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

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Abstract In many problems, one wishes to solve the Helmholtz equation in cylindrical or spherical coordinates which introduces variable coefficients within the differentiated terms. Fourth order accurate methods are desirable to reduce pollution and dispersion errors and so alleviate the points-per-wavelength constraint. However, the variable coefficients renders existing fourth order finite difference methods inapplicable. We develop a new compact scheme that is provably fourth order accurate even for these problems. The resulting system of finite difference equations is solved by a separation of variables technique based on the FFT. Moreover, in the r direction the unbounded domain is replaced by a finite domain, and an exact artificial boundary condition is specified as a closure. This global boundary condition fits naturally into the inversion of the linear system. We present numerical results that corroborate the fourth order convergence rate for several scattering problems.

Keywords Helmholtz equation · Variable coefficients · Polar coordinates · High order accuracy · Compact finite differences · Exact artificial boundary condition (ABC)

1 Introduction

The Helmholtz equation

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

Dedicated to the memory of our dear friend, David Gottlieb.

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is the Fourier transform (in time) 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 [18, 21]. 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 (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 (as 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 et al. [7] examined the Helmholtz equation and found that for a given error level the quantity $k^{p+1}h^p$ 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, 13], who labeled it as "pollution". Thus, to maintain a fixed discretization error the number of points per wavelength $\sim(kh)^{-1}$ 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. A survey of the difficulties that arise when treating the Helmholtz equation numerically is presented in [35].

Nehrbass et al. [26] 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 [20] constructed a fourth order approximation for Dirichlet boundary conditions. The method was based on Padé expansions, and was extended by Singer and Turkel in [27] 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 referred to as compact.

Note, that having a narrow stencil or in other words, having the same order of the difference equation as that of the differential equation (second order), 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 artificial boundary conditions. This has been demonstrated in [5] and will also

be shown in this paper. We should emphasize though that a sharp distinction between the finite difference scheme of [5] and the one built in this paper is that the former uses compact differencing only in one coordinate direction whereas in this study the stencil is compact in all directions.

Another method of approximating the Helmholtz equation with high order accuracy was introduced by Caruthers et al. [11] 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. Under this assumption one can even construct a sixth order accurate compact approximation, see [11, 25, 28, 30]. This implies, however, that no coordinate system except Cartesian could be used. The corresponding constraints for the method of [20, 27] were somewhat less strict in the sense that k could be a smooth function of x and y. Yet the geometric limitations were still the same, so that the method did not apply to general coordinate systems.

In addition to finite differences, the Helmholtz equation is frequently solved by finite element methods. High order finite elements require a larger stencil. An alternative approach is to consider a formally low order compact finite element basis, but to increase the resolution by introducing functions that satisfy the Helmholtz equation. A number of different finite element approaches incorporate plane waves in the basis either in an additive or multiplicative way. Some sample techniques include the partition of unity method (PUM) [23], the generalized finite elements (GFEM) [29], weak elements [17], ultra weak variational formulations [12], and the discontinuous enrichment method (DEM) [14]. Besides the volumetric approach there are infinite element approaches that lead to integral equations on the scatterer; see Harari [19] and Thompson [32] for more details on all these various techniques. Note also that the previous approaches are mainly geared toward Cartesian coordinates and so are based on plane waves. It is also possible to include Bessel-type functions in the basis instead. Preliminary results with this approach are not very encouraging though, see e.g. [16, 24]. Tsukerman [33] has introduced a finite difference approach Trefftz-FLAME that includes an analytical basis. He considered a combination of plane waves and cylindrical harmonics for constant coefficient wave propagation about a cylinder.

Finally, there are also techniques based on the ray theory. Brandt and Livshitz [9] combined ray theory with multigrid to get a fast solver. Budaev and Bogy [10] combined a ray method with a probabilistic approach.

Our central objective in this paper is to construct a fourth order yet compact 9-point finite difference approximation for the Helmholtz equation in polar coordinates:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}+k^2u=f \tag{3}$$

This example is important for both theory and applications. Its theoretical significance is in (3) has a variable coefficient under the first derivative, which renders existing fourth order compact finite difference methods inapplicable. From the standpoint of applications, (3) appears, e.g., in many scattering problems. The resulting scheme will also be easily extendable to the 3D cylindrical case, because the third, axial, direction z remains Cartesian. A similar methodology will apply to the Helmholtz equation in spherical coordinates with azimuthal symmetry:

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

Our approach to constructing the scheme for (3) exploits the same idea as the previously introduced equation based approach, see [27]. There is, however, a fundamental difference

between the two. Unlike [27], in the current paper, we treat each second order derivative on the left-hand side of (3) independently. This is precisely what allows us to obtain the overall fourth order accurate approximation for the case of variable coefficients and still stay within the compact 3×3 stencil.

The methodology that we employ for solving the resulting system of linear algebraic equations is based on the separation of variables. It uses a FFT in the circumferential direction, and tri-diagonal elimination in the radial direction. While other solvers can, of course, be used for the scheme in other settings, this particular solver is especially advantageous for the scattering applications that we have in mind, when (3) is initially formulated on an unbounded region.

