Abstract. In this paper new innovative fourth order compact schemes for Robin and Neumann boundary conditions have been developed for boundary value problems of elliptic PDEs in two and three dimensions. Different from traditional finite difference operator approach, which may not work for flux type of boundary conditions, carefully designed underdetermined coefficient methods are utilized in developing high order compact (HOC) schemes. The new methods not only can be utilized to design HOC schemes for flux type of boundary conditions but can also be applied to general elliptic PDEs including Poisson, Helmholtz, diffusion-advection, and anisotropic equations with linear boundary conditions. In the new developed HOC methods, the coefficient matrices are generally M-matrices, which guarantee the discrete maximum principle for well-posed problems, so the convergence of the HOC methods. The developed HOC methods are versatile and can cover most of high order compact schemes in the literature. The HOC methods for Robin boundary conditions and for anisotropic diffusion and advection equations with Robin or even Dirichlet boundary conditions are likely the first ones that have ever been developed. With the help of pseudo-inverse, or SVD solutions, we have also observed that the developed HOC methods usually have smaller error constants compared with traditional HOC methods when applicable. Non-trivial examples with large wave numbers and oscillatory solutions are presented to confirm the performance of the new HOC methods.

AMS Subject Classification 2000 65N06, 65N12.

Keywords: Poisson/Helmholtz, diffusion-advection/anisotropic equations, high order compact method, HOC method for flux BCs, discrete maximum principle.

1. Introduction. The original motivation of this research is to develop fourth order compact finite difference schemes for flux boundary conditions (BCs) such as Neumann and Robin for Poisson/Helmholtz equations for which one can apply the standard fourth order compact scheme at interior grid points. After initial success in developing HOC schemes for Robin/Neumann boundary conditions, we have found out that the methodology can be applied to general elliptic boundary value problems (BVP) of the following

\[
\begin{align*}
\nabla \cdot (A \nabla u) + a \cdot \nabla u + Ku &= f(x), \\
\left. u \right|_{\partial R_1} &= u_1(x), \\
\left. (A \nabla u \cdot n + \sigma u(x)) \right|_{\partial R_2} &= g(x),
\end{align*}
\]

with a few line changes in the computer codes, where \( x \) is a point in a rectangular domain \( \mathcal{R} \), \( n \) is the unit normal at the boundary pointing outside of the domain. We assume that \( A, a, K, \) and \( \sigma \) are constants, although the methodology developed in this paper can be applied to variable coefficients as well at a cost. We assume that the source term \( f(x) \in C^\nu \) and the solution \( u(x) \in C^{4+\nu} \) for a \( \nu > 0 \). For a fourth order method, we need \( \nu = 2 \) for the convergence proof. The condition \( \sigma \geq 0 \) is needed to guarantee the well-posedness of the boundary value problem. When \( \sigma = 0 \), we have a Neumann boundary condition.

One of advantages of a compact higher order method is that fewer grid points can be used for the same order accuracy as a lower order method; therefore, a smaller resulting system of algebraic equations needs to be solved. This is significant for three or higher dimensional problems to relieve the so-called memory bottleneck. Also, a compact higher order method maybe needed for highly oscillatory solutions, particularly for wave scattering characterized by Helmholtz equations with large wave numbers \( \sqrt{K} \). Furthermore, high order compact methods are important for problems with an infinite domain when a mesh size is relatively large. Moreover, HOC methods have less grid orientation effects compared with standard finite difference schemes since more neighboring grid points in different directions rather than just coordinates ones are involved. On the other hand, it is challenging to develop HOC schemes for flux BCs since there is few information outside of the domain.

One of the earlier fourth order compact finite difference (FD) schemes for Poisson equations can be found in [18]. The authors state that the fourth order compact method developed in [18] becomes third order for Neumann boundary conditions, which can be actually validated in this paper, see Section 3. Other early work can be found in [2, 7, 9, 27] and a few others. A commonly used fourth order compact finite difference

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scheme for Poisson equations, or Helmholtz equations in 2D can be found in [13, 27, 28], for example. For a Helmholtz equation with a Dirichlet boundary condition, one can simply treat the \( K u \) term as an external force in the discretization, which does not work for Neumann or Robin boundary conditions, and destroy the M-matrix property for a non-zero \( K \).

In deriving HOC schemes, often finite difference operators are employed dimension by dimension in discretizing a PDE. At the boundary of a rectangular domain, Dirichlet boundary have no effect on the accuracy of high order compact schemes. However, for many applications, flux type boundary conditions are provided. For example, in a shear flow, often no-slip \( (u = 0) \) boundary conditions are prescribed at the top and bottom walls, while at the inlet, a flux condition is prescribed. A second order accurate scheme to deal with flux boundary conditions would ruin global fourth order accuracy if a fourth order discretization is utilized in the interior. Research on HOC schemes for flux type boundary conditions can be found, for example, in [4, 6, 23] for time dependent problems based on operator splitting approaches, for Poisson and Helmholtz or wave equations [1, 5, 12, 17, 25, 26], other related HOC methods and applications [3, 10, 11, 16, 19, 23, 24, 29, 30], and for diffusion and advection equations [1, 7, 15]. However, few can be found in the literature for general elliptic partial differential equations with flux boundary conditions. Thus, it is a important problem to develop HOC schemes, particularly fourth order, for flux type of boundary conditions (Neumann or Robin).

There are two important considerations in deriving HOC schemes. The first one is the consistency, which is relatively easy to confirm. The second one is the stability, which is more challenging to address and often left out in discussions especially for elliptic PDEs in some of research in the literature. One of tools to ensure the stability is to check whether the coefficient matrix of the system of equations is an M-matrix or not. The consistence condition plus an M-matrix (stronger stability) condition will lead to the convergence of the method, see for example, [20].

In this paper, we propose a completely new approach in constructing HOC finite difference schemes for Poisson, Helmholtz, and diffusion-advection equations with constant coefficients on rectangular domains with Dirichlet, Neumann, or Robin boundary condition along a part of boundary of the domain. The idea is to use linear combinations of the solution values \((U_{ij} \text{ or } U_{ijk})\), the source term values \((f_{ij} \text{ or } f_{ijk})\), and the flux type of boundary condition restricted to the grid points in the compact finite difference stencil. The undetermined coefficients are chosen such that the local truncation errors can be as small as possible in magnitude, \(O(h^4)\) in interior and \(O(h^3)\) at the boundary, while maintaining the discrete maximum principle, that is, the coefficient matrix is an M-matrix when \(K \leq 0\). We summarize our new HOC methods in this paper below:

1) 4th order compact method for Poisson/Helmholtz equations with Neumann or Robin BCs;
2) 4th order compact method for diffusion and advection equations with constant coefficients with Dirichlet, Neumann, or Robin BCs;
3) 4th order compact method for anisotropic diffusion and advection equations with constant coefficients with Dirichlet, Neumann, or Robin BCs;
4) super 3rd order compact methods for above equations and BCs without \(f\)-extensions.

In the first three items, we assume that we can extend the source term \((f)\) to one grid line (2D) or surface (3D) outside of the boundary with \(O(h^3)\) accuracy. The extension can be easily done either continuously or discretely. For a Poisson equation, we just need to extend one \(f\) value for both 2D and 3D problems. If one prefers not to extend the source term, then there is not enough degree of freedom for fourth order compact schemes. Our HOC methods can ensure a super-third order convergence that are accurate to \(O(h^4)\) for all fourth order polynomials except for the \(x^4\) and \(y^4\) terms, which is referred as the super-third order methods in this paper.

We think the proposed new strategy is quite versatile. Just a few lines of modifications to the computer codes are needed for the different problems mentioned above. We also think that most of HOC schemes in the literature can be included in the framework of our method from the definition of HOC schemes even though the derivations may be different. The designed HOC schemes are recommended for Poisson/Helmholtz equations, diffusion and advection equations, anisotropic PDEs with constant coefficients since the finite difference coefficients just need to be computed once or twice. The proposed methods can be applied to PDEs with variable coefficients, but the computational costs may be too high to be practical. For variable coefficients problems, a Richardson extrapolation approach [29] may be the most economical way to get a fourth order method, although it would not be compact anymore.

The developed new methods can be and have been applied to Helmholtz type equations \((K > 0)\). When
$K \leq 0$, then the proposed methods always work with strict error bounds; if $K > 0$, then the proposed methods always work if $h$ is smaller enough. The computed solutions have the designed order of convergence but the error constant is promotional to $K$. If $h$ is not smaller enough and $K$ is large, the developed methods work fine as long as the coefficient matrix $A_h$ is not singular; that is, $K$ is not an eigenvalue of $A_h$, for which the probability is one. We do not have a uniform error bound in this case though and the error depends on $\| (A_h)^{-1} \|$. The rest of the paper is organized as follows. In the next section, we explain the algorithm for Poisson/Helmholtz equations with a Neumann/Robin boundary condition along part of a boundary. In Section 3, we explain the super-third algorithm and present numerical test results and comparisons. In Section 4, we discuss the fourth order compact scheme for diffusion and advection equations with constant coefficients. In Section 5, we discuss the HOC schemes for anisotropic diffusion and advection equations for Dirichlet (fourth-order) and flux (super-third) boundary conditions. In Section 6, we discuss the fourth order compact scheme for flux boundary conditions in three dimensions followed with a numerical example. We conclude in the last section.

