispersion relation

The accuracy and stability of the numerical scheme under consideration will be analyzed using discrete dispersion relations [3]. To do this, it is enough to consider how a plane wave passes through the numerical scheme. Substitute a two-dimensional plane wave of the form

$$E(x, z) = \exp\left(i\tilde{k}_x x + i k_z z \right),$$

where $k_z = k \sin\theta$ is the vertical wavenumber, θ is the angle between the direction of the wave and x-axis. For simplicity, we further consider the case of a homogeneous medium ($n(x,z) \equiv 1$). Then, the discrete horizontal wavenumber $\tilde{k}_x$ takes the form [14]

$$\tilde{k}_x \left(k_z, \Delta x, \Delta z, a_1 \dots a_p, b_1 \dots b_p \right) = k + \frac{\ln \prod_{l=1}^{p} t_l}{i \Delta x}, \tag{4}$$

$$t_l = \frac{1 - \frac{4a_l}{(k\Delta z)^2} \sin^2\left(\frac{k_z \Delta z}{2} \right)}{1 - \frac{4b_l}{(k\Delta z)^2} \sin^2\left(\frac{k_z \Delta z}{2} \right)}.$$

Latter expression is also known as the discrete dispersion relation.

Horizontal wavenumber for the original Helmholtz equation (1) is expressed as follows

$$k_x(k_z) = \begin{cases} \sqrt{k^2 - k_z^2}, & |k_z| \le k, \\ i\sqrt{k_z^2 - k^2}, & |k_z| > k. \end{cases} \tag{5}$$

4 Optimization of the numerical scheme

It is common to use the Padé approximation method [2] to obtain coefficients $a_1 \dots a_p, b_1 \dots b_p$ of rational approximation (3). The Padé approximation is local one and works well in the vicinity of zero propagation angle. As the propagation

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angle increases, its accuracy drops rapidly. To tackle this issue, it was previously proposed to use a class of rational approximation methods on an interval [16]. These methods make it possible to achieve uniform accuracy on the desired interval of propagation angles.

In this paper, the coefficients of the numerical scheme are defined by minimizing the difference between the real and discrete dispersion relation. The resulting optimization problems have a very complex structure and are hardly solvable by known deterministic optimization methods. In this connection, it is reasonable to apply evolutionary algorithms to solve them. Due to their stochastic nature, they are able to solve very complex optimization problems.

Our perspective of optimization of a numerical scheme is an increasing the speed of calculations without increasing the computational resources or reducing the applicability limits of the scheme.

4.1 Differential evolution method

In this work, we will use the differential evolution method [19] as one of the most well-known representatives of evolutionary algorithms. Let's briefly describe its main features.

Consider the following minimization problem

$$f\left(x\right) \to \min,\, x \in D \subset \mathbb{R}^n.$$

Fitness function f is a black box for the differential evolution method, no restrictions are imposed on it. The only thing required is to be able to compute its value in any point on its domain.

At each iteration, the algorithm generates a new generation of vectors by randomly combining vectors from the previous generation. For each vector x_i three different vectors v_1, v_2 and v_3 are randomly selected among the vectors from the old generation and a new mutant vector is produced

$$v = v_1 + F \cdot \left(v_2 - v_3\right), \tag{6}$$

where $F \in [0, 2]$ is a parameter called mutation. The mutation can be set by a constant or selected randomly at each iteration. Note that the formula for calculating the mutant vector (6) may differ depending on the strategy. Number of vectors in population (population size) is also a parameter of the method.

Then the crossover operation is applied: some coordinates are randomly replaced by the corresponding coordinates from the mutant vector v. If the new vector turns out to be better, then it passes to the next generation, otherwise the old one remains.

The unconditional optimization problem was considered above, but the differential evolution method can be generalized to take into account arbitrary nonlinear constraints [11] of the form

$$a \le g\left(x\right) \le b.$$

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We further use the implementation of the differential evolution method from the SciPy library [1].

