A Compact Fourth Order Scheme for the Helmholtz Equation in Polar Coordinates*

S. Britt[†] S. Tsynkov[‡] E. Turkel[§]

Abstract

In many problems, one wishes to solve the Helmholtz equation with variable coefficients and use a high order accurate method (e.g., fourth order accurate) to reduce the pollution and dispersion errors and alleviate the points-per-wavelength constraint. The variation of coefficients in the equation may be due to an inhomogeneous medium and/or the geometry. In particular, when the equation needs to be solved in cylindrical or spherical coordinates, variable coefficients are introduced within the differentiated terms. This renders existing fourth order finite difference methods inapplicable. We develop a new compact scheme that is provably fourth order accurate even for these problems. We also present numerical results that corroborate the fourth order convergence rate for several scattering problems.

Key words: Helmholtz equation, variable coefficients, polar coordinates, high order accuracy, compact finite differences.

Dedicated to the memory of our dear friend, David Gottlieb

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[†]Department of Mathematics, North Carolina State University, Box 8205, Raleigh, NC 27695, USA. E-mail: dsbritt@ncsu.edu

[‡]Corresponding author. Department of Mathematics, North Carolina State University, Box 8205, Raleigh, NC 27695, USA. Phone: +1-919-515-1877, Facsimile: +1-919-513-7336, E-mail: tsynkov@math.ncsu.edu

[§]School of Mathematical Sciences, Tel Aviv University, Ramat Aviv, Tel Aviv 69978, Israel. E-mail: turkel@post.tau.ac.il

1 Introduction

The Helmholtz equation

$$\Delta u + k^2 u = 0 \tag{1}$$

is the Fourier transform of the wave equation. Hence, accuracy requirements for the two are closely related. The first to investigate accuracy requirements for a simple advection equation were Kreiss and Oliger, see [12,15]. Given the equation $\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$ and a central difference approximation in space, they found the required number of points per wavelength $M_p = \lambda/h$ (λ is the wavelength and h is the grid size) for a $p-th$ order accurate order scheme. In particular:

$$\begin{aligned} M_2 &\approx 2\pi\left(\frac{\pi}{3}\right)^{\frac{1}{2}}\left(\frac{q}{\varepsilon}\right)^{\frac{1}{2}} \\ M_4 &\approx 2\pi\left(\frac{\pi}{15}\right)^{\frac{1}{4}}\left(\frac{q}{\varepsilon}\right)^{\frac{1}{4}} \\ M_6 &\approx 2\pi\left(\frac{\pi}{70}\right)^{\frac{1}{6}}\left(\frac{q}{\varepsilon}\right)^{\frac{1}{6}} \end{aligned} \tag{2}$$

In equations (2), ε denotes the desired accuracy and q denotes the number of periods to be calculated. In general

$$M_p = C_p\left(\frac{q}{\varepsilon}\right)^{\frac{1}{p}}$$

with

$$M_2 = 0.36M_4^2 \quad \text{and} \quad M_4 = 0.58M_6^{3/2}$$

It is important to emphasize that not only does the number of points per wavelength depend on the order of the scheme (it is expected), but it also depends on the number of oscillations to be computed. In other words, the longer the desired physical time/distance, the finer the required mesh.

Later, Bayliss, Goldstein, and Turkel [6] examined the Helmholtz equation and found that for a given error level the quantity $k^p h^{p+1}$ needs to be constant, where $k = \omega/c = 2\pi/\lambda$ is the wavenumber. Subsequently, this phenomenon was studied in more detail by Babuška and coworkers [4,10], who labeled it as "pollution." Thus, to maintain a fixed discretization error the number of points per wavelength kh must grow as $k^{1/p}$. This growth decreases as the order of the scheme increases. Hence, one way of reducing the pollution error is to increase the order of accuracy of the scheme. Surveys of the difficulties in treating the Helmholtz equation are presented in [14,25,27].

Nehrbass, Jevtic and Lee [19] studied ways of reducing the phase error when approximating the Helmholtz equation (1). They used a 5-point stencil and replaced the weight of the center node using a Bessel function. Harari and Turkel [13] constructed a fourth order approximation for Dirichlet boundary conditions. The method was based on Padé expansions, and it was extended by Singer and Turkel in [21] to Neumann boundary conditions. They also introduced a different approach named equation based. In this approach one finds the truncation error of a classical second order method and then uses the Helmholtz equation and its derivatives to eliminate this truncation error to the next order. This yields a stencil which is no wider in any coordinate direction than that of the underlying second order scheme. Accordingly, the resulting scheme is often referred to as compact. Note, that having a narrow stencil or in other words, having the same order of the difference equation (second order) as that of the differential equation, yet with higher order accurate approximation, is convenient for a number of reasons. In particular, it leads to a narrower bandwidth of the resulting matrix and also considerably simplifies setting both physical and radiation boundary conditions, as has been demonstrated in [5] and will also be shown later in this paper.

Another method of approximating the Helmholtz equation with high order accuracy was introduced by Caruthers, Steinhoff, and Engels [9] who based their finite-difference scheme on a Green's function approach and used Bessel functions. A key limitation of this technique was that all the coefficients were assumed to be constant [1].This implies that no coordinate system except Cartesian could be used. The corresponding constraints for the method of [13,21] were somewhat less strict in the sense that k could be a smooth function of x and y. However, the geometric limitations were still the same, so that the method did not apply to general coordinate systems.

In addition to the case of non-Cartesian geometry, the time-harmonic wave equation may acquire variable coefficients under the differentiated terms in the case of propagation through inhomogeneous media. In this case, the Laplacian in equation (1) is replaced by a variable coefficient operator, such as the one in the following simple equation:

$$\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}\right)+\mu\frac{\omega^2}{c^2}H_z=0 \tag{3}$$

obtained by combining the TE_z frequency Maxwell's equations:

$$-\frac{i\omega\mu}{c}H_z=\frac{\partial E_x}{\partial y}-\frac{\partial E_y}{\partial x}$$
$$\frac{i\omega}{c}E_x=-\frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}\qquad \frac{i\omega}{c}E_y=\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}$$

[1]Under this assumption one can even construct a sixth order accurate compact approximation, see [9, 18, 22, 23]

Whereas the magnetic permeability μ is constant for most materials, especially for high frequencies [16], the electric permittivity ε may vary across the medium, i.e., $\varepsilon = \varepsilon(x, y)$. Hence, none of the high order methods mentioned previously will apply to the generalized Helmholtz equation (3).