2. Constructing 4th-order compact schemes for Poisson/Helmholtz equations with a flux BC using f-extension. We first construct a fourth order compact scheme for a Helmholtz (including Poisson when $K = 0$) equation on a rectangular domain in 2D. Without loss of generality and for the convenience of presentation, we assume that the domain $\mathcal{R}$ is a square $[x_l, x_r] \times [y_l, y_r]$. We use a uniform mesh

\begin{align}
   x_i = x_l + ih, \quad i = 0, 1, \ldots, N; \quad y_j = y_l + jh, \quad j = 0, 1, \ldots, N.
\end{align}

In an interior grid point, the classical compact nine-point finite difference stencil, the finite difference coefficients and the right hand sides are illustrated in Figure 1, see for example, [13, 28]. The fourth order compact scheme can be written as

\begin{align}
   (L_h + KM_h) U_{ij} = M_h f_{ij},
\end{align}

at an interior grid point $(x_i, y_j)$, where $L_h$ is the discrete nine-point Laplacian whose coefficients at four corners are $\frac{1}{6h^2}$, at east-north-south-west grid points are $\frac{4}{6h^2}$, and at the center is $-\frac{20}{6h^2}$; $M_h$ is an averaging operator whose coefficients at east-north-south-west grid points are $\frac{1}{12}$, and at the center is $\frac{8}{12}$, that is,

\begin{align}
   M_h f_{ij} = \frac{1}{12} \left( f_{i-1,j} + f_{i+1,j} + f_{i,j-1} + f_{i,j+1} + 8f_{i,j} \right),
\end{align}

where $f_{ij} = f(x_i, y_j)$ and so on, see Figure 1 for an illustration. Assume that the coefficient matrix of the finite difference equation is $A_h$. Then, $-A_h$ is an M-matrix if $K \leq 0$ and $4/(6h^2) + K/12 \geq 0$, i.e. $1/h^2 + K/8 \geq 0$. There are several definitions of an M-matrix in the literature. We quote the definition from [8] below.
The sign conditions (2.4) and (2.5) are easy to check, but not so for the condition (2.6). We combine Theorem 6.4.10 and Lemma 6.4.12 from [8] to have the following lemma to state an equivalent definition of an M-matrix.

**Lemma 2.2.** Let the matrix \( \mathbf{A} \in \mathbb{R}^{n \times n} \) be irreducibly weakly diagonally dominant with at least one row being strictly. If the sign conditions (2.4) and (2.5) are satisfied, then \( \mathbf{A} \) is an M-matrix. Furthermore, if \( \mathbf{A} = \mathbf{A}^T \), then \( \mathbf{A} \) is also symmetric positive definite.

From the definitions of \( \mathbf{L}_h, \mathbf{M}_h \) in (2.2) and Lemma 2.2, we know that the coefficient matrix \((-A_h)\) of the finite difference equations is an M-matrix if \( K \leq 0 \) and \( 1/h^2 + K/8 \geq 0 \). The local truncation error at an interior grid point \((x_i, y_j)\) is defined as

\[
T^h_{ij} = (L_h + K \mathbf{M}_h) u(x_i, y_j) - M_h f(x_i, y_j),
\]

which is of \( O(h^4) \) if \( u \in C^6(\mathbb{R}) \). Thus, the global error is bounded by \( \|E_h\|_{\infty} = \|u(x_i, y_j) - U_{ij}\|_{\infty} \leq C h^4 \) if a Dirichlet boundary condition is specified.

Now we consider a Robin boundary condition \((\partial u/\partial n + \sigma u)|_{x=x_0} = g(y)\) to explain our idea and the new algorithm. Note that \( \mathbf{n} = (-1, 0) \) and \( \partial u/\partial x = -\partial u/\partial n \) at the boundary \( x = x_0 \). We assume that we know the source term \( f(x, y) \) at \( x = x_0 - h \), or we can use a quadratic extension that is third order accurate. In the next section, we will explain a super-third order compact algorithm that does not need to use \( f(x, y) \) at \( x = x_0 - h \).

A compact FD scheme at a boundary grid point \((x_0, y_j)\), \( j = 1, 2, \ldots, N-1 \) can be written as

\[
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} U_{i+i_k,j+j_k} = \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} f(x_{i+i_k}, y_{j+j_k}) + \sum_{j_k=-1}^{1} \gamma_{j_k} g(y_{j+j_k}),
\]

(2.8)

where \( i = 0 \) throughout this section, \( \alpha_{i_k,j_k} \) \((i_k = 0, 1, j_k = -1, 0, 1)\), \( \beta_{i_k,j_k} \) \((i_k = -1, 0, 1, j_k = -1, 0, 1)\), and \( \gamma_{j_k} \) \((j_k = -1, 0, 1)\) are undetermined coefficients. We leave the index \( i \) in the formulas so that the derivation can be applied to interior grid points as well for other problems discussed in the later sections. Thus, we have 6 coefficients for \( U_{ij} \), 9 coefficients for \( f_{ij} \), and 3 coefficients for \( g(y_j) \). The reason to have the constraint

\[
\sum_{i_k,j_k=-1}^{1} \beta_{i_k,j_k} = 1
\]

will be seen soon, which is analogous to the fourth order scheme at interior grid points.

Apparently, almost all existing high order compact schemes have the form above.

Denote the ‘local truncation error’ for the scheme at \((x_i, y_j)\) as

\[
T^h_{ij} = \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} u(x_{i+i_k}, y_{j+j_k}) - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} f(x_{i+i_k}, y_{j+j_k}) - \sum_{j_k=-1}^{1} \gamma_{j_k} g(y_{j+j_k}).
\]

We want to determine the coefficients such that the local truncation errors are zero or \( O(h^4) \) for any fourth order polynomials. To derive the system of equations for the coefficients, we expand \( u(x_{i+i_k}, y_{j+j_k}) \),

\[\text{This is because the } K u \text{ term is treated as a source. Note that if the condition is violated, that means } |K| > 8/h^2, K < 0, \text{ then the coefficient matrix is actually more diagonally dominant since the contribution to the diagonal is } 8K/12 \text{ while to each of the four off-diagonals is } K/12. \text{ The coefficient matrix is invertible and the norm } \|A_h^{-1}\|_2 \text{ will be smaller than that corresponding to } K = 0 \text{ although the sign property will be violated. In our new methods, we do not treat } K u \text{ as a source term and just need the usual } K \leq 0 \text{ condition for an M-matrix condition.}\]
\( f(x_i+i_k, y_j+k_j) \) at \((x_i, y_j)\), and \( g(y_j+k_j) \) at \(y_j\). For the \(u(x_i+i_k, y_j+k)\) terms, we apply the Taylor expansion at \((x_i, y_j)\) up to all fourth order partial derivatives,

\[
\begin{aligned}
  &u(x_{i+l}, y_{j+k}) = \sum_{0 \leq k_1+k_2 \leq 4} \frac{1}{k_1!k_2!} \frac{\partial^{k_1+k_2} u}{\partial x^{k_1} \partial y^{k_2}} (x_i, y_j) h_{i+k_1} h_{j+k_2} + O(h^5),
\end{aligned}
\]

where \(h_{i+k} = i_k h\) and \(h_{j+k} = j_k h\).

For the \(f(x_i+i_k, y_j+k_j)\) terms, we apply the Taylor expansion at \((x_i, y_j)\) up to all second order partial derivatives,

\[
\begin{aligned}
  &f(x_{i+l}, y_{j+k}) = f_0 + f_{x,0} h_{i+k} + f_{y,0} h_{j+k} + f_{x,x,0} h_{i+k} h_{j+k} + f_{x,y,0} h_{i+k} h_{j+k} + f_{y,y,0} h_{i+k} h_{j+k} + O(h^3),
\end{aligned}
\]

where \(f_0 = f(x_i, y_j)\), \(f_{x,0} = \frac{\partial f}{\partial x}(x_i, y_j)\) and so on. By differentiating the Helmholtz equation, we get the following high order PDE relations

\[
\begin{aligned}
  f_x &= u_{xxx} + u_{yy} + Ku_x, \quad f_y = u_{xy} + u_{ty} + Ku_y, \\
  f_{xx} &= u_{xxxx} + u_{yyy} + Ku_{xx}, \quad f_{xy} = u_{xyy} + u_{yy} + Ku_{xy}, \\
  f_{yy} &= u_{xxy} + u_{yy} + Ku_{yy}.
\end{aligned}
\]

(2.10)

For the \(g(y_j+k_j)\) terms, we apply the Taylor expansion at \(y_j\) with respect to \(y\) up to third order derivatives

\[
\begin{aligned}
  &g(y_{j+k}) = g(y_j) + g'(y_j) h_{j+k} + g''(y_j) \frac{h_{j+k}^2}{2} + g'''(y_j) \frac{h_{j+k}^3}{6} + O(h^4).
\end{aligned}
\]

(2.11)

Note that,

\[
\begin{aligned}
  &\left( \frac{\partial u}{\partial n} + \sigma u(x) \right) \bigg|_{x=0} = \left( \frac{\partial u}{\partial x} + \sigma u(x) \right) \bigg|_{x=0} = g(y).
\end{aligned}
\]

(2.12)

Thus, we have more relations from the boundary condition needed for the HOC scheme,

\[
\begin{aligned}
  &-u_x(0, y) + \sigma u(0, y) = g(y), \quad -u_{xy}(0, y) + \sigma u_y(0, y) = g'(y), \\
  &-u_{xyy}(0, y) + \sigma u_{yy}(0, y) = g''(y), \quad -u_{xyyy}(0, y) + \sigma u_{yy}(0, y) = g'''(y).
\end{aligned}
\]

(2.13)

These relations are utilized in deriving the fourth order compact scheme.