4.2 Unconditional optimization

Let's start with the simplest optimization problem. Consider that values of the computational grid sizes Δx and Δz are fixed. Assume also that we know maximum propagation angle θ_{max}. The numerical scheme should minimize the difference between the real (5) and discrete (4) dispersion relation for all propagation angles from interval $[0, \theta_{max}]$. Formally , this can be written as follows

$$\text{argmin}_{a_1 \ldots a_p, b_1 \ldots b_p} \left[\max_{k_z \in [0, k_z^{max}]} \frac{1}{k} \left| \tilde{k}_x \left(k_z, \Delta x, \Delta z, a_1 \ldots a_p, b_1 \ldots b_p \right) - k_x \left(k_z \right) \right| \right], \quad (7)$$

where $k_z^{max} = k \sin \theta_{max}$.

Consider an example of solving optimization problem (7) with the following parameters: $\Delta x = 50\lambda$, $\Delta z = 0.25\lambda$, rational approximation order is equal to $[6/7]$, $\theta_{max} = 22°$. Fig. 2 demonstrates the dependence of the discrete dispersion relation error on the propagation angle for various rational approximations. It is clearly observable that the proposed method gives a much more accurate solution than the Padé approximation and the rational interpolation method [16]. Note that since the computational grid and the order of approximation are the same in all three cases, the complexity of propagation computations is equivalent.

Table 1 compares various strategies of the differential evolution method for the given example. The *randtobest1bin* strategy proved to be the best in this example. A high crossover probability leads to faster convergence. Reducing the range of mutation selection increases the rate of convergence, but sometimes it leads to a less optimal solution.

Strategy	mutation	Crossover probability	error	Number of iterations
currenttobest1exp	$[0, 2]$	1.0	1e-5.77	8089
currenttobest1exp	$[0.5, 1]$	1.0	1e-5.77	4541
currenttobest1exp	$[0.5, 1]$	0.7	1e-2.86	>10000
best1bin	$[0.5, 1]$	1.0	1e-4.68	>10000
best2exp	$[0.5, 1]$	1.0	1e-1.90	>10000
rand2exp	$[0.5, 1]$	1.0	1e-1.83	>10000
best1exp	$[0.5, 1]$	1.0	1e-5.77	5856
rand1exp	$[0.5, 1]$	1.0	1e-1.9	>10000
randtobest1bin	$[0.5, 1]$	1.0	1e-5.77	3808
currenttobest1bin	$[0.5, 1]$	1.0	1e-5.77	6074

Table 1. Comparison of various optimization strategies. $\Delta x = 50\lambda$, $\Delta z = 0.25\lambda$, approximation order is equal to $[6/7]$, $\theta_{max} = 22°$. Population size is equal to 20.

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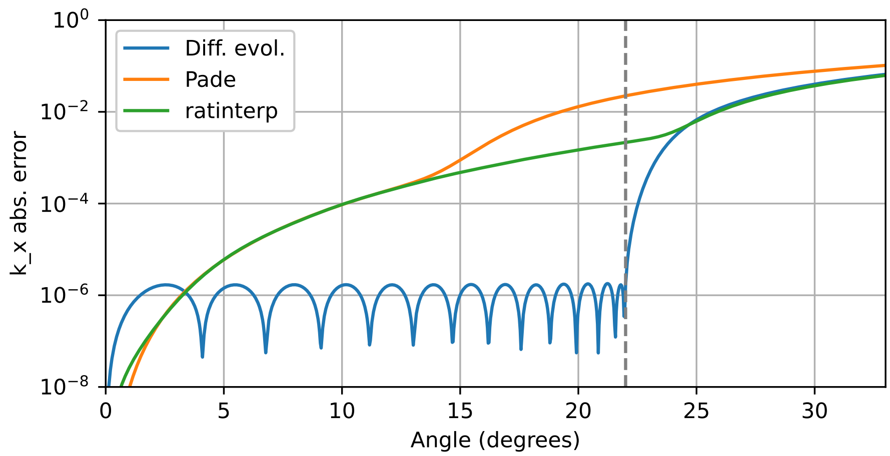

Figure 2. Dependence of the discrete dispersion relation error on the propagation angle for the Padé approximation, rational interpolation and the proposed method. In all cases $\Delta x = 50\lambda$, $\Delta z = 0.25\lambda$, approximation order is equal to [6/7], $\theta_{max} = 22°$.