The FFT/tri-diagonal solver is very fast. In addition, it couples naturally with the artificial boundary condition (ABC) set at the outer boundary of the finite computational domain, which is obtained from the original infinite domain by means of truncation. Indeed, the ABC must ensure that if the solution computed inside the bounded computational domain was extended toward its unbounded exterior, then it would satisfy the homogeneous Helmholtz equation there and the Sommerfeld radiation condition at infinity. ABCs of this type are typically obtained in the Fourier space (see, e.g., [34] for a general survey). In physical space they become nonlocal, i.e., they couple the values of the solution and derivatives along the entire artificial boundary rather. The global nature of such ABCs is "the price to pay" for their exactness, i.e., for having no error in the overall solution due to the domain truncation. In some instances, this global nature may be viewed as a shortcoming. If, however, the separation of variables is used as a solver, it rather becomes a major advantage, because the boundary condition is set straight in the Fourier space, independently for each uncoupled one-dimensional equation. Hence, there is an exact ABC, yet there is never a need to formulate this nonlocal boundary condition in physical space, let alone to deal with the resulting dense near-boundary block of the overall system matrix. In fact, this matrix never needs to be written down explicitly. Even though the solution methodology we propose is direct, it applies to the system of finite difference equations in its original form, i.e., when it is written on a two-dimensional grid.

Note also that we construct the ABC directly for the scheme, as opposed to first specifying the boundary condition for the differential equation and then approximating it on the grid. The advantage of our approach is apparent in the context of wave propagation. The waves governed by the finite difference equation on the grid are close yet not quite identical to the waves governed by the underlying differential equation; in particular, the discrepancy becomes larger for higher frequencies (e.g., with respect to azimuthal modes). The ABC built straight for the scheme makes the outer boundary transparent precisely for those "discrete" outgoing waves, whereas a continuous ABC that is subsequently discretized makes the outer boundary transparent for the continuous waves approximated on the grid. The latter approach may be prone to having additional reflection errors. We therefore interpret exactness of the ABC as exactness for a given finite difference approximation. In other words, in the framework of our methodology the accuracy of the boundary treatment always matches automatically that of the interior discretization.

The rest of the paper is organized as follows. In Sect. 2, we analyze a one-dimensional example that illustrates the key ideas of building compact high order approximations for differential equations with variable coefficients. In Sect. 3, we derive a compact fourth order accurate scheme for (3) on the 3×3 stencil. In Sect. 4, we introduce the separation of variables for the scheme, and discuss the boundary conditions (both physical and artificial) and the solver. In Sect. 5, we present the results of numerical simulations that corroborate the theoretical design properties of the scheme. In Sect. 6, we provide a summary and the conclusions.

2 One-Dimensional Example

We first consider the following inhomogeneous ODE:

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

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

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

where $F\equiv f-k^2u$ is a formal right-hand side. We first approximate (5) with second order accuracy:

$$\frac{1}{r_m}\frac{1}{h}\left(r_{m+1/2}\frac{u_{m+1}-u_m}{h}-r_{m-1/2}\frac{u_m-u_{m-1}}{h}\right)=F_m \tag{6}$$

Analysis of the truncation error for scheme (6) shows that

$$\begin{aligned}&\frac{1}{r_m}\frac{1}{h}\left(r_{m+1/2}\frac{u_{m+1}-u_m}{h}-r_{m-1/2}\frac{u_m-u_{m-1}}{h}\right)\\&\quad=\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right)\Big|_m+\frac{h^2}{12}\left(u_m^4+\frac{2}{r}u_m^3\right)+\mathcal{O}(h^4)\end{aligned} \tag{7}$$

Consequently, to achieve fourth order accuracy, we need to eliminate the term that contains $u^{(3)}$ and $u^{(4)}$ on the right-hand side of (7). Differentiating (5), we have:

$$\frac{d^3u}{dr^3}+\frac{1}{r}\frac{d^2u}{dr^2}-\frac{1}{r^2}\frac{du}{dr}=F' \tag{8}$$

and

$$\frac{d^4u}{dr^4}+\frac{1}{r}\frac{d^3u}{dr^3}-\frac{2}{r^2}\frac{d^2u}{dr^2}+\frac{2}{r^3}\frac{du}{dr}=F'' \tag{9}$$

Multiplying (8) by $\frac{1}{r}$ and adding to (9) 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 (7) we obtain:

$$\begin{aligned}&\frac{1}{r_m}\frac{1}{h}\left(r_{m+1/2}\frac{u_{m+1}-u_m}{h}-r_{m-1/2}\frac{u_m-u_{m-1}}{h}\right)\\&\quad-\frac{h^2}{12}\left(F''+\frac{1}{r}F'+\frac{1}{r^2}F-\frac{2}{r^3}\frac{du}{dr}\right)\Big|_m=\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right)\Big|_m+\mathcal{O}(h^4)\end{aligned} \tag{10}$$