After the expansions of all involved terms, we can write the local truncation error as

\[
\begin{aligned}
  &T^h_{ij} = \sum_{0 \leq k_1+k_2 \leq 4} L_{k_1,k_2} \frac{\partial^{k_1+k_2} u}{\partial x^{k_1} \partial y^{k_2}} (x_i, y_j) + O \left( \|\alpha\|_{\infty} h^5 + \|\beta\|_{\infty} h^3 + \|\gamma\|_{\infty} h^4 \right),
\end{aligned}
\]

(2.14)

where \(L_{k_1,k_2}\) are the results after we collect terms and will be seen in the linear system of equations for the coefficients soon, \(\|\alpha\|_{\infty} = \max_{0 \leq i_k \leq 1, -1 \leq j_k \leq 1} \{|\alpha_{i_k,j_k}|\}\) and so on. We want the local truncation error to be zeros or \(O(h^4)\) for all fourth order polynomials, or \(x^{k_1} y^{k_2}, 0 \leq k_1 + k_2 \leq 4\). The finite difference equation should approximate the Poisson equation well for which \(f(x, y)\) is an \(O(1)\) quantity in general. Thus, as in the standard 9-points fourth order compact scheme, we impose the constraint of \(\sum_{i_k,j_k=1}^{4} \beta_{i_k,j_k} = 1\) otherwise the minimum of \(|T^h_{ij}|\) are zero with all zero coefficients. In this way, by matching the terms of the coefficients of \(u, u_x, u_y, \cdots, u_{xxx}, u_{xxx}, \cdots, u_{yy}\), we have 15 linear equations with one constraint. The first six equations
(required for all quadratic polynomials) are,

\[
\sum_{i_k=0}^{1} \alpha_{i_k,j_k} h_{i_k} - K - \sigma \sum_{j_k=-1}^{1} \gamma_{j_k} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{i_k} = K - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} + \sum_{j_k=-1}^{1} \gamma_{j_k} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{j_k} - K \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{j_k} - \sigma \sum_{j_k=-1}^{1} \gamma_{j_k} h_{j_k} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{j_k}^2}{2} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{j_k} - K \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \frac{h_{j_k}^2}{2} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{j_k}^2}{2} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{j_k} - K \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \frac{h_{j_k}^2}{2} - \sigma \sum_{j_k=-1}^{1} \gamma_{j_k} \frac{h_{j_k}^2}{2} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{i_k} h_{j_k} - K \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} h_{j_k} + \sum_{j_k=-1}^{1} \gamma_{j_k} h_{j_k} = 0.
\]

(2.15)

The next four equations (required for cubic polynomials) are

\[
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^3}{3!} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} h_{j_k} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{j_k}^2}{2} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{j_k} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k} h_{j_k}}{2} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} + \sum_{j_k=-1}^{1} \gamma_{j_k} \frac{h_{j_k}}{2} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^3}{3!} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} + \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \frac{h_{j_k}^2}{2} - \sigma \sum_{j_k=-1}^{1} \gamma_{j_k} \frac{h_{j_k}^2}{3!} = 0.
\]

(2.16)

The next five equations (required for quartic polynomials) are

\[
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^4}{4!} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k}^2 = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^3}{3!} h_{j_k} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} h_{j_k} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^2 h_{j_k}}{4!} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( \frac{h_{i_k}^2}{2} + \frac{h_{j_k}^2}{2} \right) = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^3}{3!} h_{j_k} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} h_{j_k} + \sum_{j_k=-1}^{1} \gamma_{j_k} \frac{h_{j_k}^3}{6} = 0 \\
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}}{4!} - \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k}^2 = 0.
\]

(2.17)

There are 16 equations and 18 unknowns, which is an under-determined system of equations. In general there are infinity number of solutions. We have found out a set of coefficients analytically for Poisson equations with a Neumann BC, given at the left boundary \( x = x_l \); see Figure 2, which lists a set of coefficients \( \alpha_{i_k,j_k} \) corresponding to the finite difference coefficients \( U_{ij} \); \( \beta_{i_k,j_k} \) corresponding to the combination coefficients of \( f \); and \( \gamma_{j_k} \) corresponding to the combination coefficients of \( g \).
For a Poisson equation with a Robin BC, we need to add $-2\sigma/h$ to the coefficient $\alpha_{0,j}$ for $U_{0,j}$, which is on a diagonal of the coefficient matrix of the FD equation. Note also that, similar to the ghost point method, those coefficients at $(x_0 + h, y_j)$ are doubled compared with those at an interior grid point, see the corresponding coefficients in Fig. 1 and Fig. 2, which can be regarded as the reflection, shifting the coefficient at $(x_0 - h, y_j)$ to $(x_0 + h, y_j)$ with an appropriate adjustment for $f(x_0 - h, y_j)$ and $f(x_0 + h, y_j)$ compared with that of an interior grid point. It is worth mentioning that, for a Poisson equation and other PDEs with constant coefficients with a flux BC, the derivation of the scheme is independent of the index $j$. Thus, we can simply use the grid points $(0, \pm h), (\pm h, 0), (0, 0)$, the six particular grid points to derive the coefficients. Note also that there are other analytic sets of solutions as well.

For Helmholtz equations with a Robin boundary condition, we have also found a set of analytic coefficients below obtained from the Maple symbolic package:

\begin{align*}
U_{i,j} & : \frac{1}{\lambda h^2} \left[ 4\sigma Kh^3 + \lambda Kh^2 - 24\sigma h - 40 \right], \\
& \text{with } \lambda = 12 - Kh^2, \\
\text{corresponding to the finite difference coefficients for } U_{ij}, \text{ the combination coefficients for } f_{ij}, \text{ and } g_j \text{ of the right hand side of the flux boundary condition. Again we see the perfect symmetry in the coefficients. When } K = 0, \text{ the finite difference scheme is the same as that for Poisson equations; and when } K \leq 0, \text{ the coefficient matrix of the finite difference equations is an M-matrix and the convergence is guaranteed. While there are infinite number of solution sets to the linear system of equations for the coefficients, we show that the system of equations for the coefficients are solvable.}
\end{align*}

Next, we discuss the convergence of the fourth order compact scheme for Poisson or generalized Helmholtz equations ($K < 0$) as summarized in the following theorem. The sign property, $\alpha_{00} < 0$ and otherwise $\alpha_{i,j} \geq 0$ is the key for the convergence proof. In general, there is no guarantee for the convergence of Helmholtz equations ($K > 0$) since there is no control of the coefficient matrix of the FD equations. For instance, when $K$ is in a neighborhood of an eigenvalue of the boundary value problem, then the coefficient matrix is close to be singular.

**Theorem 2.3.** Let $U_{ij}$ be the finite difference solution obtained from the fourth order scheme with the set of the coefficients given by (2.18)-(2.19), which include the special situation listed in Figure 2. Assume that the solution to the Poisson/Helmholtz equation with non-empty $\mathcal{R}_1$ (Dirichlet) and $\mathcal{R}_2$ (Robin) in the boundary condition (1.2) is $u(x, y)$. Then, the algorithm is exact if the solution is a fourth order polynomial if $K = 0$ and $\sigma = 0$. For a general solution $u(x, y) \in C^\infty(\mathcal{R})$, we have the following error estimate assuming...
that \( K \leq 0 \) and \( \sigma \geq 0 \),

\[
\|u(x_i, y_j) - U_{ij}\|_\infty \leq C \max\{\|D^6u\|_{\infty, \mathcal{R}}, \|D^5u\|_{\infty, \partial\mathcal{R}}\} h^4,
\]

where \( D^6u \) means all possible sixth order partial derivatives of \( u(x, y) \) and so on.

**Proof:** For the fixed set of the coefficients, we know that the scheme is exact for all fourth order polynomials at all (interior and boundary) grid points from the design of the algorithm if \( K = 0 \) and \( \sigma = 0 \).