In the current paper, we will focus on addressing the issues of geometry, while more general equations of type (3), as well as those that allow for the variation of k, will be analyzed in a future publication. Specifically, our aim is to construct a fourth order yet compact 9-point finite-difference approximation for the Helmholtz equation in polar coordinates:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} + k^2 u = f \tag{4}$$

Clearly, the resulting scheme will be easily extendable to the 3D cylindrical case, because the third, axial, direction z remains Cartesian. We also expect that a very similar methodology will apply to the Helmholtz equation in spherical coordinates with azimuthal symmetry:

$$\frac{1}{r^2}\frac{\partial}{\partial r^2}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2 \sin^2(\theta)}\frac{\partial^2 u}{\partial \theta^2} + k^2 u = f$$

2 One-Dimensional Example

We first consider the following inhomogeneous ODE:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) + k^2 u = \frac{d^2 u}{dr^2} + \frac{1}{r}\frac{du}{dr} + k^2 u = f \tag{5}$$

where $f = f(r)$ is assumed given, and recast it for convenience as

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) = \frac{d^2 u}{dr^2} + \frac{1}{r}\frac{du}{dr} = F \tag{6}$$

where $F \equiv f - k^2 u$ is a formal right-hand side. We first approximate equation (6) with second order accuracy:

$$\frac{1}{r_m}\frac{1}{h}\left(r_{m+1/2}\frac{u_{m+1} - u_m}{h} - r_{m-1/2}\frac{u_m - u_{m-1}}{h}\right) = F_m \tag{7}$$

Analysis of the truncation error for scheme (7) shows that

$$\begin{aligned} &\frac{1}{r_m}\frac{1}{h}\left(r_{m+1/2}\frac{u_{m+1} - u_m}{h} - r_{m-1/2}\frac{u_m - u_{m-1}}{h}\right) \\ &= \frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right)\bigg|_m + \frac{h^2}{12}\left(u_m^{(4)} + \frac{2}{r}u_m^{(3)}\right) + \mathcal{O}(h^4) \end{aligned} \tag{8}$$

Consequently, to achieve fourth order accuracy, we need to eliminate the term that contains $u^{(4)}$ and $u^{(3)}$ on the right-hand side of (8). Differentiating equation (6), we have:

$$\frac{d^3u}{dr^3} + \frac{1}{r}\frac{d^2u}{dr^2} - \frac{1}{r^2}\frac{du}{dr} = F' \tag{9}$$

and

$$\frac{d^4u}{dr^4} + \frac{1}{r}\frac{d^3u}{dr^3} - \frac{2}{r^2}\frac{d^2u}{dr^2} + \frac{2}{r^3}\frac{du}{dr} = F''. \tag{10}$$

Multiplying (9) by $\frac{1}{r}$ and adding to (10) yields

$$\begin{aligned}\frac{d^4u}{dr^4} + \frac{2}{r}\frac{d^3u}{dr^3} &= F'' + \frac{1}{r}F' + \frac{1}{r^2}\frac{d^2u}{dr^2} - \frac{1}{r^3}\frac{du}{dr} \\ &= F'' + \frac{1}{r}F' + \frac{1}{r^2}\left(\frac{d^2u}{dr^2} - \frac{1}{r}\frac{du}{dr}\right) \\ &= F'' + \frac{1}{r}F' + \frac{1}{r^2}\left(F - \frac{2}{r}\frac{du}{dr}\right)\end{aligned}$$

Therefore, from formula (8) we obtain:

$$\begin{aligned}&\frac{1}{r_m}\frac{1}{h}\left(r_{m+1/2}\frac{u_{m+1}-u_m}{h} - r_{m-1/2}\frac{u_m - u_{m-1}}{h}\right) \\ &\quad -\frac{h^2}{12}\left(F'' + \frac{1}{r}F' + \frac{1}{r^2}F - \frac{2}{r^3}\frac{du}{dr}\right)\Bigg|_m \\ &\quad = \frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right)\Bigg|_m + \mathcal{O}(h^4)\end{aligned} \tag{11}$$

Relation (11) yields the following approximation for the original ODE (5) provided that k is constant:

$$\begin{aligned}&\frac{1}{r_m}\frac{1}{h}\left(r_{m+1/2}\frac{u_{m+1}-u_m}{h} - r_{m-1/2}\frac{u_m - u_{m-1}}{h}\right) + k^2u_m \\ &-\frac{h^2}{12}\left(f'' + \frac{1}{r}f' + \left(\frac{1}{r^2} - k^2\right)(f - k^2u) - \frac{2}{r^3}\frac{du}{dr}\right)\Bigg|_m = f_m\end{aligned} \tag{12}$$

where (5) was used to replace $\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right)$ inside the term $\sim \frac{h^2}{12}$. Equation (12) is not quite a true finite-difference scheme because it still contains continuous derivatives of f and of u. To transform (12) into a fourth order scheme, we first realize that the term multiplied by $\frac{h^2}{12}$ on the left-hand side of (12) does not need to be evaluated exactly. It is sufficient to have it approximated with second order accuracy, because of the factor of $\frac{h^2}{12}$ in front of it. This can be done for both f and u by means of the standard central differences on a 3-node stencil. If $f(r)$ is known analytically, then one can use the exact derivatives of f. In any event, once this is done the approximating relation (12) becomes a fourth order accurate scheme for equation (5) while still maintaining a compact 3-node stencil.

3 Two-Dimensional Scheme

The key consideration that enables us to extend the methodology of Section 2 to the two-dimensional equation (4) is that the fourth order accurate approximations will be built independently for the individual second order differential operators of the Laplacian. Hence, we write the following formal ODEs based on equation (4):

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) = F_r \equiv f - k^2 u - \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} \tag{13a}$$

$$\frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = F_\theta \equiv f - k^2 u - \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) \tag{13b}$$

Equation (13a) is identical to (6) up to the notation. Consequently, we can use formula (11) to obtain a fourth order accurate approximation of the radial part of the Laplacian in (4):

$$\begin{aligned}\frac{1}{r_m}\frac{1}{h_r}\left(r_{m+1/2}\frac{u_{m+1,l}-u_{m,l}}{h} - r_{m-1/2}\frac{u_{m,l}-u_{m-1,l}}{h_r}\right)\\ -\frac{h_r^2}{12}\left(F_r'' + \frac{1}{r}F_r' + \frac{1}{r^2}F_r - \frac{2}{r^3}\frac{\partial u}{\partial r}\right)\bigg|_{m,l}\\ = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)\bigg|_{m,l} + \mathcal{O}(h_r^4)\end{aligned} \tag{14}$$

where primes denote differentiation with respect to r. Relation (14) is different from its "parent" relation (11) in that the auxiliary right-hand side F_r also contains the second derivative with respect to θ, see formula (13a) so that

$$F_r' = \frac{\partial f}{\partial r} - k^2\frac{\partial u}{\partial r} - \frac{\partial}{\partial r}\left(\frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}\right)$$

$$F_r'' = \frac{\partial^2 f}{\partial r^2} - k^2\frac{\partial^2 u}{\partial r^2} - \frac{\partial^2}{\partial r^2}\left(\frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}\right)$$