4.3 Optimization for a given accuracy

In the previous example, we optimized a numerical scheme based on the known parameters of the computational grid. Usually, these parameters are unknown in advance and need to be determined. We will assume that we know acceptable error ε at distance x_{max} from the start propagation point. In this case, we need to find such parameters of the numerical scheme that would maximize the values of the grid steps (and accordingly minimize the computational time) while providing the specified accuracy. Bearing in mind that the error accumulates at each iteration of the step-by-step method, we come to the following conditional optimization problem

$$\text{argmax}_{\Delta x, \Delta z, a_1 \ldots a_p, b_1 \ldots b_p} \left[\Delta x \Delta z \right],$$

on condition

$$\max_{k_z \in [0, k_z^{max}]} \frac{1}{k \Delta x} |\tilde{k}_x \left(k_z, \Delta x, \Delta z, a_1 \ldots a_p, b_1 \ldots b_p \right) - k \left(k_z \right)| < \frac{\varepsilon}{x_{max}}.$$

Table 2 demonstrates the optimal values of the grid steps for the proposed method and the Padé approximation method with the required accuracy $\varepsilon = 3e-4$ at distance $x_{max} = 3e3\lambda$. Fig. 3 depicts the dependence of the discrete dispersion relation error on the propagation angle at distance $x_{max} = 3e3\lambda$. It can be seen that in order to achieve the same accuracy, Padé approximation method requires a much thicker computational grid, and, accordingly, more

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calculation time is required. The computational grid parameters optimization within the Padé approximation was previously suggested in [14].

	Δx	Δz
Padé	10.8λ	0.005λ
Diff.evol.	46.9λ	0.67λ

Table 2. Optimal values of the grid steps Δx и Δz for the Padé approximation and the proposed approach. $\varepsilon = 3e-4$, $x_{max} = 3e3\lambda$, $\theta_{max} = 22°$.

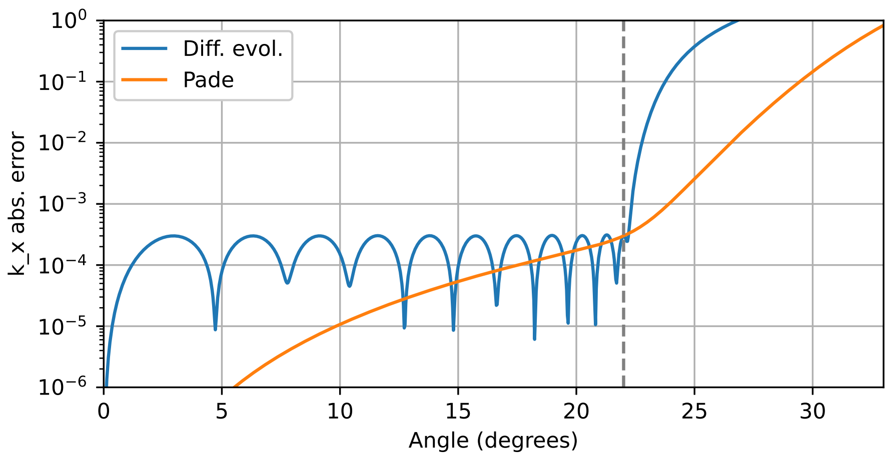

Figure 3. Dependence of the discrete dispersion relation error on the propagation angle at distance $x_{max} = 3e3$ for the Padé approximation ($\Delta x = 10.8\lambda$, $\Delta z = 0.005\lambda$) and the proposed approach ($\Delta x = 46.9\lambda$, $\Delta z = 0.67\lambda$). In all cases approximation order is equal to [6/7], $\theta_{max} = 22°$.

4.4 Stability condition

One of the most sophisticated issues in the development of numerical schemes is the determination of their stability conditions. Note that the discrete dispersion relation analysis is equivalent to the Von Neumann stability analysis. Thus, the stability condition is written as follows

$$\forall k_z \ \mathrm{Im}\left(\tilde{k}_x\left(k_z\right)\right) > 0.$$

It is equivalent to the following condition

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$$|\prod_{l=1}^{p}\frac{(k\Delta z)^2-4a_l x}{(k\Delta z)^2-4b_l x}|<1,\ x\in[0;1]. \quad (8)$$

Note that in this case, it is no longer sufficient to fulfill the condition only for the propagation angles of interest. Failure to comply with this condition contributes to the exponential growth of evanescent waves arising during diffraction [12].

