

Compact Schemes for Acoustics in the Frequency Domain

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Abstract

This article is concerned with the fourth-order compact scheme for an accurate simulation of acoustic waves in the frequency domain. The compact schemes are known for a long time; however, they have shown difficulties, in particular, in dealing with general boundary conditions. This article introduces a new formulation for the compact scheme for the Helmholtz equation and an effective strategy of incorporating absorbing boundary conditions. It has been numerically verified that the resulting compact scheme is fourth-order in general heterogeneous media and improves the accuracy of the numerical solution dramatically, by more than two-digits, over the standard second-order scheme.

1. Introduction

The propagation of waves in realistic media is often formulated in an unbounded domain. Such a problem can be solved by first truncating the domain into a tractable finite domain, imposing a suitable absorbing boundary condition (ABC) on the artificial boundary, and then solving the resulting problem using discretization methods (e.g., finite differences and finite element methods).

Let $\Omega \subset \mathbb{R}^2$ be a rectangular domain with its boundary $\Gamma = \partial\Omega$. Consider the following Helmholtz problem

$$\begin{aligned} \text{(a)} \quad & -\Delta u - K^2(\mathbf{x})u = f(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ \text{(b)} \quad & \frac{\partial u}{\partial \nu} + i\alpha(\mathbf{x})u = 0, \quad \mathbf{x} \in \Gamma, \end{aligned} \tag{1.1}$$

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where i is the imaginary unit, ν is the unit outward normal from Γ , f denotes the source, and the coefficients $K(\mathbf{x})$ and $\alpha(\mathbf{x})$ are given as

$$\begin{aligned} K &= \omega/v, \\ \alpha &= \alpha_r - i\alpha_i, \quad \alpha_r > 0, \quad \alpha_i \geq 0, \end{aligned}$$

where v denotes the sound velocity and ω is the angular frequency. The coefficient α is assumed to be properly chosen such that (1.1.b) represents the first-order ABC that allows normally incident waves to pass out of Ω transparently. Problem (1.1) models the propagation of time-harmonic waves, polarized electromagnetic waves, scattering problems, seismic waves, and ocean acoustics.

In the simulation of acoustic waves in the frequency domain, the second-order schemes requires to choose 25-40 grid points per wavelength for the numerical solutions of an acceptable accuracy for various applications [7]. So the problem size becomes too large to solve even in modern high-performance computers, in particular, for high frequency applications. This article studies *compact schemes* for the numerical solution of the Helmholtz problem. The 9-point compact difference formulas have been known for many years [2]. In recent years, many authors have derived fourth-order finite difference (FD) approximations to solve various partial differential equations (PDEs); see e.g. [1, 3, 6, 8, 9, 10] and references therein. These fourth-order schemes have been derived by substituting the Taylor series expansions at neighboring grid points (up to order four) into the PDE and by obtaining the representation for the solution of the PDE. Thus the derivation of compact schemes and its extensions to 3D and time-dependent problems are straightforward but tedious; the symbolic derivation has occasionally saved such human efforts [4]. However, these *standard* compact schemes show the following drawbacks:

- It is difficult to incorporate more general boundary conditions such as Neumann and mixed-type boundary conditions. Up to date, compact schemes have been applied either to problems of Dirichlet boundary conditions or with lower-order/one-sided difference approximations for general boundary conditions.
- Properties of the resulting algebraic system are hardly known for most cases.

In this article, we present a new approach for the derivation of fourth-order compact schemes for an accurate solution of the Helmholtz equation (1.1).