Relation (10) yields the following approximation for the original ODE (4) provided that k is constant:

$$\frac{1}{r_m}\frac{1}{h}\left(r_{m+1/2}\frac{u_{m+1}-u_m}{h}-r_{m-1/2}\frac{u_m-u_{m-1}}{h}\right)+k^2u_m - \frac{h^2}{12}\left(f''+\frac{1}{r}f'+\left(\frac{1}{r^2}-k^2\right)(f-k^2u)-\frac{2}{r^3}\frac{du}{dr}\right)\Bigg|_m = f_m \tag{11}$$

where (4) was used to replace $\frac{1}{r}\frac{d}{dr}(r\frac{du}{dr})$ inside the term $\sim\frac{h^2}{12}$. Equation (11) is not a true finite difference scheme yet because it still contains continuous derivatives of f and of u. To transform (11) into a fourth order scheme, we first realize that the term multiplied by $\frac{h^2}{12}$ on the left-hand side of (11) 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 (11) becomes a fourth order accurate scheme for (4) while still maintaining a compact 3-node stencil.

Let us emphasize that scheme (11) has been built on a uniform grid, $h = \text{const}$. If the grid becomes nonuniform, then already our "point of departure" scheme (6) loses accuracy and reduces from second order to first order. Accordingly, the methodology for achieving high order that we have presented most likely won't work in its current form, and will require modification. In Sect. 3, we extend this methodology to the two-dimensional case, and we also restrict our consideration to the case of uniform grids only, both in the radial and circumferential directions.

3 Two-Dimensional Scheme

The key consideration that enables us to extend the methodology of Sect. 2 to the two-dimensional equation (3) 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 operators based on (3):

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) = F_r \equiv f - k^2u - \frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2} \tag{12a}$$

$$\frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2} = F_\theta \equiv f - k^2u - \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) \tag{12b}$$

Equation (12a) is identical to (5) up to the notation. Consequently, we can use formula (10) to obtain a fourth order accurate approximation of the radial part of the Laplacian in (3):

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)\Bigg|_{m,l} = \frac{1}{r_m}\frac{1}{h_r}\left(r_{m+1/2}\frac{u_{m+1,l}-u_{m,l}}{h_r}-r_{m-1/2}\frac{u_{m,l}-u_{m-1,l}}{h_r}\right) - \frac{h_r^2}{12}\left(F_r''+\frac{1}{r}F_r'+\frac{1}{r^2}F_r-\frac{2}{r^3}\frac{\partial u}{\partial r}\right)\Bigg|_{m,l}+\mathcal{O}(h_r^4) \tag{13}$$

where primes denote differentiation with respect to r. Relation (13) is different from its "parent" relation (10) in that the auxiliary right-hand side F_r also contains the second derivative

with respect to θ, see formula (12a) 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

$$\begin{aligned}
F_r\big|_{m,l} &= f_{m,l} - k^2 u_{m,l} - \frac{1}{r_m^2}\frac{u_{m,l+1} - 2u_{m,l} + u_{m,l-1}}{h_\theta^2} + \mathcal{O}(h_r^2)\\
F_r'\big|_{m,l} &= \left.\frac{\partial f}{\partial r}\right|_{m,l} - k^2 \frac{u_{m+1,l} - u_{m-1,l}}{2h_r}\\
&\quad - \frac{1}{2h_r}\left(\frac{1}{r_{m+1}^2}\frac{u_{m+1,l+1} - 2u_{m+1,l} + u_{m+1,l-1}}{h_\theta^2}\right.\\
&\quad \left. - \frac{1}{r_{m-1}^2}\frac{u_{m-1,l+1} - 2u_{m-1,l} + u_{m-1,l-1}}{h_\theta^2}\right) + \mathcal{O}(h_r^2) \qquad (14)\\
F_r''\big|_{m,l} &= \left.\frac{\partial^2 f}{\partial r^2}\right|_{m,l} - k^2 \frac{u_{m+1,l} - 2u_{m,l} + u_{m-1,l}}{h_r^2}\\
&\quad - \frac{1}{h_r^2}\left(\frac{1}{r_{m+1}^2}\frac{u_{m+1,l+1} - 2u_{m+1,l} + u_{m+1,l-1}}{h_\theta^2} - \frac{2}{r_m^2}\frac{u_{m,l+1} - 2u_{m,l} + u_{m,l-1}}{h_\theta^2}\right.\\
&\quad \left. + \frac{1}{r_{m-1}^2}\frac{u_{m-1,l+1} - 2u_{m-1,l} + u_{m-1,l-1}}{h_\theta^2}\right) + \mathcal{O}(h_r^2)
\end{aligned}$$

Substituting expressions (14) into (13) and also using the approximation

$$\left.\frac{\partial u}{\partial r}\right|_{m,l} = \frac{u_{m+1,l} - u_{m-1,l}}{2h_r} + \mathcal{O}(h_r^2) \qquad (15)$$

we obtain a fourth order accurate finite difference approximation of $\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r})$ on a compact 3×3 stencil. Note that the derivatives of f in formulae (14) can be done either analytically or numerically by central differences on a 3 point stencil.