For a general solutions \( u(x, y) \in C^6(\mathcal{R}) \), we know that the local truncation errors are of \( O(\|D^6u\|_{\infty, \mathcal{R}} h^4) \) at interior grid points and are of \( O(\|D^5u\|_{\infty, \partial\mathcal{R}} h^3) \) at boundary grid points \((x_0, y_j)\) from (2.14) and the analytic expressions of the coefficients, which implies that \( \alpha_\infty = O(\frac{1}{h^4}), \beta_\infty = O(1) \) and \( \gamma_\infty = O(h) \).

If \( K \leq 0 \) and \( \sigma \geq 0 \), from (2.18) and Lemma 2.2 we know that the coefficient matrix \((-A_h)\) of the finite difference equations is an M-matrix. Thus, from Theorem 6.1 and Theorem 6.2 of Morton & Mayer's book [20], which is also valid for part of Neumann boundary condition as long as at least one point has a Dirichlet boundary condition prescribed as stated in the book, we conclude that \( \|u(x_i, y_j) - U_{ij}\|_\infty \leq Ch^4 \).

Note that, for part of Neumann or Robin boundary conditions, the related boundary grid points are regarded as an 'interior points' in the proof of the maximum principle, which implies a slightly larger error constant.

The fourth order compact scheme is not exact for Helmholtz equations because we only utilized up to all second order partial derivatives for the \( Ku \) term. Note also that for a pure Neumann boundary condition along the entire boundary, we need to assume that the solution exists. Then, we can specify the solution at one point at the boundary to make the solution unique and apply the theorem. For other well-posed situations such as \( K < 0 \), or part of Robin BC’s without a Dirichlet BC on the boundary, we believe that the method is still fourth order accurate, but the proof is an open challenge.

### 2.1. Numerical experiments of the fourth order compact scheme for Poisson and Helmholtz equations.

We have tested the proposed fourth order compact scheme for polynomials \( f_k(x, y), k \leq 4 \), the computed solutions are accurate to \( \epsilon \log(\|A_h\|) \) when \( K = \sigma = 0 \), where \( \epsilon \sim 10^{-16} \) is the machine precision and \( A_h \) is the coefficient matrix of the finite difference equations. Next we test two constructed examples with genuine non-linear solutions, in which one is a relatively smooth, and the other can be oscillatory.

**Example 1. An example with a smooth solution.**

\[
\begin{align*}
  u(x, y) &= e^{-\pi} \sin(\pi y), & (x, y) \in (0, 1)^2, \\
  f(x, y) &= e^{-\pi} \sin(\pi y)(1 - \pi^2), & (x, y) \in (0, 1)^2, \\
  \left( \frac{\partial u}{\partial n} + \sigma u \right)_{x=0} &= (1 + \sigma) \sin(\pi y), & y \in (0, 1).
\end{align*}
\]

In this example, the Robin BC is a non-zero function of \( y \). The solution and the source term are relatively smooth.

**Example 2. An example with an oscillatory solution.**

\[
\begin{align*}
  u(x, y) &= \sin(k_1 x) \cos(k_2 y), & (x, y) \in (0, 1)^2, \\
  f(x, y) &= -\left(k_1^2 + k_2^2\right) \sin(k_1 x) \cos(k_2 y), & (x, y) \in (0, 1)^2, \\
  \left( \frac{\partial u}{\partial n} + \sigma u \right)_{x=0} &= -k_1 \cos(k_2 y) + \sigma \sin(k_1 x) \cos(k_2 y), & y \in (0, 1).
\end{align*}
\]

In this example, we can choose \( k_1 \) and \( k_2 \) to make the solution more oscillatory. For a typical test, we choose \( k_1 = 5 \) and \( k_2 = 50 \), so \( f(x, y) \sim 2525 \). This is a relatively tough problem to compute for large \( k_1 \) or \( k_2 \) since \( \frac{\partial u}{\partial y} \sim 3.125 \times 10^8 \). The mesh needs to be fine enough to resolve the solution.

We assume Dirichlet boundary conditions on other parts of the boundary from the exact solution. In Table 1, we show some experimental results. The top table lists results for Example 1. The second-third columns are the results for the Poisson equation with a Neumann BC, while the fourth-fifth columns list the results for the Helmholtz equation with \( K = 2000 \) and a Robin boundary condition with \( \sigma = -20 < 0 \) to test our method for an extreme case. In the table, \( N \) is the number of grid lines in one coordinate direction so \( h = 1/N \); and the order is the computed convergence order using two consecutive errors,

\[
\text{order} = \frac{\log(\|E_N\|_{\infty}/\log |E_{2N}\|_{\infty})}{\log 2}.
\]
We see clearly fourth order convergence. From $N = 256$ to $N = 512$, we observe better than expected convergence order for which we think it just a coincidence. The results using $N = 510$ or $N = 513$ are in line of a fourth order method. Also note that around $N = 512$, the mesh $h$ is close to the best possible before the round-off errors become dominant to ruin the convergence if $h$ decreases further.

### Table 1

Grid refinement analysis of the fourth order compact scheme. The top table lists the results for Example 1 with a Neumann BC and $K = 0$ in the column 2-3, and a Robin BC ($\sigma = -20$) in the columns 4-5. The bottom table lists the results for Example 2 for the Helmholtz equation with $K = 2000$, $k_1 = 5$, $k_2 = 50$, and a Neumann BC in the columns 2-3, and a Robin BC ($\sigma = -20$) in the columns 4-5. In both cases, we see clearly fourth order convergence.

| $N$ | $\|E\|_\infty$ Neumann order | $\|E\|_\infty$ Robin order |
|-----|-------------------------------|----------------------------|
| 16  | 2.2943e-05                    | 1.6933e-05                 |
| 32  | 1.4127e-06                    | 4.0215                     |
| 64  | 8.7602e-08                    | 4.0114                     |
| 128 | 5.4524e-09                    | 4.0060                     |
| 256 | 3.3800e-10                    | 4.0118                     |
| 512 | 2.1125e-11                    | 4.7221                     |

| $N$ | $\|E\|_\infty$ Neumann order | $\|E\|_\infty$ Robin order |
|-----|-------------------------------|----------------------------|
| 16  | 1.0920e-00                    | 2.8336                     |
| 32  | 4.7754e-02                    | 4.5152                     |
| 64  | 2.7619e-03                    | 4.1119                     |
| 128 | 1.6941e-04                    | 4.0271                     |
| 256 | 1.0539e-05                    | 4.0067                     |
| 512 | 6.5794e-07                    | 4.0016                     |

In the bottom table of Table 1, we show the grid refinement analysis for the Helmholtz equation using Example 2 with $K = 2000$, $k_1 = 5$, $k_2 = 50$. The second-third columns are the results for the Neumann BC, while the fourth-fifth columns list the results for a Robin boundary condition with $\sigma = -20$. We see errors are larger compared with that for Example 1 due to the nature of the oscillatory solutions and large amplitudes of high order partial derivatives. The mesh needs to be fine enough to resolve the solution. Still, we see clearly fourth order convergence. Also, the coefficient $\sigma$ has little effect on the convergence unless it is very large.

In Figure 3, we show the solution and error plots of Example 1 for the Poisson equation with a Neumann BC obtained using a 64 by 64 grid. Both the solution and error are smooth and the error is small, $\|E\|_\infty = 8.7602 \times 10^{-8}$.

![Fig. 3](image)

**Fig. 3.** (a): A plot of the computed solution of Example 1 for the Poisson equation and a Neumann BC obtained from a 64 by 64 grid. (b): The error plot where $\|E\|_\infty = 8.7602 \times 10^{-8}$.

In Figure 4 (a), we show an error plot from a 64 by 64 grid of Example 1 for the Helmholtz equation...
with $K = 200$, $k_1 = 5$, $k_2 = 50$, and a Neumann BC. The error now has mild oscillations. In Figure 4 (b), we show the error plot when the wave number is relatively large $K = 2000$. We see the error is oscillatory even though the solution is smooth.

![Fig. 4](image1.png)

**Fig. 4.** (a): Error plots of the computed solution using the compact fourth order schemes for Example 1 for the Helmholtz equation. (a): $K = 200$ and the error has mild oscillation. (b): $K = 2000$, the error is more oscillatory.

![Fig. 5](image2.png)

**Fig. 5.** (a): The computed solution using the fourth order compact schemes for Helmholtz equations applied to Example 2 with $K = 2000$, $k_1 = 5$, $k_2 = 50$. (b): The error plot ($\|E\|_\infty = 2.7619 \times 10^{-3}$). Both the solution and the error are oscillatory with some boundary effect at $x = 0$ where a Robin BC is specified.

In Figure 5 (a), we show a solution plot of Example 2 for the Helmholtz equation with $k_1 = 5$, $k_2 = 50$ from a 64 by 64 grid and a Neumann boundary condition at $x = 0$ and the Dirichlet boundary condition elsewhere. The solution is oscillatory. In Figure 5 (b) we show the error plot when the wave number is $K = 2000$. We see that the error is also oscillatory, and some boundary effect at $x = 0$.