Then, approximating the derivatives of u with second order accuracy by central differences we get

$$\begin{aligned}
F_r\big|_{m,l} &= f_{m,l} - k^2 u_{m,l} - \frac{1}{r_m^2}\frac{u_{m,l+1} - 2u_{m,l} + u_{m,l-1}}{h_\theta^2} + \mathcal{O}(h_\theta^2)\\
F_r'\big|_{m,l} &= \frac{\partial f}{\partial r}\bigg|_{m,l} - k^2\frac{u_{m+1,l} - u_{m-1,l}}{2h_r}\\
&\quad - \frac{1}{2h_r}\Big(\frac{1}{r_{m+1}^2}\frac{u_{m+1,l+1} - 2u_{m+1,l} + u_{m+1,l-1}}{h_\theta^2}\\
&\quad - \frac{1}{r_{m-1}^2}\frac{u_{m-1,l+1} - 2u_{m-1,l} + u_{m-1,l-1}}{h_\theta^2}\Big) + \mathcal{O}(h_r^2 + h_\theta^2)\\
F_r''\big|_{m,l} &= \frac{\partial^2 f}{\partial r^2}\bigg|_{m,l} - k^2\frac{u_{m+1,l} - 2u_{m,l} + u_{m-1,l}}{h_r^2}\\
&\quad - \frac{1}{h_r^2}\Big(\frac{1}{r_{m+1}^2}\frac{u_{m+1,l+1} - 2u_{m+1,l} + u_{m+1,l-1}}{h_\theta^2}\\
&\quad - \frac{2}{r_m^2}\frac{u_{m,l+1} - 2u_{m,l} + u_{m,l-1}}{h_\theta^2}\\
&\quad + \frac{1}{r_{m-1}^2}\frac{u_{m-1,l+1} - 2u_{m-1,l} + u_{m-1,l-1}}{h_\theta^2}\Big) + \mathcal{O}(h_r^2 + h_\theta^2)
\end{aligned} \tag{15}$$

Substituting expressions (15) into (14) and also using the approximation

$$\frac{\partial u}{\partial r}\bigg|_{m,l} = \frac{u_{m+1,l} - u_{m-1,l}}{2h_r} + \mathcal{O}(h_r^2) \tag{16}$$

we obtain a fourth order accurate finite-difference approximation of $\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)$ on a compact 3×3 stencil. Note that the derivatives of f in formulae (15) can be done either analytically or also numerically by central differences, depending on how the right-hand side is defined.

The treatment of the second derivative with respect to θ, which will be based on equation (13b), is even more straightforward. We begin with the standard second order accurate central difference scheme:

$$\frac{1}{r_m^2}\frac{u_{m,l+1} - 2u_{m,l} + u_{m,l-1}}{h_\theta^2} = F_\theta\big|_{m,l}$$

The analysis of its truncation error shows that

$$\frac{1}{r_m^2}\frac{u_{m,l+1} - 2u_{m,l} + u_{m,l-1}}{h_\theta^2} = \frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2} + \frac{1}{r^2}\frac{h_\theta^2}{12}\frac{\partial^4 u}{\partial\theta^4} + \mathcal{O}(h_\theta^4)$$

Consequently,

$$\frac{1}{r_m^2}\frac{u_{m,l+1} - 2u_{m,l} + u_{m,l-1}}{h_\theta^2} - \frac{h_\theta^2}{12}F_\theta''\bigg|_{m,l} = \frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2}\bigg|_{m,l} + \mathcal{O}(h_\theta^4) \tag{17}$$

where primes denote differentiation with respect to θ. All the derivatives in F''_θ shall be approximated with second order accuracy by central differences:

$$\begin{aligned} F''_\theta\big|_{m,l} = \frac{\partial^2 f}{\partial\theta^2}\bigg|_{m,l} &- k^2\frac{u_{m,l+1}-2u_{m,l}+u_{m,l-1}}{h_\theta^2} \\ &- \frac{1}{r_m}\frac{1}{h_r^2}\Big(r_{m+1/2}\frac{u_{m+1,l+1}-2u_{m+1,l}+u_{m+1,l-1}}{h_\theta^2} \\ &- 2r_m\frac{u_{m,l+1}-2u_{m,l}+u_{m,l-1}}{h_\theta^2} \\ &+ r_{m-1/2}\frac{u_{m-1,l+1}-2u_{m-1,l}+u_{m-1,l-1}}{h_\theta^2}\Big) + \mathcal{O}(h_r^2+h_\theta^2) \end{aligned} \tag{18}$$

Substituting expression (18) into (17), we obtain a fourth order accurate finite-difference approximation of $\frac{\partial^2 u}{\partial\theta^2}$ on a compact 3×3 stencil.

The overall fourth order accurate compact scheme for the Helmholtz equation (4) is then obtained by combining (14) and (17):

$$\begin{aligned} &\frac{1}{r_m}\frac{1}{h_r}\left(r_{m+1/2}\frac{u_{m+1,l}-u_{m,l}}{h} - r_{m-1/2}\frac{u_{m,l}-u_{m-1,l}}{h_r}\right) \\ &\qquad + \frac{1}{r_m^2}\frac{u_{m,l+1}-2u_{m,l}+u_{m,l-1}}{h_\theta^2} + k^2 u_{m,l} \\ &- \frac{h_r^2}{12}\left(\frac{\partial^2 F_r}{\partial r^2} + \frac{1}{r}\frac{\partial F_r}{\partial r} + \frac{1}{r^2}F_r - \frac{2}{r^3}\frac{\partial u}{\partial r}\right)\bigg|_{m,l} - \frac{h_\theta^2}{12}\frac{\partial^2 F_\theta}{\partial\theta^2}\bigg|_{m,l} = f_{m,l} \end{aligned} \tag{19}$$

where the correction terms $\sim \frac{h_r^2}{12}$ and $\sim \frac{h_\theta^2}{12}$ are to be evaluated according to (15), (16), and (18).

4 Boundary Conditions and the Solver

4.1 Continuous Boundary Conditions

We will solve the Helmholtz equation (4) on an annular domain

$$\{(r,\theta)\mid R_0\le r\le R_1,\ 0\le\theta<2\pi\} \tag{20}$$

This will allow a comparison of our numerical results against exact solutions that are available in the literature [8] for the scattering of plane waves off cylindrical shapes, see Section 5. The boundary condition on the surface of the cylinder $r = R_0$ can be either Dirichlet or Neumann. If the unknown variable u in equation (4) is interpreted as acoustic pressure, then the former corresponds to sound-soft scattering and the latter corresponds to sound-hard scattering. Other boundary conditions can also be considered, and we will report on their implementation in a future publication.

The boundary condition at the outer boundary $r = R_1$ requires special attention. As we are going to solve scattering problems, this boundary condition must guarantee the reflectionless propagation of all the scattered (i.e., outgoing) waves. To attain this capability, we will use the exact nonlocal artificial boundary condition (ABC) at $r = R_1$ which will be equivalent to the Sommerfeld radiation condition at infinity.

To derive the ABC, we will use a natural assumption that even though inside the domain (20) we generally allow $f \neq 0$, in the far field, i.e., for $r \geq R_1$ equation (4) becomes homogeneous, $f = 0$. Then, after the azimuthal Fourier transform we obtain a collection of uncoupled ODEs that govern the individual modes $\hat{u}_j = \hat{u}_j(r)$:

$$\begin{gathered}\frac{1}{r}\frac{d}{dr}\left(r\frac{d\hat{u}_j}{dr}\right) - \frac{j^2}{r^2}\hat{u}_j + k^2\hat{u}_j = 0 \\ j = 0, \pm 1, \pm 2, \ldots, \quad r \geq R_1\end{gathered} \tag{21}$$

Each equation (21) is a Bessel equation, and has two linearly independent solutions that can be taken in the form of the Hankel functions $H_j^{(1)}(kr)$ and $H_j^{(2)}(kr)$. Out of the two, only $H_j^{(2)}(kr)$ satisfies the radiation condition at infinity.[2] Hence, an equivalent boundary condition at $r = R_1$ for a given j can be written in the form of a Wronskian:

$$\det \begin{bmatrix} \hat{u}_j(r) & H_j^{(2)}(kr) \\ \frac{d}{dr}\hat{u}_j(r) & \frac{d}{dr}H_j^{(2)}(kr) \end{bmatrix}\Bigg|_{r=R_1} = 0$$

which yields

$$\frac{d\hat{u}_j}{dr}\bigg|_{r=R_1} = \hat{u}_j(r)\frac{\frac{d}{dr}H_j^{(2)}(kr)}{H_j^{(2)}(kr)}\Bigg|_{r=R_1} \tag{22}$$