The treatment of the second derivative with respect to θ, which will be based on (12b), 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, by differentiating (12b) we arrive at

$$\frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2}\bigg|_{m,l} = \frac{1}{r_m^2}\frac{u_{m,l+1}-2u_{m,l}+u_{m,l-1}}{h_\theta^2} - \frac{h_\theta^2}{12}F_\theta''\bigg|_{m,l} + \mathcal{O}(h_\theta^4) \tag{16}$$

where primes denote differentiation with respect to θ. All the derivatives in F_θ'' shall be approximated with second order accuracy

$$\begin{aligned} F_\theta''|_{m,l} = {} & \frac{\partial^2 f}{\partial\theta^2}\bigg|_{m,l} - k^2\frac{u_{m,l+1}-2u_{m,l}+u_{m,l-1}}{h_\theta^2} \\ & - \frac{1}{r_m}\frac{1}{h_\theta^2 h_r^2}\left[r_{m+1/2}\left(u_{m+1,l+1}-u_{m,l+1}\right) - r_{m-1/2}\left(u_{m,l+1}-u_{m-1,l+1}\right)\right. \\ & - 2\left(r_{m+1/2}\left(u_{m+1,l}-u_{m,l}\right) - r_{m-1/2}\left(u_{m,l}-u_{m-1,l}\right)\right) \\ & \left. + r_{m+1/2}\left(u_{m+1,l-1}-u_{m,l-1}\right) - r_{m-1/2}\left(u_{m,l-1}-u_{m-1,l-1}\right)\right] + \mathcal{O}(h_\theta^2) \end{aligned} \tag{17}$$

Substituting expression (17) into (16), 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 (3) is then obtained by combining (13) and (16):

$$\begin{aligned} & \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{\partial^2 u}{\partial\theta^2} + k^2 u \\ & = \frac{1}{r_m}\frac{1}{h_r}\left(r_{m+1/2}\frac{u_{m+1,l}-u_{m,l}}{h_r} - r_{m-1/2}\frac{u_{m,l}-u_{m-1,l}}{h_r}\right) \\ & \quad + \frac{1}{r_m^2}\frac{u_{m,l+1}-2u_{m,l}+u_{m,l-1}}{h_\theta^2} \\ & \quad - \frac{h_r^2}{12}\left(\frac{\partial^2 F_r}{\partial r^2} + \frac{1}{r}\frac{\partial F_r}{\partial r} + \frac{1}{r^2}F_r - \frac{2}{r^3}\frac{\partial u}{\partial r}\right)\bigg|_{m,l} - \frac{h_\theta^2}{12}\frac{\partial^2 F_\theta}{\partial\theta^2}\bigg|_{m,l} + k^2 u_{m,l} = f_{m,l} \end{aligned} \tag{18}$$

The terms multiplying $\frac{h_r^2}{12}$ and $\frac{h_\theta^2}{12}$ are evaluated to second order accuracy according to (14), (15), and (17). We thus obtain

$$\begin{aligned} & \frac{1}{r_m}\frac{1}{h_r}\left(r_{m+1/2}\frac{u_{m+1,l}-u_{m,l}}{h_r} - r_{m-1/2}\frac{u_{m,l}-u_{m-1,l}}{h_r}\right) \\ & \quad + \frac{1}{r_m^2}\frac{u_{m,l+1}-2u_{m,l}+u_{m,l-1}}{h_\theta^2} \\ & \quad - \frac{h_r^2}{12}\left[\frac{\partial^2 f}{\partial r^2}\bigg|_{m,l} - k^2\frac{u_{m+1,l}-2u_{m,l}+u_{m-1,l}}{h_r^2}\right] \\ & \quad + \frac{1}{12h_\theta^2}\left[\frac{1}{r_{m+1}^2}\left(u_{m+1,l+1}-2u_{m+1,l}+u_{m+1,l-1}\right) - \frac{2}{r_m^2}\left(u_{m,l+1}-2u_{m,l}+u_{m,l-1}\right)\right. \\ & \quad \left. + \frac{1}{r_{m-1}^2}\left(u_{m-1,l+1}-2u_{m-1,l}+u_{m-1,l-1}\right)\right] \end{aligned}$$

$$
\begin{aligned}
&- \frac{h_r^2}{12r_m}\left[\left.\frac{\partial f}{\partial r}\right|_{m,l} - k^2\frac{u_{m+1,l}-u_{m-1,l}}{2h_r}\right.\\
&- \frac{1}{2h_r h_\theta^2}\left(\frac{1}{r_{m+1}^2}\left(u_{m+1,l+1}-2u_{m+1,l}+u_{m+1,l-1}\right)\right.\\
&\left.\left.- \frac{1}{r_{m-1}^2}\left(u_{m-1,l+1}-2u_{m-1,l}+u_{m-1,l-1}\right)\right)\right]\\
&- \frac{h_r^2}{12r_m^2}\left(f_{m,l}-k^2u_{m,l}-\frac{1}{r_m^2h_\theta^2}\left(u_{m,l+1}-2u_{m,l}+u_{m,l-1}\right)\right)\\
&+ \frac{h_r}{12r_m^3}\left(u_{m+1,l}-u_{m-1,l}\right) - \frac{h_\theta^2}{12}\left[\left.\frac{\partial^2 f}{\partial\theta^2}\right|_{m,l} - k^2\frac{u_{m,l+1}-2u_{m,l}+u_{m,l-1}}{h_\theta^2}\right]\\
&+ \frac{1}{12h_r^2r_m}\left[r_{m+1/2}(u_{m+1,l+1}-u_{m,l+1}) - r_{m-1/2}(u_{m,l+1}-u_{m-1,l+1})\right.\\
&- 2\left(r_{m+1/2}(u_{m+1,l}-u_{m,l}) - r_{m-1/2}(u_{m,l}-u_{m-1,l})\right)\\
&\left.+ r_{m+1/2}(u_{m+1,l-1}-u_{m,l-1}) - r_{m-1/2}(u_{m,l-1}-u_{m-1,l-1})\right] + k^2u_{m,l} = f_{m,l}
\end{aligned}
\tag{19}
$$