3. **Super-third order compact schemes for flux BCs without $f$-extension.** If we do not use any extension of $f(x, y)$, then we can seek a high order compact scheme of the following form

$$
\sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} U_{i+i_k,j+j_k} = \sum_{i_k=0}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} f(x_{i+i_k}, y_{j+j_k}) + \sum_{j_k=-1}^{1} \gamma_{j_k} g(y_{j+j_k}),
$$

(3.1)

Now the indexes for $f_{ij}$ and $U_{ij}$ range from $i = 0, 1$ and $j = -1, 0, 1$. The degree of freedom is 15 which is not enough for a fourth-order scheme. Another consideration is the stability. We want the coefficient matrix
is an M-matrix if $K \leq 0$.

It is important to have both consistency and stability. Thus, we give up two equations corresponding to $x^4$ and $y^4$ while keep other equations. In the modified system of equations, we will have HOC schemes that are better than third but not fully fourth order accurate. Therefore, we call such schemes super third-accurate methods.

For the stability concern, we use a maximum principle preserving scheme to enforce the sign property. Let the system of linear equations for the coefficients be $Ax = b$, where $A \in \mathbb{R}^{14 \times 15}$. We impose the sign restrictions on the coefficients $\alpha_{i_k,j_k}$ in (3.1)

\begin{align}
\alpha_{i_k,j_k} & \geq 0 \quad \text{if} \quad (i_k,j_k) \neq (0,0), \\
\alpha_{i_k,j_k} & < 0 \quad \text{if} \quad (i_k,j_k) = (0,0),
\end{align}

along the equality constraints.

We form the following quadratic constrained optimization problem to determine the coefficients of the finite difference scheme, see for example [14],

\begin{align}
\min_x \left\{ \frac{1}{2} x^T H x - x^T w \right\}, \\
\text{s.t.} \quad A x = b \\
\alpha_{i_k,j_k} & \geq 0 \quad \text{if} \quad (i_k,j_k) \neq (0,0), \\
\alpha_{i_k,j_k} & < 0 \quad \text{if} \quad (i_k,j_k) = (0,0),
\end{align}

where $x$ is the vector composed of the coefficients of the finite difference equation, the coefficients of the combination of $f_{ij}$, and the coefficients of the combination of $g(y_{jk})$. In the implementation, we take $H = A^T A$, and $w = A^T b$, and use the Matlab quadratic programming function ‘quadprog’ to solve the optimization problem with the initial guess $x_0 = A^+b$, where $A^+$ is the pseudo-inverse of $A$. It is possible to have better $H$ and $w$.

![Finite difference coefficients](image)

**Fig. 6.** The finite difference coefficients for $U_{0j}$ without (the filled red circles); and with the optimization process (the blue diamonds). The coefficient matrix of the FD equations using the second one is an M-matrix. The six coefficients $\alpha_k$’s correspond to the grid points $(0,y_j - h), (h,y_j - h), (0,y_j), (h,y_j), (0,y_j + h), (h,y_j + h)$, where $(0,y_j)$ is the master grid point.

In Figure 6 we show a computed set of the finite difference coefficients for $U_{0j}$ at a grid point, say $(x_0, y_j)$ where a Neumann or Robin boundary condition is prescribed. The third coefficient is the one on the diagonal. The data marked with the filled red circles is obtained directly from $x_0 = A^+b$ without optimization, where $A^+$ is the pseudo-inverse of the coefficient matrix $A$. We can see that the coefficients of the diagonals can be positive or negative. The data marked with the blue diamonds is obtained from the optimization process. We can see that the coefficients off the diagonals now are all non-negative.

Once again, there are infinite number of solution sets to the linear system of equations. We list one
particular ideal set below,

\[ U_{i,j} : \frac{1}{\lambda h^2} \begin{bmatrix} 2\sigma Kh^3 + (\lambda + 2)K h^2 - 12\sigma h - 20 & 2 \\ 4 - K h^2 & 2 \end{bmatrix}, \]  

\[ f_{i,j} : \frac{1}{\lambda} \begin{bmatrix} 0 & 0 \\ 4 - K h^2 & 2 \\ 0 & 0 \end{bmatrix}, \ g_j : \frac{1}{h} \begin{bmatrix} 0 \\ -2 \\ 0 \end{bmatrix}, \]

where \( \lambda = 6 - K h^2 \). Note that, if \( K \leq 0, \sigma \geq 0 \), then the coefficient matrix is an M-matrix and the HOC scheme preserve the discrete maximum principle.

Similar to the error estimates in the previous section, we have the convergence theorem for the super-third compact method for the particular set of coefficients list above as stated below.

**Theorem 3.1.** Let \( U_{ij} \) be the finite difference solution obtained from the super-third order compact scheme with a set of coefficients given by (3.5)-(3.6). Assume that the solution to the Poisson/Helmholtz equation with non-empty \( \mathbb{R}_1 \) (Dirichlet) and \( \mathbb{R}_2 \) (Robin) in the boundary condition (1.2) is \( u(x,y) \). Then, the algorithm is exact if the solution is any fourth order polynomials without \( x^4 \) and \( y^4 \) terms when \( K = 0 \) and \( \sigma = 0 \). For general solutions, assuming \( u(x,y) \in C^6(\mathbb{R}) \), we have the following error estimate

\[ \|u(x_i,y_j) - U_{ij}\|_\infty \leq C \max\{\|D^6u\|_{\infty,\mathbb{R}}, \|D^5u\|_{\infty,\partial\mathbb{R}}\} h^3+. \]

The proof is similar to that of Theorem 2.3. From the PDE theory we know that, if \( K \leq 0 \) and \( \sigma \geq 0 \), then the continuous problem is wellposed, while \( K > 0 \) is not guaranteed.

**Table 2**

Grid refinement analysis of the super-third order compact scheme for Helmholtz equations with a Neumann BC. (a): Example 1 with \( K = 200 \). The average convergence order is 3.3118. (b): Example 2 with \( K = 2000, k_1 = 5, k_2 = 50 \). The convergence order is clean fourth order. (c): Example 2 with \( K = 2000, k_1 = 25, k_2 = 5 \). The average for the last column is 4.0393.

| \( N \) | \( \|E\|_\infty \) | order | \( N \) | \( \|E\|_\infty \) | order | \( N \) | \( \|E\|_\infty \) | order |
|-------|-----------------|------|-------|-----------------|------|-------|-----------------|------|
| 8     | 7.9660e-03      |      | 16    | 1.0922e-00      |      | 16    | 0.5620e-00      |      |
| 16    | 5.6584e-04      | 3.8154 | 32    | 4.7754e-02      | 4.5138 | 32    | 1.1471e-02      | 5.6145 |
| 32    | 6.5175e-05      | 3.1180 | 64    | 2.7660e-03      | 4.1114 | 64    | 7.7896e-04      | 3.8803 |
| 64    | 7.8505e-06      | 3.0508 | 128   | 1.7023e-04      | 4.0222 | 128   | 4.1507e-05      | 4.2301 |
| 128   | 1.2122e-06      | 2.6978 | 256   | 1.0526e-05      | 4.0155 | 256   | 2.7972e-06      | 3.8913 |
| 256   | 1.4943e-07      | 3.0201 | 512   | 6.6300e-07      | 3.9888 | 512   | 1.5868e-07      | 4.1398 |
| 512   | 8.3095e-09      | 4.1686 |       |                 |      |       |                 |      |

We have repeated numerical tests for the same examples in the previous section without extension \( f(x,y) \) using the super-third compact method with a flux type BC. In Table 2, we show grid refinement results for the Helmholtz equation. In Table 2 (a), we list the results for Example 1 with \( K = 200 \). The order of convergence fluctuates between three and four and the average is 3.3118. In Table 2 (b), the test is for Example 2 with \( K = 2000, k_1 = 5, k_2 = 50 \). The results show a fourth order convergence. One of explanations is that the error is dominated in the \( y \) direction \( (k_2 = 50) \) rather than from the Neumann BC at \( x = 0 \). In Table 2 (c), the test is for Example 2 with \( K = 2000, k_1 = 25, k_2 = 5 \). The order of convergence fluctuate between three and four and the average is 4.0393, which shows some natures of the super-third compact method.