The ABC (22) is formulated in the Fourier space for every $j = 0, \pm 1, \pm 2, \ldots$ and is exact. It provides superior numerical accuracy, as demonstrated by the experiments of Section 5. If transformed back into the configuration space, the ABC (22) becomes nonlocal, i.e., it couples the points along the entire artificial boundary $r = R_1$. This nonlocality, however, is by no means a disadvantage.[3] In fact, it never manifests itself because the ABC (22) needs to be implemented only in the transformed space when

[2] Choosing $H_j^{(2)}(kr)$ or $H_j^{(1)}(kr)$ depends on the sign in the time Fourier transform used to reduce the wave equation to the Helmholtz equation.

[3] More detail on the local vs. nonlocal artificial boundary conditions for a large variety of problems in scientific computing can be found in the review paper [26].

combined with our solver, which is based on the separation of variables. The latter, in turn, is an obvious logical choice for equation (4), which is written in polar coordinates and hence suggests the use of the azimuthal Fourier transform.

Note also that the well-known local first order Bayliss-Turkel radiation boundary condition of [7] can be obtained from (22) as an approximation. This is done by disregarding all the modes except $j = 0$ and employing asymptotic expressions for the Hankel functions of large arguments.

4.2 Solution by Separation of Variables

Scheme (19) is implemented on the polar grid uniform in each direction:

$$\begin{gathered}\{(r_m,\theta_l)\mid r_m = R_0 + mh_r,\ \theta_l = lh_\theta\}\\ h_r = \frac{R_1 - R_0}{M},\quad m = 0,1,\dots,M\\ h_\theta = \frac{2\pi}{L},\quad l = 0,1,\dots,L-1\end{gathered}\tag{23}$$

The number of cells in the azimuthal direction L is chosen as a power of 2 to facilitate efficient application of the FFT. The forward and backward discrete azimuthal Fourier transforms are taken in the complex form:

$$\hat{u}_{m,j} = \sum_{l=0}^{L-1} u_{m,l} e^{-ijlh_\theta}\tag{24a}$$

$$u_{m,l} = \frac{1}{L}\sum_{j=0}^{L-1} \hat{u}_{m,j} e^{ijlh_\theta}\tag{24b}$$

because the solution of equation (4) is expected to be complex.

Application of the Fourier transform (24) to scheme (19) allows us to separate the variables. Namely, we substitute the solution $u_{m,l}$ in the form of the sum (24b) and then apply (24a) to obtain a system of uncoupled ordinary difference equations in the radial direction:

$$\begin{gathered}\frac{1}{r_m}\frac{1}{h_r}\left(r_{m+1/2}\frac{\hat{u}_{m+1,j} - \hat{u}_{m,j}}{h_r} - r_{m-1/2}\frac{\hat{u}_{m,j} - \hat{u}_{m-1,j}}{h_r}\right)\\ + \left(k^2 + \frac{\nu_j^2}{r_m^2}\right)\hat{u}_{m,j} - \frac{h_r^2}{12}\left(\frac{\partial^2 \hat{F}_r}{\partial r^2} + \frac{1}{r}\frac{\partial \hat{F}_r}{\partial r} + \frac{1}{r^2}\hat{F}_r\right)\Big|_{m,j}\\ + \frac{h_r^2}{12}\frac{2}{r_m^3}\frac{\hat{u}_{m+1,j} - u_{m-1,j}}{2h_r} - \frac{h_\theta^2}{12}\nu_j^2 \hat{F}_\theta\big|_{m,j} = \hat{f}_{m,j}\\ j = 0,1,\dots,L-1\end{gathered}\tag{25}$$

In formula (25), the quantity

$$\nu_j^2 = -\frac{4}{h_\theta^2}\sin^2\left(\frac{jh_\theta}{2}\right) \tag{26}$$

is the eigenvalue of the second order central difference operator with respect to θ that corresponds to the j-th eigenfunction e^{ijlh_θ}, see (24b).

Similarly to scheme (19), the correction terms that enable fourth order accuracy need to be defined for (25). To do that, we use equations (15), (18) and substitute the expressions

$$\begin{aligned}
\hat{F}_r\big|_{m,j} &= \hat{f}_{m,j} - \left(k^2 + \frac{\nu_j^2}{r_m^2}\right)\hat{u}_{m,j} \\
\frac{\partial \hat{F}_r}{\partial r}\bigg|_{m,j} &= \frac{\partial \hat{f}}{\partial r}\bigg|_{m,j} - \left(k^2 + \frac{\nu_j^2}{2h_r}\right)\left(\frac{\hat{u}_{m+1,j}}{r_{m+1}^2} - \frac{\hat{u}_{m-1,j}}{r_{m-1}^2}\right) \\
\frac{\partial^2 \hat{F}_r}{\partial r^2}\bigg|_{m,j} &= \frac{\partial^2 \hat{f}}{\partial r^2}\bigg|_{m,j} - \left(k^2 + \frac{\nu_j^2}{h_r^2}\right)\left(\frac{\hat{u}_{m+1,j}}{r_{m+1}^2} - \frac{2\hat{u}_{m,j}}{r_m^2} + \frac{\hat{u}_{m-1,j}}{r_{m-1}^2}\right)
\end{aligned} \tag{27}$$

and

$$\begin{aligned}
\hat{F}_\theta\big|_{m,j} &= \hat{f}_{m,j} - k^2\hat{u}_{m,j} \\
&\quad - \frac{1}{r_m}\frac{1}{h_r}\left(r_{m+1/2}\frac{\hat{u}_{m+1,j} - \hat{u}_{m,j}}{h_r} - r_{m-1/2}\frac{\hat{u}_{m,j} - \hat{u}_{m-1,j}}{h_r}\right)
\end{aligned} \tag{28}$$

into (25), which completes the difference equation at every node m.

Altogether, formulae (25), (26), (27), and (28) define a system of L independent difference equations with respect to the unknown variables $\hat{u}_{m,j}$. The subscript m in (25) plays the role of the argument, whereas j is the Fourier parameter. We emphasize that since the original two-dimensional scheme (19) is written on a compact 3×3 stencil, each equation (25) is a second order difference equation. Hence, it can be solved efficiently by the standard tri-diagonal elimination, which is an important advantage.