4 Boundary Conditions and the Solver

4.1 Continuous Boundary Conditions

We will solve the Helmholtz equation (3) 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 Sect. 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 (3) 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 $r\ge R_1$ (3) becomes homogeneous, $f=0$. Then, after the azimuthal Fourier transform we obtain a collection of uncoupled ODEs that govern the individual modes $\hat{u}_j=\hat{u}_j(r)$:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\hat{u}_j}{dr}\right) - \frac{j^2}{r^2}\hat{u}_j + k^2\hat{u}_j = 0 \quad j=0,\pm1,\pm2,\ldots,\ r\ge R_1 \tag{21}$$

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.[1] 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

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

The ABC (22) is formulated in the Fourier space for every $j = 0, \pm 1, \pm 2, \ldots$ and is exact. Its discrete counterpart derived in Sect. 4.3.1 provides superior numerical accuracy, as demonstrated by the experiments of Sect. 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.[2] In fact, it never manifests itself because the ABC (22) needs to be implemented only in the transformed space when combined with our solver, which is based on the separation of variables. The latter, in turn, is an obvious logical choice for (3), which is written in polar coordinates and hence suggests the use of the azimuthal Fourier transform.

Note, that the well-known local first order Bayliss-Turkel radiation boundary condition of [6] 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 (18) is implemented on the polar grid uniform in each direction:

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

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:

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

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

[1] 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.

[2] 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 [34].

because the solution of (3) is expected to be complex.

Application of the Fourier transform to scheme (18) (or, equivalently, (19)) allows a separation of 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:

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

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).

Similar to scheme (18), the correction terms that enable fourth order accuracy need to be defined for (25). To do that, we use (14), (17) and substitute the expressions

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

and

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

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 (18) 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 solve (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 fol-

lowing semi-discrete version of (3) for $f = 0$ and for every $l = 0, 1, \ldots, L-1$:

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

In (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 applied to (29) yields:

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

or equivalently:

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

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:

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

We note that we use the half-node location only for convenience, and this is not necessary. 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 (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

$$\hat{u}'_{M-1/2,\,j} = \frac{\hat{u}_{M,j} - \hat{u}_{M-1,j}}{h_r} - \frac{h_r^2}{24}u'''_{M-1/2,\,j} + \mathcal{O}(h_r^4)$$

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

and

$$\begin{aligned}\hat{u}_{M-1/2,j} &= \frac{\hat{u}_{M,j} + \hat{u}_{M-1,j}}{2} - \frac{h_r^2}{8}u''_{M-1/2,j} + \mathcal{O}(h_r^4) \\ &= \frac{\hat{u}_{M,j} + \hat{u}_{M-1,j}}{2} - \frac{h_r^2}{8}\left[-\frac{1}{r_{M-1/2}}\frac{\hat{u}_{M,j} - \hat{u}_{M-1,j}}{h_r} - \left(\frac{\tilde{\nu}_j^2}{r_{M-1/2}^2} + k^2\right)\frac{\hat{u}_{M,j} + \hat{u}_{M-1,j}}{2}\right] + \mathcal{O}(h_r^4)\end{aligned} \tag{33}$$

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

$$\alpha_j = \left.\frac{\frac{d}{dr}H^2_{|\tilde{\nu}_j|}(kr)}{H^2_{|\tilde{\nu}_j|}(kr)}\right|_{r=R_1-h_r/2} \tag{34}$$

Then, substituting expressions (32) and (33) into (31) and dropping the $\mathcal{O}(h_r^4)$ terms, we arrive at

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

which yields the following fourth order accurate discrete ABC:

$$\hat{u}_{M,j} = \hat{u}_{M-1,j}\left(\frac{\beta_j}{h_r} + \frac{\gamma_j}{2}\right)\left(\frac{\beta_j}{h_r} - \frac{\gamma_j}{2}\right)^{-1} \quad j = 0, 1, \ldots, L-1 \tag{35}$$

In practical terms, for every given j (35) 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 (35) completes the lower right corner of the corresponding tri-diagonal matrix. Note, that a simpler, second order, version of the ABC (35) was constructed in [22, Sect. 3.3].

Let us also emphasize that as scheme (18) 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 [15].