2. Preliminaries

In this section, we review the standard compact schemes. For simplicity, let $\Omega = (0, 1)^2$, the unit square in \mathbb{R}^2 . Let n_x and n_y be the numbers of equally partitioned elements in the x - and y -directions, respectively, and $\{\mathbf{x}_{ij} := (ih_x, jh_y)\}$ the grid

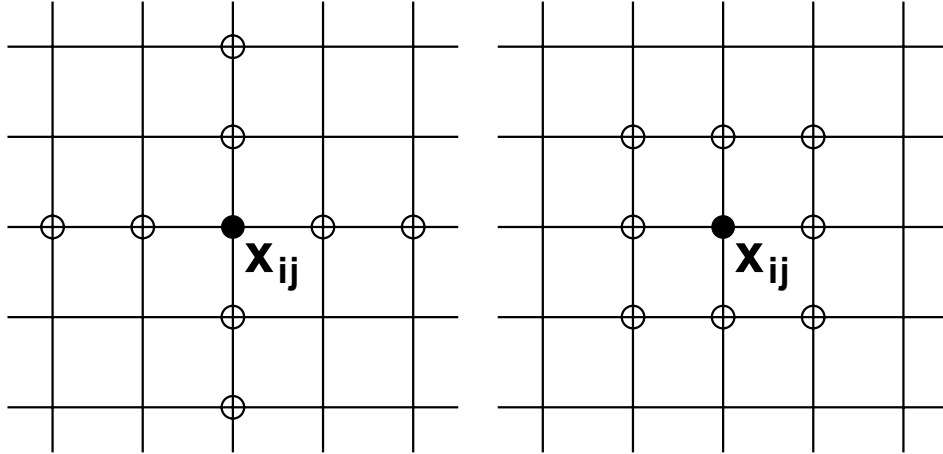


Figure 1: Stencils for $-\Delta u$ at the reference point \mathbf{x}_{ij} for the conventional fourth-order scheme (left) and the fourth-order compact scheme (right).

points in Ω , where $h_x = 1/n_x$ and $h_y = 1/n_y$, for some positive integers n_x and n_y . Define $u_{ij} = u(\mathbf{x}_{ij})$ and $h = \max(h_x, h_y)$.

The conventional fourth-order scheme for $-\Delta u$ incorporates five points in each direction, as shown in Figure 1 (left). The fourth-order compact scheme is formulated on a compact set of nine grid points as in Figure 1 (right). To derive the nine-point fourth-order compact scheme, the solution u is assumed to satisfy the Taylor series expansion

$$u(\xi, \eta) = \sum c_{pq} \xi^p \eta^q \quad (2.1)$$

locally on the local mesh points, with a local center at the reference grid point $(0, 0)$ and the nearest eight neighboring grid points. The force term f is also assumed to have a similar Taylor series expansion locally at the grid points under consideration. The fourth-order compact scheme can be obtained by substituting the Taylor series expansions into the differential equation and by setting all the Taylor series coefficients of u_{pq} and f_{pq} to be zero for $(p + q) > 4$. When $h = h_x = h_y$, the resulting compact scheme for the Poisson equation at the reference grid point \mathbf{x}_{ij} reads (see e.g. [5])

$$\frac{1}{h^2} \begin{bmatrix} \frac{-1}{6} & \frac{-2}{3} & \frac{-1}{6} \\ \frac{-2}{3} & \frac{10}{3} & \frac{-2}{3} \\ \frac{-1}{6} & \frac{-2}{3} & \frac{-1}{6} \end{bmatrix} u_{ij} \approx \begin{bmatrix} 0 & \frac{1}{12} & 0 \\ \frac{1}{12} & \frac{2}{3} & \frac{1}{12} \\ 0 & \frac{1}{12} & 0 \end{bmatrix} f_{ij} \quad (2.2)$$

corresponding to the nine point stencil. This formula is often called ‘‘Mehrstellen’’ and has been known for a long time [2]. The idea for the derivation of Mehrstellen has been applied to various PDEs along with the development of efficient computational

algorithms; see [3, 6, 8, 9, 10] and references therein. However, none of these articles have considered *compact* fourth-order approximations for Neumann/mixed-type boundary conditions. Furthermore, properties of the resulting matrices obtainable from the fourth-order compact schemes are hardly known, in particular, when the problem coefficients are not constant and/or when $h_x \neq h_y$.