This condition can also be taken into account within the differential evolution method. Fig. 4 and 5 demonstrate the dependence of the horizontal wave number $\tilde{k}_x$ on vertical wavenumber k_z without stability condition (8) and with its accounting. Parameters from the previous subsection were used. The effect of the stability condition on the resulting solution will be demonstrated in the next section.

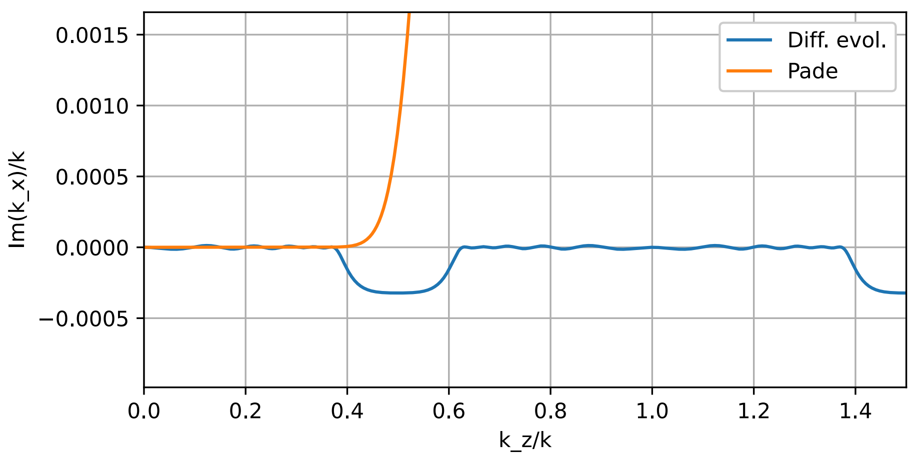

Figure 4. Dependence of the horizontal wave number $\tilde{k}_x$ on vertical wavenumber k_z without stability condition.

5 Numerical results

We will demonstrate the application of the proposed method to the classical wedge diffraction problem. The harmonic wave source is located at an altitude of 200 m and emits a signal at a frequency of 1 GHz. A wedge with a height of 200 m is located at a distance of 1500 m from the source. A transparent boundary condition is imposed on the upper boundary of the computational domain [17,7]. The wedge is approximated by a staircase function [12].

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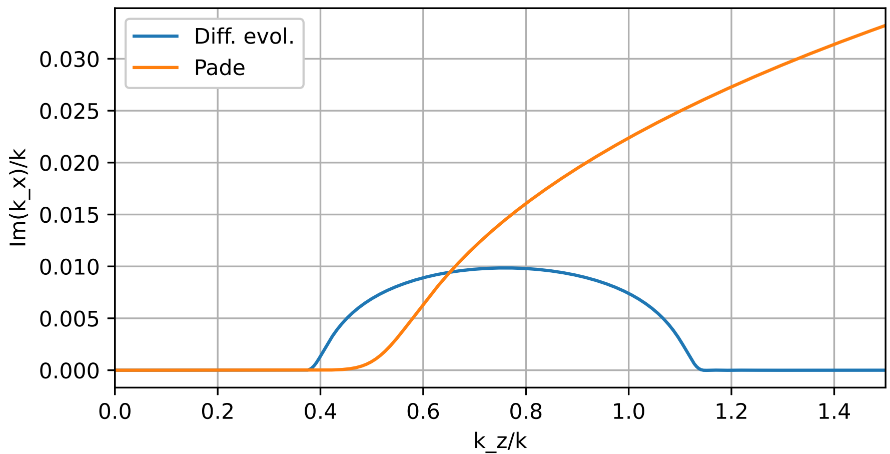

Figure 5. Dependence of the horizontal wave number $\tilde{k}_x$ on vertical wavenumber k_z with stability condition.