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 Sect. 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, $R_0 = r_{1/2}$ (again, this modification is not necessary and is only done for convenience):

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

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

$$\hat{u}'_{1/2,j} = \frac{\hat{u}_{1,j} - \hat{u}_{0,j}}{h_r} - \frac{h_r^2}{24}\left[\left(\frac{-\tilde{\nu}_j^2 + 2}{r_{1/2}^2} - k^2\right)\frac{\hat{u}_{1,j} - \hat{u}_{0,j}}{h_r} + \left(\frac{3\tilde{\nu}_j^2}{r_{1/2}^3} + \frac{k^2}{r_{1/2}}\right)\frac{\hat{u}_{1,j} + \hat{u}_{0,j}}{2}\right] + \mathcal{O}(h_r^4) \tag{36}$$

Using the approximation (36), 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,

$$\hat{u}_{0,j} = \hat{u}_{1,j}\frac{\tilde{\gamma}_j}{\tilde{\beta}_j} - \frac{\hat{g}_j}{\tilde{\beta}_j} \quad j = 0, 1, \ldots, L-1 \tag{37}$$

Similar to (35), for every given j (37) 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 (35), relation (37) is inhomogeneous if the Neumann boundary data are non-zero. Relation (37) allows the completion of the upper left corner of the tri-diagonal matrix of (25).

As in the case of the ABC, see Sect. 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 [31]. 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:

$$H_\nu^{(2)}(x) \approx \sqrt{\frac{2}{\pi\mu}} e^{-\mu+\nu \tanh^{-1}\frac{\mu}{\nu}} \tag{38}$$

where $\mu = \sqrt{\nu^2 - x^2}$ and $\tanh^{-1} z = \frac{1}{2}\ln\frac{1+z}{1-z}$. Using (38), we find for the coefficient α_j of (34):

$$\alpha_j \approx -\sqrt{\frac{|\nu_j|}{|\nu_j|+1}} \frac{|\nu_j|+1}{r}\Bigg|_{r=R_1-h_r/2} \tag{39}$$

Expression (39) is substituted into (35) via β_j and γ_j whenever the Hankel subroutine of `Algorithm 644` fails. This is a fully automated procedure that does not require any user intervention. Failure of `Algorithm 644` means that it cannot achieve the desired accuracy when computing a particular Hankel function. In that case, it returns a certain value of the special flag variable, and based on this value, our code substitutes the appropriate asymptotic expression for this Hankel function.

5 Test Solutions and Numerical Results

In all the simulations given below, we take $R_0 = 1$ and $R_1 = 2$. To study the grid convergence and the complexity of the solver, we take $k = 8$ and run a series of simulations on a sequence of grids. To study the behavior of the scheme as the wavenumber k varies, we maintain $k^{p+1}h^p = \text{const}$ and verify that the error stays at the same level.

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 homogeneous Dirichlet boundary condition on the circle. This translates into the following Dirichlet boundary condition for the scattered field:

$$u(r,\theta)\big|_{r=R_0} = -e^{ikR_0\cos\theta} \tag{40}$$

For this scattering problem there are no sources inside the domain, and the Helmholtz equation is homogeneous, i.e., $f = 0$ in (3). The general solution that satisfies the Sommerfeld radiation condition at infinity is given by the Fourier/Hankel series:

$$v(r,\theta) = \sum_{j=-\infty}^{\infty} c_j e^{ij\theta} H^{(2)}_{|j|}(kr) \tag{41}$$

To find a particular solution that satisfies (40), we need to choose c_j so that the quantities $c_j H^{(2)}_{|j|}(kR_1)$ be equal to the Fourier coefficients of the Dirichlet data in (40):

$$c_j = \frac{1}{H^{(2)}_{|j|}(kR_0)} \int_{-\pi}^{\pi} -e^{ikR_0\cos\theta} e^{-ij\theta} d\theta \quad j = 0, \pm 1, \pm 2, \ldots \tag{42}$$

The resulting exact solution with the coefficients c_j of (42) substituted into (41) is equivalent to the one given in [8].

To evaluate this solution, we replace the integral in (42) 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 (40) is smooth, the coefficients c_j of (42) are expected to decay very rapidly (exponentially). This is what we indeed observe, and even though the series (41) is formally infinite, in practice it appears sufficient to keep only about 30 of its leading coefficients (for $k = 8$) 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 (41). In the next section, we study convergence of our numerical approximations to this exact solution.

5.1.2 Grid Convergence and Computational Complexity

We compute the sound-soft scattered solution subject to boundary condition (40) on a sequence of eight grids and summarize the results in Table 1. The third column of Table 1 clearly demonstrates fourth order grid convergence of the proposed scheme. A slight slowdown of convergence on the finest grid, 4096×4096, should probably be attributed to the loss of significant digits that already starts to manifest itself when the error is about 10^{-10} and the computations are done with double precision (approximately 16 decimal digits). The fourth column of Table 1 shows the actual execution times needed to compute the solution on the grid (those do not include the time needed to evaluate the exact solution).[3] The fifth

[3] All the computations were performed on a 2×2.93 GHz Qaud-core Intel Xeon Mac Pro with 32 Gb of RAM, using the Intel Fortran Compiler Professional Edition for Mac OS X, Version 11.