4.3 Discrete Boundary Conditions

4.3.1 Discrete ABC at the Outer Boundary

To actually solve equation (25) for a given j, one needs to supplement it with the boundary conditions. To obtain a discrete fourth order accurate counterpart of the ABC (22), we begin with the following semi-discrete version of equation (4) for for $f=0$ and for every $l=0,1,\ldots,L-1$:

$$\begin{aligned} &\frac{1}{r}\frac{d}{dr}\left(r\frac{du_l}{dr}\right)+\frac{1}{r^2}\frac{u_{l+1}-2u_l+u_{l-1}}{h_\theta^2} \\ &+\frac{h_\theta^2}{12}\left\{\frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right)+k^2\right\}\frac{u_{l+1}-2u_l+u_{l-1}}{h_\theta^2}+k^2u_l=0 \end{aligned} \tag{29}$$

In equation (29), we have kept continuous differentiation with respect to r and introduced fourth order compact finite differences with respect to θ. The discrete Fourier transform (24) applied to (29) yields:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\hat{w}_j}{dr}\right)+\frac{\nu_j^2}{r^2}\hat{u}_j+k^2\hat{w}_j=0$$
$$j=0,1,\ldots,L-1,\qquad \hat{w}_j\overset{\text{def}}{=}\hat{u}_j\left(1+\frac{h_\theta^2}{12}\nu_j^2\right)$$

or equivalently:

$$\begin{gathered} \frac{1}{r}\frac{d}{dr}\left(r\frac{d\hat{u}_j}{dr}\right)+\frac{\tilde{\nu}_j^2}{r^2}\hat{u}_j+k^2\hat{u}_j=0 \\ j=0,1,\ldots,L-1 \end{gathered} \tag{30}$$

where the modified eigenvalue is defined as [cf. formula (26)]

$$\tilde{\nu}_j^2=\nu_j^2\left(1+\frac{h_\theta^2}{12}\nu_j^2\right)^{-1}$$

Each equation (30) is also a Bessel equation (recall, ν_j^2 is negative), and repeating the previous analysis we arrive at the semi-discrete ABC that will be convenient to apply at a half-node radial location:

$$\begin{gathered} \left.\frac{d\hat{u}_j}{dr}\right|_{r=R_1-h_r/2}=\hat{u}_j(r)\left.\frac{\frac{d}{dr}H^{(2)}_{|\tilde{\nu}_j|}(kr)}{H^{(2)}_{|\tilde{\nu}_j|}(kr)}\right|_{r=R_1-h_r/2} \\ l=0,1,\ldots,L-1 \end{gathered} \tag{31}$$

Boundary condition (31) differs from the previous continuous version, see formula (22), in two aspects. First, the range of j is finite, and second, the Hankel functions involved are of a non-integer order.

What remains is to approximate relations (31) on the grid with fourth order accuracy using compact finite differences. Differentiating equation (30) and replacing the second derivative via the equation itself, we find:

$$\hat{u}_j''=-\frac{1}{r}\hat{u}_j'-\frac{\tilde{\nu}_j^2}{r^2}\hat{u}_j-k^2\hat{u}_j$$
$$\hat{u}_j'''=\left(\frac{-\tilde{\nu}_j^2+2}{r^2}-k^2\right)\hat{u}_j'+\left(\frac{3\tilde{\nu}_j^2}{r^3}+\frac{k^2}{r}\right)\hat{u}_j$$

Then, at the cell center $M-1/2$ of the grid (23), which corresponds to $r = r_{M-1/2} = R_1 - h_r/2$, we can write

$$
\begin{aligned}
\hat{u}'_{M-1/2,j} &= \frac{\hat{u}_{M,j} - \hat{u}_{M-1,j}}{h_r} - \frac{h_r^2}{24} u'''_{M-1/2,j} + \mathcal{O}(h_r^4) \\
&= \frac{\hat{u}_{M,j} - \hat{u}_{M-1,j}}{h_r} - \frac{h_r^2}{24} \left[\left(\frac{-\tilde{\nu}_j^2 + 2}{r_{M-1/2}^2} - k^2 \right) \frac{\hat{u}_{M,j} - \hat{u}_{M-1,j}}{h_r} \right. \\
&\left. + \left(\frac{3\tilde{\nu}_j^2}{r_{M-1/2}^3} + \frac{k^2}{r_{M-1/2}} \right) \frac{\hat{u}_{M,j} + \hat{u}_{M-1,j}}{2} \right] + \mathcal{O}(h_r^4)
\end{aligned}
\tag{32a}
$$

and

$$
\begin{aligned}
\hat{u}_{M-1/2,j} &= \frac{\hat{u}_{M,j} + \hat{u}_{M-1,j}}{2} - \frac{h_r^2}{8} u''_{M-1/2,j} + \mathcal{O}(h_r^4) \\
&= \frac{\hat{u}_{M,j} + \hat{u}_{M-1,j}}{2} - \frac{h_r^2}{8} \left[- \frac{1}{r_{M-1/2}} \frac{\hat{u}_{M,j} - \hat{u}_{M-1,j}}{h_r} \right. \\
&\left. - \left(\frac{\tilde{\nu}_j^2}{r_{M-1/2}^2} + k^2 \right) \frac{\hat{u}_{M,j} + \hat{u}_{M-1,j}}{2} \right] + \mathcal{O}(h_r^4)
\end{aligned}
\tag{32b}
$$

Finally, let us introduce a new notation [see formula (31)]:

$$
\alpha_j = \left. \frac{\frac{d}{dr} H^{(2)}_{|\tilde{\nu}_j|}(kr)}{H^{(2)}_{|\tilde{\nu}_j|}(kr)} \right|_{r = R_1 - h_r/2}
\tag{33}
$$

Then, substituting expressions (32a) and (32b) into (31) and dropping the $\mathcal{O}(h_r^4)$ terms, we arrive at

$$
\frac{\hat{u}_{M,j} - \hat{u}_{M-1,j}}{h_r} \Big[\underbrace{1 - \frac{h_r^2}{24} \left(\frac{-\tilde{\nu}_j^2 + 2}{r_{M-1/2}^2} - k^2 \right) - \alpha_j \frac{h_r^2}{8} \frac{1}{r_{M-1/2}}}_{\beta_j} \Big]
$$

$$
= \frac{\hat{u}_{M,j} + \hat{u}_{M-1,j}}{2} \Big[\underbrace{\alpha_j + \frac{h_r^2}{24} \left(\frac{3\tilde{\nu}_j^2}{r_{M-1/2}^3} + \frac{k^2}{r_{M-1/2}} \right) + \alpha_j \frac{h_r^2}{8} \left(\frac{\tilde{\nu}_j^2}{r_{M-1/2}^2} + k^2 \right)}_{\gamma_j} \Big]
$$

which yields the following fourth order discrete ABC:

$$
\begin{gathered}
\hat{u}_{M,j} = \hat{u}_{M-1,j} \left(\frac{\beta_j}{h_r} + \frac{\gamma_j}{2} \right) \left(\frac{\beta_j}{h_r} - \frac{\gamma_j}{2} \right)^{-1} \\
j = 0, 1, \ldots, L-1
\end{gathered}
\tag{34}
$$

In practical terms, for every given j equation (34) provides a missing relation between the last and second to last components of the vector $[\hat{u}_{0,j}, \hat{u}_{1,j}, \ldots, \hat{u}_{M-1,j}, \hat{u}_{M,j}]^T$ which is to be determined by solving the tri-diagonal system (25). In other words, relation (34) completes the lower right corner of the corresponding tri-diagonal matrix. Note, that a simpler, second order, version of the ABC (34) was constructed in [17, Sec. 3.3].

Let us also emphasize that as scheme (19) is compact and, accordingly, each difference equation (25) is second order, it does not need any additional boundary conditions at the outer surface $r = R_1$ beyond the radiation conditions required by physics. A fourth order scheme built on a wider stencil would require additional, purely numerical, boundary conditions, as constructed, for example, in [11].