Fig. 6 and 7 depicts the two-dimensional distribution of the field amplitude, computed by the proposed method and the Padé approximation method. It is clear that both methods yield indistinguishable results, while the computation using the proposed method is faster due to a sparser computational grid. Namely, the proposed method allows to use a 4 times more sparse grid on x coordinate and a 130 times more sparse grid on z coordinate which gives a performance increase of more than 500 times in this particular case.

Fig. 8 shows the field distribution obtained by the Padé method on a sparse grid. It is clearly seen that in this case, the Padé method gives an incorrect solution in the diffraction zone behind the obstacle. Finally, Fig. 9 shows the field distribution calculated by the proposed method without taking into account the stability condition (8). One can see that the solution actually diverged due to the exponentially growing field components with high propagation angles.

6 Conclusion

The main disadvantage of the proposed method is the computational cost for solving the optimization problem, which is several times higher than the computation by the numerical scheme itself. Generally speaking, this problem can be tackled by preprocessing and tabulating the coefficients for various values of the maximum propagation angle and the required accuracy of calculations. Nevertheless, increasing the convergence rate of the proposed optimization problems is an urgent task.

Since the topology of the numerical scheme does not change in the proposed approach, it automatically obtains many useful properties. In particular, the

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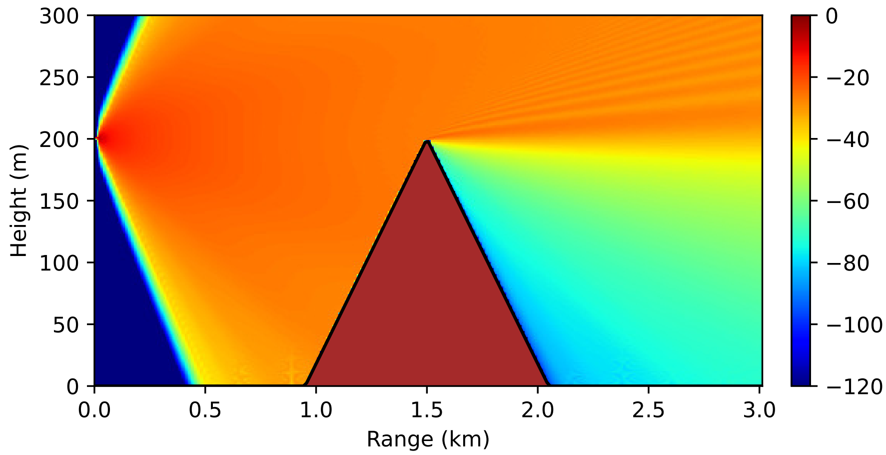

Figure 6. Wedge diffraction. Spatial distribution of the filed amplitude ($20 \log |\psi|$), obtained by the proposed method. $\Delta x = 46.9\lambda$, $\Delta z = 0.67\lambda$, approximation order is equal to [6/7].

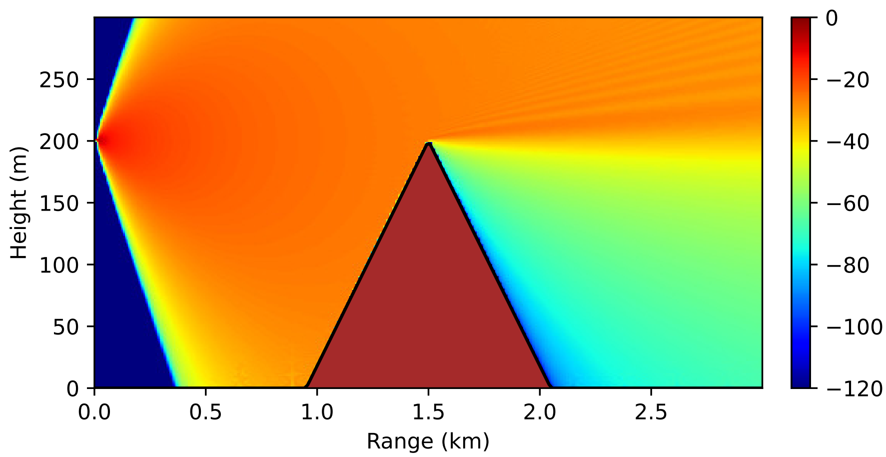

Figure 7. Wedge diffraction. Spatial distribution of the filed amplitude ($20 \log |\psi|$), obtained by the Padé method. $\Delta x = 10.8\lambda$, $\Delta z = 0.005\lambda$, approximation order is equal to [6/7].