4. **HOC schemes for diffusion and advection equations.** In this section, we show that the same idea can be applied to diffusion and advection equations with constant coefficients,

\[ \Delta u + au_x + bu_y + Ku = f. \]
Using the same approach, the finite difference equation for an interior grid point can be written as

\begin{equation}
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} U_{i+i_k,j+j_k} = \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} f(x_{i+i_k}, y_{j+j_k}),
\end{equation}

\begin{equation}
\sum_{i_k,j_k=-1}^{1} \beta_{i_k,j_k} = 1.
\end{equation}

The coefficients are determined in a similar way as discussed in previous sections. We list additional PDE relations and the system of linear equations for the coefficients in Appendix. There are infinite number of solutions of the coefficients. With the Matlab/Maple symbolic package, we have obtained a set of solution relations and the system of linear equations for the coefficients in Appendix. There are infinite number of solutions of the coefficients. With the Matlab/Maple symbolic package, we have obtained a set of solution relations and the system of linear equations for the coefficients in Appendix.

\begin{equation}
\alpha = \frac{A_{\text{diff}}}{h^2} + \frac{B_{\text{advec}}(a, b)}{h} + C_{\text{other}}(K),
\end{equation}

\begin{equation}
A_{\text{diff}} \sim O(1), \quad B_{\text{advec}}(a, b) \sim O(a, b), \quad C_{\text{other}} \sim O(K),
\end{equation}

where \( \frac{A_{\text{diff}}}{h^2} \) is the leading terms in the FD coefficients which has the symmetry in terms of the four corner and west-east-north-south grid points in reference to the master grid point. When \( a = 0 \) and \( b = 0 \), \( \frac{A_{\text{diff}}}{h^2} \) is the same as that listed in (2.18)-(2.19).

The FD coefficients corresponding to \( U_{ij} \) of the HOC scheme for diffusion and advection equations computed with the Maple are shown in Figure 9 in Appendix. The solution set is obtained using the pseudo-inverse of the coefficient matrix, also called the SVD solution. The computation can be done almost instantly with numerical solutions but took quite a while to return the symbolic (analytic) solution. As expected, the SVD solution is often the best compared with other set of solutions even if the convergence order is the same. We have seen that the error constant can be several order magnitude smaller using the SVD solution than with numerical solutions but took quite a while to return the symbolic (analytic) solution. As expected, the inverse of the coefficient matrix, also called the SVD solution. The computation can be done almost instantly with numerical solutions but took quite a while to return the symbolic (analytic) solution. As expected, the inverse of the coefficient matrix, also called the SVD solution. The computation can be done almost instantly with numerical solutions but took quite a while to return the symbolic (analytic) solution. As expected, the inverse of the coefficient matrix, also called the SVD solution. The computation can be done almost instantly with numerical solutions but took quite a while to return the symbolic (analytic) solution. As expected, the inverse of the coefficient matrix, also called the SVD solution. The computation can be done almost instantly with numerical solutions but took quite a while to return the symbolic (analytic) solution.

If a Robin or Neumann boundary condition, say, is defined at \( x = x_1 \), then we find another set of FD coefficients of the form as in (2.8) with different PDE, high order PDE relations, and resulting linear system of equations for the coefficients assuming that we have an extension of \( f(x, y) \). We also list those relations in Appendix. The FD coefficients for \( U_{ij} \) also have the form,

\begin{equation}
\alpha_{\text{Robin}} = \frac{\tilde{A}_{\text{diff}}}{h^2} + \frac{\tilde{B}_{\text{advec}}(a, b, \sigma)}{h} + \tilde{C}_{\text{other}}(K).
\end{equation}

The coefficient matrix of the FD is a M-matrix unless extreme situations when \( K, |a|, |b| \) is so large that the optimization process fails to return a feasible solution. The local truncation error is of \( O(h^3) \) which would not affect the global fourth order convergence.

### 4.1. Convergence analysis of the HOC method for diffusion and advection equations.

The discussion of the convergence for the developed HOC scheme is challenging since it depends on the advection coefficients and boundary conditions. Using the computed sets of coefficients, and the fact that the local truncation errors at boundary grid points can be one order lower than that of interior grid points without affecting the global accuracy of the computed solution, we can obtain asymptotic fourth order convergence theorem.

**Theorem 4.1.** Let \( U_{ij} \) be the finite difference solution obtained from the derived HOC scheme for the diffusion and advection equation with non-empty \( R_1(\text{Dirichlet}) \) and \( R_2(\text{Robin}) \) in the boundary condition (1.2). Assume that the solution \( u(x, y) \in C^0(\mathcal{R}) \), if \( h \) is small enough, \( K \leq 0 \), and \( \sigma \geq 0 \), then the following error estimates hold

\begin{equation}
\| T_h \|_\infty \leq \begin{cases} 
C_1 \| D^6 u \|_{\infty, \mathcal{R}} h^4 & \text{interior grid points}, \\
C_2 \| D^3 u \|_{\infty, \partial \mathcal{R}} h^3 & \text{flux boundary grid points}, \\
C_3 \| u(x, y) - U_{ij} \|_\infty \leq \bar{C} h^4,
\end{cases}
\end{equation}

for Dirichlet, or Dirichlet with part of Robin, or Neumann boundary conditions.
Proof: At an interior point, we carry out the Taylor expansion at a grid \((x_i, y_j)\) of the local truncation error for all terms \((u(x_i, y_j))\) and \(f(x_i, y_j))\) involved. Thus, we should have

\[
T^n_{ij} = T_{\text{diff}}h^3 + T_{\text{advec}}(a, b)h^4 + C_{\text{other}}(K)h^4 + O(h^5),
\]

according to \((4.4)\). Furthermore, since \(A_{\text{diff}}\) is symmetric, or centered discretization in reference \((x_i, y_j)\), the terms in the expansion involving odd partial derivatives are canceled out, which leads to \(\|T_h\|_{\infty} \sim O(h^3)\) if \(h\) is small enough. Thus, for a Dirichlet boundary condition, the HOC scheme is asymptotically fourth order convergent.

If part of flux boundary condition is given, then there are no cancellations from \(1/h^2\) terms, thus, we have \(\|T_h\|_{\infty} \sim O(h^3)\). Since the coefficient matrix is an M-matrix which is true if \(K \leq 0, h \leq C/\max \{|a|, |b|\}\), and \(\sigma \geq 0\), we apply the convergence theorem in [20] to get the asymptotically fourth order convergence. \(\Box\)

4.2. Numerical examples of the HOC method for diffusion and advection equations. We carried out numerical experiments for Example 1 and Example 2 using the resultant source terms and the boundary conditions. In Table 3, we show numerical experiments results and the grid refinement analysis. The left and middle tables are the results of the method applied to Example 1 while the right table lists results of the method applied to Example 2. In the left table, the parameters are \(K = 20, a = 1, b = 2\) in which the convection is not very large. The results show clearly fourth order convergence starting from a rather coarse grid \(N = 16\). In the middle of table, the parameters are \(K = 20, a = 100, b = 5\) in which the convection is relatively strong. The fourth order convergence was affected at the coarse grids level until \(N \geq 128\). In the right table, the parameters are \(K = 20, a = 1, b = 100, k_1 = 5, k_2 = 10\). With modest \(k_1\) and \(k_2\), Example 2 is tougher to compute due to the oscillations and larger magnitudes of the partial derivatives and the source term. Nevertheless, when the grid is fine enough, we see clearly fourth order convergence.

| \(N\) | \(\|E\|_{\infty}\) | \(\text{order}\) | \(\|E\|_{\infty}\) | \(\text{order}\) | \(\|E\|_{\infty}\) | \(\text{order}\) |
|---|---|---|---|---|---|---|
| 16 | 1.0772e-04 | | 16 | 7.2039e-05 | | 16 | 1.0018e-02 | |
| 32 | 6.7160e-06 | 4.0035 | 32 | 8.3145e-06 | 3.1151 | 32 | 1.5245e-03 | 2.7162 |
| 64 | 4.1993e-07 | 3.9994 | 64 | 7.1788e-07 | 3.5338 | 64 | 1.4749e-04 | 3.3696 |
| 128 | 2.6249e-08 | 3.9998 | 128 | 5.1167e-08 | 3.8105 | 128 | 1.0652e-05 | 3.7914 |
| 256 | 1.6666e-09 | 3.9773 | 256 | 3.3067e-09 | 3.9517 | 256 | 6.9281e-07 | 3.9425 |
| 512 | 7.3411e-11 | 4.5048 | 512 | 1.6823e-10 | 4.2969 | 512 | 4.3801e-08 | 3.9834 |

In Figure 7, we show two error plots with different parameters and a strong advection in the \(y\)-direction for Example 2 using a 80 by 80 grid. In both cases, the errors in the infinity norm are small, \(10^{-5}\) and \(10^{-8}\). In Figure 7 (a), the oscillation is dominant compared with the advection effect. In Figure 7 (b), the solution is oscillatory, we see the boundary layer effect clearly from the strong advection.

In Table 4, we present numerical example for Example 1 with a Robin boundary condition. The second-third columns are the results for Example 1 with \(K = 50\), and \(a = 1, b_1 = -5\). The errors are small even with coarse grids since the advection is relatively small and we observe clean fourth order convergence. The fourth-fifth columns are the results for the same example with \(K = 50\), and \(a = 5, b_1 = -100\), a relatively strong advection. We observe asymptotic fourth order convergence.