3. The Compact Scheme

3.1. A new derivation

For a simpler presentation, we first define $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$ to be the central second-order difference operator for $-\Delta$, where

$$\begin{aligned}\mathcal{L}_1 u_{ij} &:= \frac{-u_{i-1,j} + 2u_{ij} - u_{i+1,j}}{h_x^2}, \\ \mathcal{L}_2 u_{ij} &:= \frac{-u_{i,j-1} + 2u_{ij} - u_{i,j+1}}{h_y^2}.\end{aligned}\tag{3.1}$$

Then, we have

$$\begin{aligned}-\Delta u(\mathbf{x}_{ij}) &\approx \mathcal{L}u_{ij} \\ &+ \frac{h_x^2}{12}u_{xxxx}(\mathbf{x}_{ij}) + \frac{h_y^2}{12}u_{yyyy}(\mathbf{x}_{ij}) + \mathcal{O}(h^4).\end{aligned}\tag{3.2}$$

To obtain a fourth-order scheme, one has to approximate u_{xxxx} and u_{yyyy} in (3.2) by FD schemes of at least second-order. Also the utilized grid points must be on the 9-point box enclosing the reference point \mathbf{x}_{ij} . Note that the equation (1.1.a) reads

$$u_{xx} = -u_{yy} - K^2u - f, \quad u_{yy} = -u_{xx} - K^2u - f.$$

By differentiating the equations and approximating the resulting equations by the central second-order scheme, we have

$$\begin{aligned}u_{xxxx}(\mathbf{x}_{ij}) &= (-u_{yy} - K^2u - f)_{xx}(\mathbf{x}_{ij}) \\ &\approx -\mathcal{L}_1[\mathcal{L}_2 u_{ij} - (K^2u)_{ij} - f_{ij}] + \mathcal{O}(h^2), \\ u_{yyyy}(\mathbf{x}_{ij}) &= (-u_{xx} - K^2u - f)_{yy}(\mathbf{x}_{ij}) \\ &\approx -\mathcal{L}_2[\mathcal{L}_1 u_{ij} - (K^2u)_{ij} - f_{ij}] + \mathcal{O}(h^2).\end{aligned}\tag{3.3}$$

Thus from (3.2) and (3.3), the *fourth-order compact scheme* for $-\Delta u - K^2u$ can be formulated as

$$\begin{aligned}(-\Delta u - K^2u)(\mathbf{x}_{ij}) &\approx \left(\mathcal{L}_1 + \mathcal{L}_2 - \frac{h_x^2}{12}\mathcal{L}_1\mathcal{L}_2 - \frac{h_y^2}{12}\mathcal{L}_2\mathcal{L}_1 \right) u_{ij} \\ &- \left(1 - \frac{h_x^2}{12}\mathcal{L}_1 - \frac{h_y^2}{12}\mathcal{L}_2 \right) (K^2u)_{ij} \\ &+ \left(\frac{h_x^2}{12}\mathcal{L}_1 + \frac{h_y^2}{12}\mathcal{L}_2 \right) f_{ij} + \mathcal{O}(h^4).\end{aligned}\tag{3.4}$$

The corresponding fourth-order algorithm for the Helmholtz equation in 2D reads: Find \mathbf{u} ($:= \{u_{ij}\}$) satisfying

$$\mathcal{P}\mathbf{u} = \mathbf{b}, \quad (3.5)$$

where

$$\begin{aligned} \mathcal{P} &:= \left(1 - \frac{h_y^2}{12}\mathcal{L}_2\right)\mathcal{L}_1 + \left(1 - \frac{h_x^2}{12}\mathcal{L}_1\right)\mathcal{L}_2 \\ &\quad - \left(1 - \frac{h_x^2}{12}\mathcal{L}_1 - \frac{h_y^2}{12}\mathcal{L}_2\right)K^2, \\ \mathbf{b} &:= \left(1 - \frac{h_x^2}{12}\mathcal{L}_1 - \frac{h_y^2}{12}\mathcal{L}_2\right)f. \end{aligned}$$