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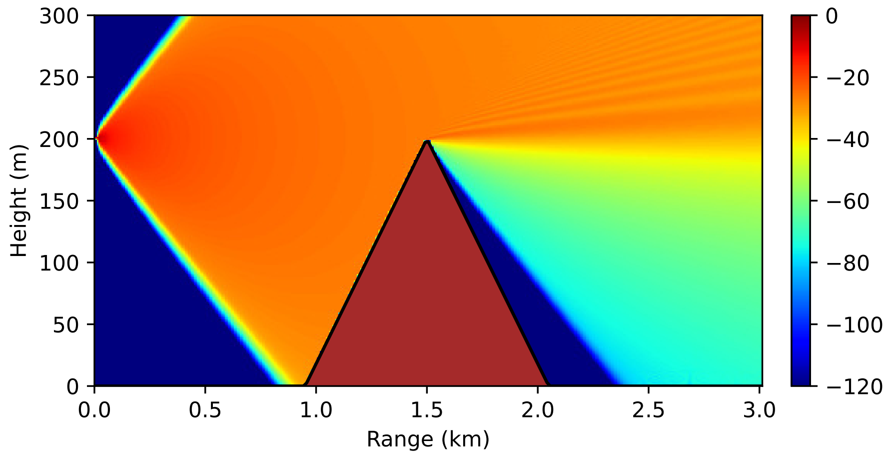

Figure 8. Wedge diffraction. Spatial distribution of the filed amplitude ($20 \log |\psi|$), obtained by the Padé method. $\Delta x = 46.9\lambda$, $\Delta z = 0.67\lambda$, approximation order is equal to [6/7].

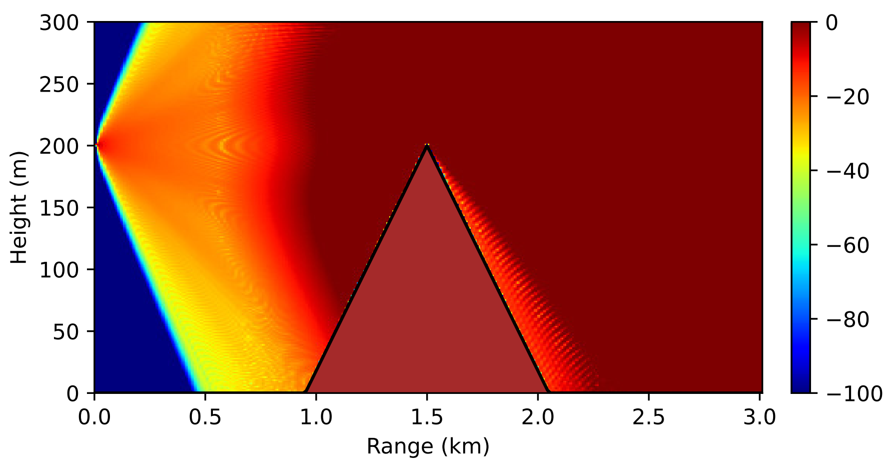

Figure 9. Wedge diffraction. Spatial distribution of the filed amplitude ($20 \log |\psi|$), obtained by the proposed method without stability condition. $\Delta x = 46.9\lambda$, $\Delta z = 0.67\lambda$, approximation order is equal to [6/7].

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methods of constructing the non-local boundary conditions are fully applicable to the proposed method. In addition, no significant changes are required to the existing software implementations.

Note that the proposed approach goes far beyond solving the Helmholtz equation. Similarly, it is possible to optimize almost any higher-order numerical scheme with a number of coefficients and computational parameters. With the classical approach, a numerical scheme is first developed, and then its accuracy and stability are analyzed. In the proposed approach, the required properties of the numerical scheme can be specified a priori.

Other configurations of the numerical scheme should be investigated, as well as other optimization methods should be applied in future studies.

Acknowledgements

This study was supported by the Russian Science Foundation grant No. 21-71-00039.

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