Table 1 Grid convergence and CPU times for sound-soft scattering, $k = 8$

Grid, $M \times M$	L_∞ error	Conv. rate	CPU time, sec	time/$M^2 \ln M$	time/M^2
32×32	3.140×10^{-2}		3.100×10^{-4}	8.7351×10^{-8}	3.0273×10^{-7}
64×64	1.912×10^{-3}	4.0376	9.399×10^{-4}	5.5175×10^{-8}	2.2947×10^{-7}
128×128	1.169×10^{-4}	4.0317	3.431×10^{-3}	4.3160×10^{-8}	2.0941×10^{-7}
256×256	7.294×10^{-6}	4.0026	1.364×10^{-2}	3.7533×10^{-8}	2.0813×10^{-7}
512×512	4.553×10^{-7}	4.0019	5.831×10^{-2}	3.5656×10^{-8}	2.2243×10^{-7}
1024×1024	2.846×10^{-8}	3.9995	0.242	3.3296×10^{-8}	2.3079×10^{-7}
2048×2048	1.791×10^{-9}	3.9901	1.008	3.1520×10^{-8}	2.4033×10^{-7}
4096×4096	1.349×10^{-10}	3.731	4.028	2.8860×10^{-8}	2.4009×10^{-7}

Table 2 Behavior of the scheme for sound-soft scattering and various k

Grid dimension	k	L_∞ error
128×128	4.595	1.098×10^{-5}
256×256	8.0	7.293×10^{-6}
512×512	13.928	6.674×10^{-6}
1024×1024	24.249	6.854×10^{-6}
2048×2048	42.218	7.251×10^{-6}
4096×4096	73.501	7.866×10^{-6}

column of Table 1 shows that the execution time scales somewhat better than the theoretically predicted log-linear rate with respect to the total number of grid nodes (the log-linear rate characterizes the FFT). The sixth column of Table 1 shows that for low grid dimensions the scaling is even better than linear, which, perhaps, has to do with the cache and memory management in the computer. For higher grid dimensions, the CPU time grows slightly faster than linear yet still slower than log-linear.

5.1.3 Variation of k

As mentioned in Sect. 1, to maintain the same level of error for different values of the wavenumber k, the quantity $k^{p+1}h^p$ must remain constant. For a fourth order accurate method ($p=4$), we conclude, in particular, that if the grid is refined in all coordinate directions by a factor of 2, then the same level of error should be expected if the wavenumber k increases by a factor of $2^{4/5} \approx 1.741$. In Table 2, we present numerical results that corroborate this theoretical finding. Namely, we take one specific grid, 256×256, and $k = 8$ from Sect. 5.1.2 (this corresponds to $k^5 h_r^4 = 2^{15} 2^{-32} = 2^{-17}$), and then repeatedly change the grid dimension by a factor of 2 in each direction while varying the wavenumber k accordingly.

5.2 Sound-Hard Scattering

5.2.1 Exact Solution

We consider the same setup as in Sect. 5.1, $f = 0$ in (3), 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:

$$\left.\frac{\partial u(r,\theta)}{\partial r}\right|_{r=R_0} = -ik\cos\theta e^{ikR_0\cos\theta} \tag{43}$$

Differentiating (41) with respect to r, we obtain:

$$\frac{\partial v(r,\theta)}{\partial r} = \sum_{j=-\infty}^{\infty} c_j e^{ij\theta} k H_{|j|}^{(2)\prime}(kr) \tag{44}$$

Consequently, to satisfy the Neumann boundary condition (43), we choose the coefficients c_j according to

$$c_j = \frac{1}{kH_{|j|}^{(2)\prime}(kR_0)} \int_{-\pi}^{\pi} -ik\cos\theta e^{ikR_0\cos\theta} e^{-ij\theta} d\theta \quad j = 0, \pm 1, \pm 2, \ldots \tag{45}$$

Substituting the coefficients c_j of (45) into (41) we obtain the solution to the homogeneous Helmholtz equation on $r \geq R_0$ subject to the Neumann boundary condition (43). 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 (45) differ from zero within the machine precision. Hence, the exact solution is again obtained in the form of a truncated series (41).

5.2.2 Results of Computation

We compute the sound-hard scattered solution subject to boundary condition (43) on a sequence of eight grids and summarize the results in Table 3. Similarly to the case of the Dirichlet boundary condition, the third column of Table 3 clearly indicates a fourth order grid convergence of the proposed scheme. As far as the computational complexity, the results are also very similar to those of Sect. 5.1.2. For larger grids, the CPU time grows somewhat faster than linear yet slower than the log-linear law, which is characteristic of the FFT, see the fourth, fifth, and sixth columns of Table 3.

Moreover, in the case of sound-hard scattering we have also studied the behavior of the scheme for different values of k, and the results are very similar to those presented in Sect. 5.1.3.