Here we have to incorporate the boundary condition appropriately, which will be discussed in the next subsection. Note that $(1 - \frac{h_x^2}{12}\mathcal{L}_1)$ and $(1 - \frac{h_y^2}{12}\mathcal{L}_2)$ are 3-point averaging operators having the weights $(\frac{1}{12}, \frac{5}{6}, \frac{1}{12})$ in the x - and y -directions, respectively, and $(1 - \frac{h_x^2}{12}\mathcal{L}_1 - \frac{h_y^2}{12}\mathcal{L}_2)$ is the averaging operator whose weights are $\frac{2}{3}$ and $\frac{1}{12}$ respectively at the reference point \mathbf{x}_{ij} and its four neighboring points. When $K = 0$ and $h_x = h_y$, the above scheme turns out to be Mehrstellen (2.2).

3.2. The absorbing boundary condition

In this subsection, we incorporate a fourth-order approximation of the ABC (1.1.b) into the algebraic system (3.5). One may try fourth-order one-sided approximations for the normal derivative u_ν ; however, it will destroy the compactness structure near the boundary. A *compact* approximation of the boundary condition is preferred.

We begin with defining

$$\mathcal{D}_x u_{ij} := \frac{u_{i+1,j} - u_{i-1,j}}{2h_x}, \quad \mathcal{D}_y u_{ij} := \frac{u_{i,j+1} - u_{i,j-1}}{2h_y},$$

and letting \mathcal{D}_x^B and \mathcal{D}_y^B be the restrictions at boundary points for \mathcal{D}_x and \mathcal{D}_y , respectively. Then,

$$u_x(\mathbf{x}_{ij}) \approx \mathcal{D}_x^B u_{ij} - \frac{h_x^2}{6} u_{xxx}(\mathbf{x}_{ij}) + \mathcal{O}(h_x^4). \quad (3.6)$$

Since $u_{xxx} = (-u_{yy} - K^2 u - f)_x$, we have

$$\begin{aligned} u_{xxx} &\approx \mathcal{D}_x^B \left(\mathcal{L}_2 u - \frac{1}{2} K^2 u - f \right) \\ &\quad - \frac{1}{2} (K^2 u)_x(\mathbf{x}_{ij}) + \mathcal{O}(h^2), \end{aligned} \quad (3.7)$$

and therefore (3.6) reads

$$\begin{aligned} u_x(\mathbf{x}_{ij}) &\approx \mathcal{D}_x^B \left(1 - \frac{h_x^2}{6} \mathcal{L}_2 \right) u_{ij} + \frac{h_x^2}{12} \mathcal{D}_x^B (K^2 u)_{ij} \\ &\quad + \frac{h_x^2}{12} (K^2 u)_x(\mathbf{x}_{ij}) + \frac{h_x^2}{6} \mathcal{D}_x^B f_{ij} + \mathcal{O}(h^4). \end{aligned} \quad (3.8)$$

It should be noticed that in (3.7), only the half of $(K^2u)_x$ is approximated by a second-order *difference* and the other half is remained as a *derivative*; the reader will figure out the reason soon.

Define

$$\begin{aligned}\mathcal{L}_\tau &:= \begin{cases} \mathcal{L}_2, & \text{if } \nu = (\pm 1, 0), \\ \mathcal{L}_1, & \text{if } \nu = (0, \pm 1), \end{cases} \\ \mathcal{D}_\nu^B &:= (\mathcal{D}_x^B, \mathcal{D}_y^B) \cdot \nu, \\ h_\nu &:= |(h_x, h_y) \cdot \nu|.\end{aligned}$$