4.3.2 Discrete Boundary Conditions on the Surface

Implementation of a Dirichlet boundary condition at $r = R_0$ is straightforward. If in the configuration space we have

$$u_{0,l} = g_l, \quad l = 0, 1, \ldots, L-1$$

then in the Fourier space we have

$$\hat{u}_{0,j} = \hat{g}_j, \quad j = 0, 1, \ldots, L-1$$

The latter relation completes the upper left corner of the tri-diagonal matrix of system (25).

Implementation of a Neumann boundary condition at $r = R_0$

$$\left.\frac{\partial u}{\partial r}\right|_{r=R_0} = g(\theta)$$

is a little bit more involved, although it is very similar to the implementation of the discrete ABC in Section 4.3.1. First, we slightly modify the grid (23) so that the location of the boundary $r = R_0$ is at a half-node, $R_0 = r_{1/2}$:

$$\begin{gathered}\{(r_m, \theta_l) \mid r_m = R_0 + (m - 1/2)h_r,\ \theta_l = lh_\theta\} \\ h_r = \frac{R_1 - R_0}{M - 1/2}, \quad m = 0, 1, \ldots, M \\ h_\theta = \frac{2\pi}{L}, \quad l = 0, 1, \ldots, L-1\end{gathered}$$

After the Fourier transform we only have derivatives with respect to r. We then employ a direct analogue of expression (32a) that yields a fourth order accurate approximation of the first derivative with respect to r:

$$\begin{aligned}\hat{u}'_{1/2,j} = \frac{\hat{u}_{1,j} - \hat{u}_{0,j}}{h_r} - \frac{h_r^2}{24}\Bigg[\left(\frac{-\tilde{\nu}_j^2 + 2}{r_{1/2}^2} - k^2\right)\frac{\hat{u}_{1,j} - \hat{u}_{0,j}}{h_r} \\ + \left(\frac{3\tilde{\nu}_j^2}{r_{1/2}^3} + \frac{k^2}{r_{1/2}}\right)\frac{\hat{u}_{1,j} + \hat{u}_{0,j}}{2}\Bigg] + \mathcal{O}(h_r^4)\end{aligned} \tag{35}$$

Using the approximation (35), we can write the discrete fourth order Neumann boundary condition as follows:

$$\hat{u}_{0,j}\underbrace{\left(\frac{1}{h_r} + \frac{h_r^2}{24}\left[-\frac{1}{h_r}\left(\frac{-\tilde{\nu}_j^2 + 2}{r_{1/2}^2} - k^2\right) + \frac{1}{2}\left(\frac{3\tilde{\nu}_j^2}{r_{1/2}^3} + \frac{k^2}{r_{1/2}}\right)\right]\right)}_{\tilde{\beta}_j}$$

$$= \hat{u}_{1,j}\underbrace{\left(\frac{1}{h_r} - \frac{h_r^2}{24}\left[\frac{1}{h_r}\left(\frac{-\tilde{\nu}_j^2 + 2}{r_{1/2}^2} - k^2\right) + \frac{1}{2}\left(\frac{3\tilde{\nu}_j^2}{r_{1/2}^3} + \frac{k^2}{r_{1/2}}\right)\right]\right)}_{\tilde{\gamma}_j} - \hat{g}_j$$

or equivalently,

$$\begin{aligned}\hat{u}_{0,j} = \hat{u}_{1,j}\frac{\tilde{\gamma}_j}{\tilde{\beta}_j} - \frac{\hat{g}_j}{\tilde{\beta}_j} \\ j = 0, 1, \ldots, L-1\end{aligned} \tag{36}$$

Similarly to (34), for every given j equation (36) provides a missing relation between the zeroth and first components of the vector $[\hat{u}_{0,j}, \hat{u}_{1,j}, \ldots, \hat{u}_{M-1,j}, \hat{u}_{M,j}]^T$. Unlike (34), relation (36) is inhomogeneous if the Neumann boundary data are non-zero. In practice, relation (36) allows the completion of the upper left corner of the tri-diagonal matrix of (25).

Note, that as in the case of the ABC, see Section 4.3.1, no additional boundary conditions (beyond Dirichlet or Neumann) are required for the fourth order accurate scheme because the difference equation (25) is second order.

4.4 Additional Implementation Details

The implementation was done in Fortran. All numerical simulations were conducted in complex arithmetic with double precision (`complex*16`). Fourier transforms were computed using the publicly available software library `dfftpack`, see [24]. The Hankel functions were computed using another publicly available software package, `Algorithm 644`, see [1–3]. Note that on fine grids the order $|\nu_j|$ of the required Hankel functions, see formula

(31), may become rather high, even though the coefficients in front of the corresponding terms in the Fourier/Hankel expansion of the solution will be negligibly small because of the smoothness. Nonetheless, we have to keep all the terms in the expansion to maintain a full basis for the separation of variables. In doing so, in some instances `Algorithm 644` may fail to compute the Hankel function of a high order. In this case, we employ the asymptotic expression for Hankel functions of a high order ν:

$$H_\nu^{(2)}(x) \approx \sqrt{\frac{2}{\pi\mu}} e^{-\mu+\nu \tanh^{-1} \frac{\mu}{\nu}} \tag{37}$$

where $\mu = \sqrt{\nu^2 - x^2}$ and $\tanh^{-1} z = \frac{1}{2} \ln \frac{1+z}{1-z}$. Using formula (37), we find for the coefficient α_j of (33):

$$\alpha_j \approx -\sqrt{\frac{|\nu_j|}{|\nu_j|+1}} \frac{|\nu_j|+1}{r} \bigg|_{r=R_1-h_r/2} \tag{38}$$

Expression (38) is substituted into formula (34) via β_j and γ_j whenever the Hankel subroutine of `Algorithm 644` fails.

5 Test Solutions and Numerical Results

In the simulations given below, we take $R_0 = 1$, $R_1 = 2$, and $k = 8$.

5.1 Sound-Soft Scattering

5.1.1 Exact Solution

We consider scattering of a plane wave e^{ikx} off a cylinder (circle) of radius $r = R_0 = 1$. Then, the overall field is given by the sum of the impinging field e^{ikx} and the (yet unknown) scattered field u. We require that this overall field $e^{ikx} + u$ satisfies a zero Dirichlet boundary condition on the circle, which immediately translates into the following Dirichlet boundary condition for the scattered field:

$$u(r,\theta)\big|_{r=R_0} = -e^{ikR_0\cos\theta} \tag{39}$$

For this scattering problem there are no sources of the field inside the domain, and the Helmholtz equation is homogeneous, i.e., $f = 0$ in (4). Its general solution that satisfies the Sommerfeld radiation condition at infinity is given by the Fourier/Hankel series:

$$v(r,\theta) = \sum_{j=-\infty}^{\infty} c_j e^{ij\theta} H_{|j|}^{(2)}(kr) \tag{40}$$

To find a particular solution that satisfies (39), we need to choose c_j in such a way that the quantities $c_j H^{(2)}_{|j|}(kR_0)$ be equal to the Fourier coefficients of the Dirichlet data in (39):

$$c_j = \frac{1}{H^{(2)}_{|j|}(kR_0)} \int_{-\pi}^{\pi} -e^{ikR_0 \cos\theta} e^{-ij\theta} d\theta \qquad j = 0, \pm 1, \pm 2, \ldots \tag{41}$$

The resulting exact solution with the coefficients c_j of (41) substituted into (40) is equivalent to the one given in [8].