Table 3 Grid convergence and CPU times for sound-hard scattering, $k = 8$

Grid, $M \times M$	L_∞ error	Conv. rate	CPU time, sec	time$/M^2 \ln M$	time$/M^2$
32×32	8.876×10^{-2}		3.400×10^{-4}	9.5804×10^{-8}	3.3203×10^{-7}
64×64	5.061×10^{-3}	4.1322	1.106×10^{-3}	6.4926×10^{-8}	2.7002×10^{-7}
128×128	3.089×10^{-4}	4.0342	4.186×10^{-3}	5.2657×10^{-8}	2.5549×10^{-7}
256×256	1.920×10^{-5}	4.0087	1.665×10^{-2}	4.5816×10^{-8}	2.5406×10^{-7}
512×512	1.198×10^{-6}	4.0016	6.959×10^{-2}	4.2554×10^{-8}	2.6546×10^{-7}
1024×1024	7.484×10^{-8}	4.0008	0.286	3.9350×10^{-8}	2.7275×10^{-7}
2048×2048	4.663×10^{-9}	4.0045	1.202	3.7586×10^{-8}	2.8658×10^{-7}
4096×4096	3.208×10^{-10}	3.861	4.787	3.4303×10^{-8}	2.8533×10^{-7}

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 (3) is compactly supported on the annulus (20). Otherwise, one cannot apply the ABC of Sects. 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

$$u(r,\theta) = p(r) \sum_{j=0}^{J} \frac{1}{2^j} e^{ij\theta} H^{(2)}(kr) \tag{46}$$

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

$$\begin{aligned} p(r) &= \begin{cases} 0, & r \leq R_0 \\ 1, & r \geq \frac{R_0+R_1}{2} \end{cases} \\ p' = p'' &= \cdots = p^{(6)}\big|_{r=R_0} = 0 \\ p' = p'' &= \cdots = p^{(6)}\big|_{r=\frac{R_0+R_1}{2}} = 0 \end{aligned} \tag{47}$$

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 (46), then $u(r,\theta)$ would have been a solution to the homogeneous Helmholtz equation (3). With the multiplier (47), 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 (47), $f(r,\theta)$ is compactly supported on a smaller annulus than (20), namely

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

5.3.2 Results of Computation

We reconstruct the test solution $u(r,\theta)$ of (46) numerically from the backward engineered right-hand side $f(r,\theta)$ on a sequence of eight grids and summarize the results in Table 4. As before, we observe a fourth order grid convergence. The only exception is the last line of Table 4. The breakdown of convergence is clearly attributable to the loss of significant digits when evaluating the error with double precision. Similar to the previous results the CPU time grows somewhat faster than linear and somewhat slower than log-linear as the total number of grid nodes increases. We also note that the absolute CPU times are somewhat higher in the case of inhomogeneous Helmholtz equation, especially on fine grids. The difference occurs because when there is a non-zero right-hand side on the entire grid, the FFT requires more CPU time and so has a greater influence on the total CPU time.

Table 4 Grid convergence and CPU times for the inhomogeneous Helmholtz equation, $k = 8$

Grid, $M \times M$	L_∞ error	Conv. rate	CPU time, sec	time$/M^2 \ln M$	time$/M^2$
32×32	1.541×10^{-4}		4.040×10^{-4}	1.1384×10^{-7}	3.9453×10^{-7}
64×64	9.465×10^{-6}	4.0251	1.218×10^{-3}	7.1501×10^{-8}	2.9736×10^{-7}
128×128	5.923×10^{-7}	3.9982	4.458×10^{-3}	5.6079×10^{-8}	2.7209×10^{-7}
256×256	3.699×10^{-8}	4.0011	1.766×10^{-2}	4.8595×10^{-8}	2.6947×10^{-7}
512×512	2.313×10^{-9}	3.9993	7.833×10^{-2}	4.7898×10^{-8}	2.9881×10^{-7}
1024×1024	1.445×10^{-10}	4.0006	0.326	4.4853×10^{-8}	3.1090×10^{-7}
2048×2048	9.515×10^{-12}	3.9247	1.384	4.3277×10^{-8}	3.2997×10^{-7}
4096×4096	5.857×10^{-12}	0.7000	5.699	4.0839×10^{-8}	3.3969×10^{-7}

6 Discussion

We have constructed 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. The 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.

To facilitate the solution of scattering problems that are initially formulated on an unbounded region, the scheme is supplemented by the exact nonlocal ABC that is specified at the outer boundary of the finite computational domain. The latter is obtained from the original unbounded domains by means of truncation. The ABC is built using the Fourier transform directly for the discretization. The accuracy of this ABC automatically matches that of the interior scheme, and it guarantees reflectionless propagation of all the outgoing waves. This ABC also couples naturally with the FFT-based solver (separation of variables) that we use for the scheme. This solver appears very efficient, because after the FFT has been performed in the azimuthal direction, the narrow bandwidth, which is due to the compact stencil, enables an easy application of the tri-diagonal elimination.

The performance of the scheme has been tested by solving several scattering problems. Numerical experiments corroborate the fourth order grid convergence and a (log-)linear computational complexity of the solver. Moreover, the method displays a correct behavior for large k, i.e., it maintains the same level of error provided that $k^5 h^4 = \text{const}$.

The compact fourth order accurate scheme that we have designed in this paper is built on a uniform grid. Obtaining a similar scheme on a non-uniform grid will require a modification of our approach. In many cases though, the scheme with a variable grid size can be re-interpreted as a scheme with a constant grid size, but for a new equation with appropriately changed variable coefficients. This issue will be studied in the future.

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