Then, (3.8) and its analogues can be written as

$$\begin{aligned}u_\nu(\mathbf{x}_{ij}) &\approx \mathcal{D}_\nu^B \left(1 - \frac{h_\nu^2}{6} \mathcal{L}_\tau \right) u_{ij} + \frac{h_\nu^2}{12} \mathcal{D}_\nu^B (K^2u)_{ij} \\ &\quad + \frac{h_\nu^2}{12} (K^2u)_\nu(\mathbf{x}_{ij}) + \frac{h_\nu^2}{6} \mathcal{D}_\nu^B f_{ij} + \mathcal{O}(h^4),\end{aligned}\tag{3.9}$$

for $\mathbf{x}_{ij} \in \Gamma$. Note that from the ABC (1.1.b), one can have

$$(K^2u)_\nu = 2KK_\nu + K^2u_\nu = 2KK_\nu - i\alpha K^2u.\tag{3.10}$$

Thus it follows from (3.9) and (3.10) that the fourth-order approximation of the ABC at $\mathbf{x}_{ij} \in \Gamma$ reads

$$\begin{aligned}\mathcal{D}_\nu^B \left(1 - \frac{h_\nu^2}{6} \mathcal{L}_\tau \right) u_{ij} &+ \frac{h_\nu^2}{12} \mathcal{D}_\nu^B (K^2u)_{ij} \\ &+ \left[i\alpha \left(1 - \frac{h_\nu^2}{12} K^2 \right) + \frac{h_\nu^2}{6} KK_\nu \right] u_{ij} \\ &\approx -\frac{h_\nu^2}{6} \mathcal{D}_\nu^B f_{ij} + \mathcal{O}(h^4).\end{aligned}\tag{3.11}$$

Now, to see how (3.5) can incorporate (3.11), we have to look at the equations in detail. Consider a reference point \mathbf{x}_{ij} on the left edge, Γ_1 , for example. Then when $h = h_x = h_y$, the coefficients of the contribution from the three points outside the domain become

$$\begin{bmatrix} \frac{-1}{6h^2} \\ \frac{-2}{3h^2} - \frac{1}{12} \cdot K_{i-1,j}^2 \\ \frac{-1}{6h^2} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \frac{1}{2h} \cdot \frac{1}{6} \\ \frac{1}{2h} \cdot \frac{2}{3} + \frac{h^2}{12} \cdot \frac{K_{i-1,j}^2}{2h} \\ \frac{1}{2h} \cdot \frac{1}{6} \end{bmatrix}\tag{3.12}$$

for (3.5) and (3.11), respectively. Thus one can easily check that the right-hand column in (3.12) multiplied by $-2/h_x$ is exactly the same as the left-hand column. This implies that the $(2/h_x)$ -multiple of (3.11) can be added to (3.5) for the *outer bordering*, the inward contribution of outside coefficients via the reflection along the

boundary. Since the inward coefficients of (3.11) is the negation of the outside ones, the outer bordering would double the inward coefficients of (3.5), canceling out the first two terms in the left side of (3.11). When $h_x = h_y$, this procedure can be applied to all four edges, except for the four corner points; the second-order scheme can be applied at the corners.

The overall scheme incorporating the outer bordering reads

$$\widehat{\mathcal{P}} \mathbf{u} = \widehat{\mathbf{b}}, \quad (3.13)$$

where

$$\begin{aligned} \widehat{\mathcal{P}} &:= \left(1 - \frac{h_y^2}{12} \widehat{\mathcal{L}}_2\right) \widehat{\mathcal{L}}_1 + \left(1 - \frac{h_x^2}{12} \widehat{\mathcal{L}}_1\right) \widehat{\mathcal{L}}_2 \\ &\quad - \left(1 - \frac{h_x^2}{12} \widehat{\mathcal{L}}_1 - \frac{h_y^2}{12} \widehat{\mathcal{L}}_2\right) K^2 \\ &\quad + \frac{2}{h_\nu} \left[i\alpha \left(1 - \frac{h_\nu^2}{12} K^2\right) + \frac{h_\nu^2}{6} K K_\nu \right]^B, \quad \mathbf{x} \in \overline{\Omega}, \\ \widehat{\mathbf{b}} &:= \left(1 - \frac{h_x^2}{12} \widehat{\mathcal{L}}_1 - \frac{h_y^2}{12} \widehat{\mathcal{L}}_2 - \frac{h_\nu}{3} \mathcal{D}_\nu^B\right) f, \end{aligned}$$

where $\widehat{}$ on the matrices indicate the inward reflection of the outside coefficients along the boundary and the superscript B denotes the boundary restriction. The above scheme is fourth-order at the boundary grid points, except for the four corner points, when $h_x = h_y$; it is always fourth-order for interior points.