To actually evaluate this solution, we replace the integral in (41) by the discrete Fourier transform and compute it on an excessively fine azimuthal grid of 8192 nodes. As the boundary function $-e^{ikR_0 \cos\theta}$ in (39) is smooth, the coefficients c_j of (41) are expected to decay very rapidly (exponentially). This is what we indeed observe, and even though the series (40) is formally infinite, in practice it appears sufficient to keep only about 30 of its leading coefficients and disregard all other coefficients as they fall below the machine precision (for `complex*16`). Consequently, the exact solution for sound-soft scattering is obtained as a finite (truncated) Fourier/Hankel sum of type (40). In the next section, we study convergence of our numerical approximations to this exact solution.

5.1.2 Results of Computation

We compute the sound-soft scattered solution subject to boundary condition (39) on a sequence of six grids and summarize the results in Table 1.

Grid dimension	L_∞ error	Convergence rate
32×32	3.140×10^{-2}	
64×64	1.912×10^{-3}	4.0376
128×128	1.169×10^{-4}	4.0317
256×256	7.293×10^{-6}	4.0026
512×512	4.552×10^{-7}	4.0019
1024×1024	2.846×10^{-8}	3.9995

Table 1: Grid convergence for the Dirichlet boundary condition

The rightmost column of Table 1 clearly indicates a fourth order grid convergence of the proposed scheme. The execution time for the scheme scales linearly with the grid dimension. On the finest grid that we have used,

1024×1024, the total CPU time was 3.185 seconds,[4] out of which the computation of the exact solution (many Hankel function evaluations) took 2.9 seconds, and the numerical solution itself took only 0.285 seconds.

5.2 Sound-Hard Scattering

5.2.1 Exact Solution

We consider the same setup as in Section 5.1, $f = 0$ in equation (4), except that the overall field is required to satisfy a zero Neumann boundary condition on the circle, which translates into the following Neumann boundary condition for the scattered field:

$$\left.\frac{\partial u(r,\theta)}{\partial r}\right|_{r=R_0} = -ik\cos\theta e^{ikR_0\cos\theta} \tag{42}$$

The general solution is still taken in the form (40). To satisfy the Neumann boundary condition, we need to select the coefficients c_j so that the derivative of the series (40) at $r = R_0$ will match the data on the right-hand side of (42). Differentiating (40) with respect to r, we obatain:

$$\frac{\partial v(r,\theta)}{\partial r} = \sum_{j=-\infty}^{\infty} c_j e^{ij\theta} k H_{|j|}^{(2)\prime}(kr)$$

Consequently, to satisfy the Neumann boundary condition (42), we choose the coefficients c_j according to

$$\begin{gathered} c_j = \frac{1}{kH_{|j|}^{(2)\prime}(kR_0)} \int_{-\pi}^{\pi} -ik\cos\theta e^{ikR_0\cos\theta} e^{-ij\theta} d\theta \\ j = 0, \pm 1, \pm 2, \dots \end{gathered} \tag{43}$$

Substituting the coefficients c_j of (43) into (40) we obtain a solution to the homogeneous Helmholtz equation on $r \geq R_0$ subject to the Neumann boundary condition (42). This solution is equivalent to the one given in [8]. As in the case of the Dirichlet boundary condition, only a small number of coefficients c_j of (43) differ from zero within the machine precision. Hence, the exact solution is again obtained in the form of a truncated series (40).

5.2.2 Results of Computation

We compute the sound-hard scattered solution subject to boundary condition (42) on a sequence of six grids and summarize the results in Table 2.

[4] 2.8 GHz Intel Core 2 Duo MacBook Pro with 4 Gb of RAM; Intel Fortran Compiler Professional Edition for Mac OS X.

Grid dimension	L_∞ error	Convergence rate
32×32	8.875×10^{-2}	
64×64	5.061×10^{-3}	4.1322
128×128	3.089×10^{-4}	4.0342
256×256	1.919×10^{-5}	4.0087
512×512	1.198×10^{-6}	4.0016
1024×1024	7.483×10^{-8}	4.0008

Table 2: Grid convergence for the Neumann boundary condition

Similarly to the case of the Dirichlet boundary condition, the rightmost column of Table 2 clearly indicates a fourth order grid convergence of the proposed scheme. The CPU times for the Neumann boundary condition are also very similar to those reported in Section 5.1.

5.3 Inhomogeneous Helmholtz Equation

5.3.1 Exact Solution

To test the algorithm for the inhomogeneous case, we need to assume that the right-hand side $f = f(r, \theta)$ of the Helmholtz equation (4) is compactly supported on the annulus (20). Otherwise, one cannot apply the ABC of Sections 4.1, 4.3.1 that require homogeneity of the equation on the exterior region, i.e., for $r \geq R_1$. Note that the assumption of compactly supported sources is met by many important practical settings.

We introduce a test solution in the form

$$u(r, \theta) = p(r) \cdot \sum_{j=0}^{J} \frac{1}{2^j} e^{ij\theta} H^{(2)}(kr) \tag{44}$$

where the number of modes $J = 8$, and $p(r)$ is a function-multiplier:

$$\begin{aligned} p(r) &= \begin{cases} 0, & r \leq R_0 \\ 1, & r \geq \frac{R_0+R_1}{2} \end{cases} \\ p' = p'' = \ldots &= p^{(6)}\Big|_{r=R_0} = 0 \\ p' = p'' = \ldots &= p^{(6)}\Big|_{r=\frac{R_0+R_1}{2}} = 0 \end{aligned} \tag{45}$$

which we take as a polynomial of degree 13 on the interval $R_0 \leq r \leq \frac{R_0+R_1}{2}$ (it is unique). If there was no multiplier $p(r)$ on the right-hand side of (44), then $u(r, \theta)$ would have been a solution to the homogeneous Helmholtz equation (4). With the multiplier (45), it is still a solution that satisfies the radiation ABC (22) and the zero Dirichlet boundary condition at $r = R_0$, but the equation it solves becomes inhomogeneous. The corresponding "backward engineered" right-hand side $f(r, \theta)$ can be easily computed analytically and mapped onto the grid (23). The Hankel functions are evaluated numerically. According to the definition of the multiplier (45), $f(r, \theta)$ is compactly supported on a smaller annulus than (20), namely

$$\operatorname{supp} f(r,\theta) \subseteq \left\{ (r,\theta) \mid R_0 \le r \le \frac{R_0 + R_1}{2},\ 0 \le \theta \le 2\pi \right\}$$

5.3.2 Results of Computation

We reconstruct the test solution $u(r, \theta)$ of (44) numerically from the backward engineered right-hand side $f(r, \theta)$ on a sequence of six grids and summarize the results in Table 3.

Grid dimension	L_∞ error	Convergence rate
32×32	1.541×10^{-4}	
64×64	9.465×10^{-6}	4.0251
128×128	5.923×10^{-7}	3.998
256×256	3.585×10^{-8}	3.943
512×512	2.312×10^{-9}	3.955
1024×1024	1.445×10^{-10}	4.000

Table 3: Grid convergence for the inhomogeneous Helmholtz equation

As before, we observe a fourth order grid convergence. The CPU time for the numerical solution on the 1024×1024 grid was 0.39 seconds. The difference compared to the previously reported shorter time, see Section 5.1.2, is accounted for by the fact that when there is a non-trivial right-hand side on the entire grid, the application of FFT takes some additional effort.