In Table 5, we show the numerical result for a Robin boundary condition with \(\sigma = 20\) for Example 2 (solution is oscillatory). The second-third columns are the results with \(K = 50\), \(k_1 = 5, k_2 = 50\), and \(a = 1, b_1 = -5\). A clean fourth order convergence can be seen since the advection is relatively small. The fourth-fifth columns are the results for the same example with \(K = 50\), and \(a = 5, b_1 = -100\), a relatively strong advection. We observe asymptotic fourth order convergence. The sixth-seventh columns are the results of the local truncation errors which also has an asymptotic fourth order. The last two columns are the results with switched advection coefficients, \(a = -100\) and \(b_1 = 5\). We observe the similar convergence behavior. In both cases, the errors due to the convections are dominated than the errors from the flux BC.
To approach, we have also developed a HOC scheme for anisotropic elliptic partial differential equations

\[ \sum_{i=1}^{m} \sum_{j=-1}^{1} \alpha_{i,j} x_{i,j} U_{i+1,j} + f_{i,j-1} + f_{i,j} + f_{i+1,j} + f_{i,j+1} + 8f_{i,j} = \gamma(f_{i+1,j} - f_{i-1,j}) + \delta(f_{i,j+1} - f_{i,j-1}) \]

where \( \gamma = ah/2 \) and \( \delta = bh/2 \), and \( \alpha_{i,j} \) are the coefficients of the nine-point stencil shown in Figure 8.

\[ \frac{1}{6h^2} \begin{pmatrix} 1 - \gamma + \delta - \gamma \delta & 4 + 4\delta + 2\delta^2 & 1 + \gamma + \delta + \gamma \delta \\ 4 - 4\gamma + 2\gamma^2 & -(20 + 4\gamma^2 + 4\delta^2) & 4 + 4\gamma + 2\gamma^2 \\ 1 - \gamma - \delta + \gamma \delta & 4 - 4\delta + 2\delta^2 & 1 + \gamma - \delta - \gamma \delta \end{pmatrix} \]

**Fig. 8.** The compact nine-point coefficients of the FD scheme from [7].

5. High order compact schemes for anisotropic elliptic PDEs. Using the same idea and approach, we have also developed a HOC scheme for anisotropic elliptic partial differential equations

\[ A_{11} u_{xx} + 2A_{12} u_{xy} + A_{22} u_{yy} + au_x + bu_y + K u = f, \]

with constant coefficients, and Dirichlet, Neumann, and Robin boundary conditions. The method is exact for any fourth order polynomials if \( K = 0 \). For well-posedness of the PDE, we assume that \( A_{11}^2 - A_{11} A_{22} < 0 \).
As before, the HOC scheme uses the 9-point stencil at interior grid points can be written as

$$U_{i,j} = \frac{1}{\lambda h^2} \left[ \begin{array}{c} 2(A_{11} - 2A_{12})(A_{11} - A_{12}) \\ 8(A_{11}^2 - A_{12}^2) \\ 2(A_{11} + A_{12})(A_{11} + 2A_{12}) \\ 2(A_{11} + A_{12})(A_{11} + A_{12}) \\ \lambda Kh^2 - 8(5A_{11}^2 - 2A_{12}^2) \\ 8(A_{11}^2 - A_{12}^2) \\ 2(A_{11} - 2A_{12})(A_{11} - A_{12}) \end{array} \right],$$

(5.4)

$$f_{i,j} = \frac{1}{2\lambda} \left[ \begin{array}{c} A_{11} - A_{12} \\ 0 \\ 20A_{11} - 2K\lambda^2 \\ 0 \\ A_{11} + A_{12} \\ 0 \end{array} \right],$$

(5.5)

where $\lambda = 12A_{11} - Kh^2$. We can see that when $A_{11} > 2|A_{12}|$ and $K \leq 0$, the coefficient matrix of the FD scheme is an M-matrix. For non-zero convection coefficients, the expressions for the set of coefficients are complicated, it is easier to use and store numerical solutions.

**Theorem 5.1.** Let $u(x,y) \in C^6(\mathbb{R})$ be the solution to (5.1) with a Dirichlet boundary condition, $U_{i,j}$ be the finite difference solution obtained from the HOC scheme. Then, the finite difference scheme with a set of coefficients given by (5.4)-(5.5) is fourth order accurate if $A_{11} > 2|A_{12}|$, $K \leq 0$, $a = 0$, $b = 0$.

---

**Table 5**

Grid refinement analysis of the HOC scheme for a diffusion and advection equation with a Robin BC for Example 2. The parameters are $K = 50$, $k_1 = 5$, $k_2 = 50$, and $a = 1, b_1 = -5$ for the results in the second-third columns, and $K = 50$, $k_1 = 5$, $k_2 = 50$, and $a = 5, b_1 = -100$ for the fourth-seventh columns. $\|T_h\|_{\infty}$ measures the local truncation errors. The last two columns are the results with switched advection coefficients, $a = -100$ and $b_1 = 5$.

| $N$ | $\|E\|_{\infty}$ | order | $\|E\|_{\infty}$ | order | $\|T_h\|_{\infty}$ | order | $\|E\|_{\infty}$ | order |
|-----|------------------|-------|------------------|-------|-------------------|-------|------------------|-------|
| 16  | 5.9061e-04       |       | 5.5602e+03       |       | 8.7058e00         |       | 1.4970e00        |       |
| 32  | 3.7512e-05       | 3.9768| 1.1095e-01       | 15.6129| 1.2100e00         | 2.8470| 6.1313e-02       | 4.6097|
| 64  | 2.3546e-06       | 3.9938| 9.2102e-03       | 3.5905 | 1.2352e-01         | 3.2922| 3.4927e-03       | 4.1338|
| 128 | 1.4734e-07       | 3.9983| 6.3934e-04       | 3.8486 | 9.0471e-04         | 3.9779| 2.1341e-04       | 4.0326|
| 256 | 9.2020e-09       | 4.0011| 4.1108e-05       | 3.9591 | 5.9032e-04         | 3.9379| 1.3891e-05       | 3.9414|
| 512 | 4.4578e-10       | 4.3675| 2.5880e-06       | 3.9895 | 3.6881e-05         | 4.0005| 8.7529e-07       | 3.9882|

We have found that the HOC scheme works better when $A_{11} = A_{22}$. If this condition is not true, we can use a scaling in one coordinate direction to transform the PDE so that $A_{11} = A_{22}$.
2) the finite difference scheme is asymptotically fourth order convergent if $A_{11} > 2|A_{12}|$ and $K \leq 0$ with general constants $a$ and $b$.

**Proof:** For the first case, from the construction of the finite difference coefficients, we know that the local truncation errors are at least $O(h^3)$ since we have matched all terms of fourth order partial derivatives. We can see that the FD scheme for $U_{ij}$ has the central symmetry, which means that all the coefficients in odd partial derivatives canceled out in the Taylor expansion of the local truncation errors. When $A_{11} > 2|A_{12}|$ and $K \leq 0$, the coefficient matrix of the FD equations is an M-matrix. Thus, from the convergence theorem in [20], we conclude the fourth order convergence.

For general anisotropic diffusion and advection equations with a Dirichlet boundary condition, from the continuity of the FD coefficients and the fact that the coefficients involving advection terms are of $O(||a||\|\sigma\|h^5) \sim O(h^4)$ in the local truncation errors, we can conclude asymptotic fourth order convergence. □

### 5.2. Finite difference coefficients for flux boundary conditions.

If a Robin boundary condition is specified, we need to solve another set of coefficients to take into account the boundary condition. The procedure is the same as before except that the linear system of equations and the high order PDE relations are different. Unfortunately, the linear system of equations using the same approach is not consistent. Nevertheless, the inconsistency comes from fourth order partial derivatives. Thus, we can simply use the singular value solution (SVD) or ignore some terms such as $x^4$ and $y^4$ to get a consistent system. With the second approach, we have obtained a set of coefficients below when $K = 0$, $a = 0$, $b = 0$ assuming a Robin BC at the left boundary using the Maple package:

\[
U_{i,j} : \frac{1}{6A_{13}h^2} \begin{bmatrix} -A_{11}\sigma h + (3A_{11}^3 + 6A_{11}A_{12} - 4A_{12}^2) & 3A_{11}^2 + 6A_{11}A_{12} + 4A_{12}^2 \\ -10A_{11}\sigma h + (8A_{12}^2 - 18A_{11}^2) & 6A_{11}^2 - 8A_{12}^2 \\ -A_{11}\sigma h + (3A_{11}^3 - 6A_{11}A_{12} - 4A_{12}^2) & 3A_{11}^2 - 6A_{11}A_{12} + 4A_{12}^2 \end{bmatrix},
\]

\[
f_{i,j} : \frac{1}{48A_{11}(A_{11}^2 - 2A_{12}^2)} \begin{bmatrix} \lambda + \mu & 0 & 0 \\ 0 & 4A_{11}(9A_{12}^2 - 20A_{12}^2) & 0 \\ \lambda - \mu & 0 & \zeta - \eta \end{bmatrix},
\]

\[
g_j : \frac{1}{6h} \begin{bmatrix} -1 \\ -10 \\ -1 \end{bmatrix},
\]

where

\[
\lambda = -A_{11}^3 + 4A_{11}A_{12}^2, \quad \mu = 3A_{11}^2A_{12} - 4A_{12}^3,
\]

\[
\zeta = 7A_{11}^3 - 12A_{11}A_{12}^2, \quad \eta = 5A_{11}^2A_{12} - 12A_{12}^3.
\]

Note that the coefficient matrix from this set of FD coefficients and (5.4) is an M-matrix if $h$ is small enough, $K \leq 0$, and $A_{11} > 1 + \frac{2\sqrt{2}}{3}|A_{12}| \approx 2.5275|A_{12}|$, a stronger condition than that of interior grid points. We have a super-third convergence theorem of the finite difference scheme.