4. Numerical Experiments

This section shows numerical results for solving the Helmholtz equation by the fourth-order compact scheme (3.13). It is not intended to present efficient iterative solvers for the resulting algebraic system; the CGNR (the conjugate gradient method applied to the normal equation) is adopted with an ILU (incomplete LU factorization) preconditioner. Here we will focus on the accuracy of the compact scheme.

For the accuracy analysis, we choose $\Omega = (0, 1)^2$ and select the following solution

$$u_{\text{true}}(x, y) = \phi(x)\phi(y), \quad \phi(x) = e^{i\omega(x-1)} + e^{-i\omega x} - 2,$$

where ω is the angular frequency, i.e., $\omega = 2\pi\mu$, where μ is the frequency. Then the source $f(x, y)$ can be set for u_{true} to satisfy (1.1.a) exactly. Note that u_{true} satisfies the ABC (1.1.b) when $\alpha = \omega$. We choose three different velocities

$$\begin{aligned} v_1(x, y) &= 2, \\ v_2(x, y) &= 1.6 + |\sin(3\pi x) \cdot \cos(4\pi y)|, \\ v_3(x, y) &= \begin{cases} 2, & \text{if } x \leq 0.5, \\ 2 + \sin(5\pi xy), & \text{else.} \end{cases} \end{aligned} \quad (4.1)$$

Table 1: The least-squares error for the standard 5-point scheme and the 9-point compact scheme, for $\mu = 10$ ($\omega = 20\pi$).

$n_x \times n_y$	5-Point			9-Point		
	$v = v_1$	$v = v_2$	$v = v_3$	$v = v_1$	$v = v_2$	$v = v_3$
100 \times 100	2.70E-01	3.08E-01	5.74E-01	4.99E-03	5.64E-03	1.11E-02
200 \times 200	6.72E-02	7.46E-02	1.41E-01	3.12E-04	3.58E-04	6.91E-04
200 \times 100	1.93E-01	1.94E-01	4.21E-01	3.54E-03	3.38E-03	7.89E-03
400 \times 200	4.87E-02	4.77E-02	1.04E-01	2.21E-04	2.13E-04	4.82E-04

In Table 1, we present the least-squares errors for the 5-point and compact schemes. We select the frequency $\mu = 10$ (thus, $\omega = 20\pi$). As one can see from the table, the compact scheme computes the solution in fourth-order accuracy, although the velocity is not homogeneous and although the mesh elements are not squares ($h_x \neq h_y$). For the case $h_x \neq h_y$, the compact scheme is not fourth-order along the boundary. However, its overall accuracy turns out to be fourth-order; the accuracy degradation from the boundary dose not seem to affect the overall accuracy to be altered visibly. The fourth-order compact scheme improves the solution accuracy dramatically, at least two-digit for problems of reasonable sizes, over the second-order scheme. We have found from various experiments that it suffices to choose 6-12 grid points per wavelength for an acceptable accuracy.

5. Conclusions and Discussion

The fourth-order compact scheme has been derived for the numerical solution of the Helmholtz equation in 2D. Strategies for incorporating a fourth-order compact approximation of the absorbing boundary condition is fully discussed. When $h_x = h_y$, the resulting scheme is analyzed to be fourth-order (except for the corner points). It has been observed from various numerical experiments that the compact scheme shows a fourth-order accuracy, in general heterogeneous media, although the condition $h_x = h_y$ is violated. Extensions to 3D problems and/or problems of general diffusion (density) coefficients are straightforward.

Acknowledgment

The computational code utilized in this article has been implemented for the modelcode library at the University of Kentucky: *Graduate Research and Applications for Differential Equations* (GRADE), and is available through internet access to www.ms.uky.edu/~skim/GRADE/ or by asking the author (skim@ms.uky.edu).

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