6 Discussion

We have built and tested a fourth order accurate compact finite-difference approximation for the Helmholtz equation in polar coordinates. A novel feature of our method is that it can handle the variation of coefficients within the differentiated terms, which is typical for non-Cartesian geometries. A compact 3×3 stencil that we have employed presents at least two important advantages over other high order discretizations — simplified setting of the boundary conditions and narrow bandwidth of the resulting matrix. The latter, in particular, allows one to apply the standard tri-diagonal elimination after the Fourier transform. Numerical experiments corroborate the fourth order grid convergence and linear computational complexity of our solver which is based on the separation of variables.

In the future, we plan to extend the proposed methodology to the case of variable coefficients due to the physical inhomogeneity of the medium across which the waves propagate. We will address smooth variation of the coefficients both within the differentiated terms and in front of the non-differentiated term. Note, that having variable coefficients in more than one coordinate direction is likely to require a replacement of the current FFT-based solver by an iterative Krylov-type solver.

Our ultimate goal, however, is not only to simulate the propagation of waves across the media with smoothly varying characteristics, but also to be able to handle the material discontinuities. Then, the coefficients of the equation may undergo jumps along some surfaces. Building a fourth order accurate approximation in the case of material discontinuities becomes a particularly challenging issue when those surfaces are not aligned with the discretization grid. This problem is often encountered in applications. We plan to solve it using Calderon's projections and the method of difference potentials [20]. In doing so, the scheme and the solver presented in the current paper will be used for fast computation of Calderon's operators on interfaces of general shape.

References

[1] Amos, D.E. (1986). Algorithm 644, a portable package for Bessel functions of a complex argument and nonnegative order. ACM Transactions on Mathematical Software 12(3), 265–273

[2] Amos, D.E. (1990). Remark on algorithm 644. ACM Transactions on Mathematical Software 16(4), 404

[3] Amos, D.E. (1995). A remark on Algorithm 644: A portable package for Bessel functions of a complex argument and nonnegative order. ACM Transactions on Mathematical Software 21(4), 388–393

[4] Babuška, I.M. and Sauter, S.A. (2000). Is the pollution effect of the FEM avoidable for the Helmholtz equation considering high wave numbers? SIAM Rev. 42(3), 451–484 (electronic). Reprint of SIAM J. Numer. Anal. 34 (1997), no. 6, 2392–2423 [MR1480387 (99b:65135)]

[5] Baruch, G., Fibich, G., and Tsynkov, S. (2009). A high-order numerical method for the nonlinear Helmholtz equation in multidimensional layered media. J. Comput. Physics 228, 3789–3815

[6] Bayliss, A., Goldstein, C.I., and Turkel, E. (1985). On accuracy conditions for the numerical computation of waves. J. Comput. Phys. 59(3), 396–404

[7] Bayliss, A. and Turkel, E. (1980). Radiation boundary conditions for wave-like equations. Comm. Pure Appl. Math. 33(6), 707–725

[8] Bowman, J.J., Senior, T.B.A., and Uslenghi, P.L.E. (eds.) (1987). Electromagnetic and Acoustic Scattering by Simple Shapes. A Summa Book. Hemisphere Publishing Corp., New York. Revised reprint of the 1969 edition

[9] Caruthers, J.E., Steinhoff, J.S., and Engels, R.C. (1999). An optimal finite difference representation for a class of linear PDE's with application to the Helmholtz equation. J. Comput. Acoust. 7(4), 245–252

[10] Deraemaeker, A., Babuška, I.M., and Bouillard, P. (1999). Dispersion and pollution of the FEM solution for the Helmholtz equation in one, two and three dimensions. Int. J. Numer. Meth. Engnr. 46, 471–499

[11] Fibich, G. and Tsynkov, S.V. (2005). Numerical solution of the nonlinear Helmholtz equation using nonorthogonal expansions. J. Comput. Phys. 210(1), 183–224

[12] Gustafsson, B., Kreiss, H.O., and Oliger, J. (1995). Time Dependent Problems and Difference Methods. Pure and Applied Mathematics (New York). John Wiley & Sons Inc., New York. A Wiley-Interscience Publication

[13] Harari, I. and Turkel, E. (1995). Accurate finite difference methods for time-harmonic wave propagation. J. Comput. Phys. 119(2), 252–270

[14] Harari, I. (2006). A survey of finite element methods for time-harmonic acoustics. Comput. Methods Appl. Mech. Engrg. 195(13-16), 1594–1607

[15] Kreiss, H.O. and Oliger, J. (1972). Comparison of accurate methods for the integration of hyperbolic equations. Tellus 24, 199–215

[16] Landau, L.D. and Lifshitz, E.M. (1984). Course of Theoretical Physics. Vol. 8, Electrodynamics of Continuous Media. Pergamon International Library of Science, Technology, Engineering and Social Studies. Pergamon Press, Oxford. Translated from the second Russian edition by J. B. Sykes, J. S. Bell and M. J. Kearsley, Second Russian edition revised by Lifshits and L. P. Pitaevskii

[17] Lončarić, J. and Tsynkov, S.V. (2003). Optimization of acoustic source strength in the problems of active noise control. SIAM J. Applied Math. 63(4), 1141–1183

[18] Nabavi, M., Siddiqui, K., and Dargahi, J. (2007). A new 9-point sixth-order accurate compact finite-difference method for the Helmholtz equation. J. Sound Vibration 307, 972–982

[19] Nehrbass, J.W., Jevtic, J.O., and Lee, R. (1998). Reducing the phase error for finite-difference methods without incresing the order. IEEE Trans. Antennas and Propagation 46, 1194–1201

[20] Ryaben'kii, V.S. (2002). Method of Difference Potentials and Its Applications, volume 30 of Springer Series in Computational Mathematics. Springer-Verlag, Berlin

[21] Singer, I. and Turkel, E. (1998). High-order finite difference methods for the Helmholtz equation. Comput. Methods Appl. Mech. Engrg. 163(1-4), 343–358

[22] Singer, I. and Turkel, E. (2006). Sixth-order accurate finite difference schemes for the Helmholtz equation. J. Comput. Acoust. 14(3), 339–351

[23] Sutmann, G. (2007). Compact finite difference schemes of sixth order for the Helmholtz equation. J. Comput. Appl. Math. 203(1), 15–31

[24] Swarztrauber, P.N. (1982). Vectorizing the FFTs. In G. Rodrigue (ed.), Parallel Computations, pp. 51–83. Academic Press, San-Diego

[25] Thompson, L.L. (2006). A survey of finite-element methods for time-harmonic acoustics. J. Acoust. Soc. Am. 199, 1315–1330

[26] Tsynkov, S.V. (1998). Numerical solution of problems on unbounded domains. A review. Appl. Numer. Math. 27, 465–532

[27] Turkel, E. (2001). Numerical difficulties solving time harmonic equations. In A. Brandt, J. Bernholc, and K. Binder (eds.), Multiscale Computational Methods in Chemistry and Physics, pp. 319–337. IOS Press, Ohmsha