**Theorem 5.2.** Let $u(x, y) \in C^5(\mathbb{R})$ be the solution to (5.1) with a Robin boundary condition, $U_{ij}$ be the finite difference solution obtained from the HOC scheme. Then,

1) the finite difference scheme with a set of coefficients given by (5.4)-(5.5) at interior grid points, (5.6)-(5.8) at boundary grid points, is super-third accurate if $A_{11} > 1 + \frac{2\sqrt{2}}{3}|A_{12}|$, $K = 0$, $a = 0$, $b = 0$;

2) the finite difference scheme is at least asymptotically super-third convergent if $A_{11} > 1 + \frac{2\sqrt{2}}{3}|A_{12}|$, $K \leq 0$, and $\sigma \geq 0$ with general constants $a$ and $b$.

We show two numerical examples in Table 6 using Example 2, the tougher example with oscillatory solutions. The second to fifth columns show grid refinement results of the global and local truncation errors, and the convergence orders of Example 2 when the parameters are $A_{11} = A_{22} = 3$, $A_{12} = 0.5$, $K = 20$, $k_1 = 3$, $k_2 = 15$, $a = 50$, $b = -1$, and a Dirichlet boundary condition. We observe asymptotic fourth order convergence in the local truncation as well as the global errors.
Grid refinement analysis of the HOC scheme for an anisotropic diffusion and advection equation using Example 2. The results in columns 2-5 are the global and local truncation errors and convergence order of a Dirichlet BC, while columns 6-7 are the global error and order of a Robin boundary condition.

| N  | $\|E\|_\infty$     | order | $\|T_h\|_\infty$ | order | $\|E\|_\infty$ | order |
|----|------------------|------|------------------|------|----------------|------|
| 16 | 2.3762e-03       | 1.7131| 1.6756e-05       |       |                |       |
| 32 | 1.6156e-04       | 3.8777| 1.1523e-06       | 3.8621|                |       |
| 64 | 1.0492e-05       | 3.9455| 8.4485e-08       | 3.7697|                |       |
| 128| 6.6211e-07       | 3.9861| 6.8592e-09       | 3.6226|                |       |
| 256| 4.2280e-08       | 3.9690| 6.3350e-10       | 3.4366|                |       |
| 512| 2.6740e-09       | 3.9975| 4.8299e-11       | 3.7133|                |       |

In the last two columns of Table 6, we show the result when a Robin boundary condition is prescribed at $x = 0$. The parameters are $A_{11} = A_{22} = 1$, $A_{12} = 0.25$, $K = -2$, $k_1 = 2$, $k_2 = 1$, and the convection coefficients $a = 1$, $b = -5$, and $\sigma = -3$. The results show a super-third convergence order (better than 3.5) but not complete fourth order. It is still ongoing project to see whether it is possible to get a full fourth order convergence for anisotropic diffusion and advection equations with flux boundary conditions.

**6. The fourth order compact scheme for flux BCs in 3D.** The same idea and methodology have also been applied to three dimensional (3D) problems with flux type of boundary conditions

\[
\begin{align*}
(6.1) & \quad u_{xx} + u_{yy} + u_{zz} + Ku = f(x, y, z), \quad x \in \mathcal{R}, \\
(6.2) & \quad u \bigg|_{\partial \mathcal{R}_1} = u_1(x), \quad \left( \frac{\partial u}{\partial n} + \sigma u(x) \right) \bigg|_{\partial \mathcal{R}_2} = g(x).
\end{align*}
\]

The main challenge probably is in the implementation and indexing.

Without loss of generality, we assume that domain is a cubic $[x_l, x_r] \times [y_l, y_r] \times [z_l, z_r]$, and a Robin boundary condition is specified at $x = x_1$, and Dirichlet boundary conditions on other parts of the boundary. With a uniform mesh, the 19-point fourth-order compact FD scheme for a Poisson equation on an interior point $(x_i, y_j, z_k)$ with mesh-size $h$ is given by [27]

\[
\begin{align*}
(6.3) & \quad -\frac{4}{h^2} U_{ijk} + \frac{1}{3h^2} (U_{i+1,j,k} + U_{i-1,j,k} + U_{i,j+1,k} + U_{i,j-1,k} + U_{i,j,k+1} + U_{i,j,k-1}) \\
& \quad + \frac{1}{6h^2} (U_{i+1,j+1,k} + U_{i+1,j-1,k} + U_{i-1,j+1,k} + U_{i-1,j-1,k} + U_{i,j+1,k+1} + U_{i,j,k+1} + U_{i,j,k-1}) \\
& \quad + U_{i-1,j,k+1} + U_{i-1,j,k-1} + U_{i,j+1,k+1} + U_{i,j-1,k+1} + U_{i,j-1,k-1} + U_{i,j,k+1} + U_{i,j,k-1}) \\
& \quad = \frac{1}{12} (6f_{ijk} + f_{i+1,j,k} + f_{i-1,j,k} + f_{i,j+1,k} + f_{i,j-1,k} + f_{i,j,k+1} + f_{i,j,k-1}).
\end{align*}
\]

The $Ku$ term is treated as a source term. The stencil notation for the approximation is

\[
\begin{align*}
(6.4) & \quad U_{i,j,k} : \quad \frac{1}{6h^2} \begin{bmatrix} 1 & 2 & 2 & 1 \\ 2 & -24 & 2 & 1 \\ 1 & 2 & 1 & 1 \end{bmatrix}, \quad U_{i \pm 1,j,k} : \quad \frac{1}{6h^2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \\
(6.5) & \quad f_{i,j,k} : \quad \frac{1}{12} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 6 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad f_{i \pm 1,j,k} : \quad \frac{1}{12} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix},
\end{align*}
\]

where for example, $j = j_c - 1, j_c, j_c + 1$ and $k = k_c - 1, k_c, k_c + 1$. Note that there are seven $f_{ijk}$‘s in the scheme.

For a grid point $(x_i, y_j, z_k)$ at the boundary $x = x_q$ where a Robin boundary condition is prescribed,
similar to the 2D case, the fourth order FD equation has the following form,

\[
\sum_{i_l=0}^{1} \sum_{j_l=-1}^{1} \sum_{k_l=-1}^{1} \alpha_{i_l,j_l,k_l} U_{i_l,j_l+k_l} = \sum_{i_l=-1}^{1} \sum_{j_l=-1}^{1} \sum_{k_l=-1}^{1} \beta_{i_l,j_l,k_l} f(x_{i_l}, y_{j_l+k_l}, z_{k_l} + k_l)
\]

\[
(6.6)
\]

\[
+ \sum_{j_l=-1}^{1} \sum_{k_l=-1}^{1} \gamma_{j_l,k_l} g(y_{j_l+k_l}, z_{k_l} + k_l),
\]

\[
(6.7)
\]

Thus, if all points are involved, then the total degree of freedom is 18 + 27 + 9 = 54. We want the FD method is exact (when \(K = \sigma = 0\)) if the solution is any fourth order polynomials \(\sum_{0 \leq i+j+k \leq 4} x^i y^j z^k\) that would lead to 35 equations in addition to the constraint. Thus, we have an under-determined linear system of equations. To enforce the discrete maximum principle, we enforce the sign property so that the coefficient matrix for the finite difference scheme is an M-matrix. In general, we have infinite number of solutions and we can pick up good ones that can have expected symmetries and the least non-zero coefficients. For a Poisson equation \(3.5\) equations in addition to the constraint. Thus, we have an under-determined linear system of equations.

\[
U_{0,j,k} : \frac{1}{6h^2} \begin{bmatrix}
1 & 2 & 1 \\
2 & -12(2+\sigma) & 2 \\
1 & 2 & 1
\end{bmatrix},
\]

\[
U_{1,j,k} : \frac{1}{6h^2} \begin{bmatrix}
0 & 2 & 0 \\
2 & 4 & 2 \\
0 & 2 & 0
\end{bmatrix},
\]

\[
(6.8)
\]

\[
f_{0,j,k} : \frac{1}{12} \begin{bmatrix}
0 & 1 & 0 \\
1 & 6 & 1 \\
0 & 1 & 0
\end{bmatrix},
\]

\[
f_{-1,j,k} : \frac{1}{12} \begin{bmatrix}
0 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 0
\end{bmatrix},
\]

\[
f_{1,j,k} : \frac{1}{12} \begin{bmatrix}
0 & 0 & 0 \\
0 & 3 & 0 \\
0 & 0 & 0
\end{bmatrix},
\]

\[
(6.9)
\]

\[
g_{j,k} : \frac{1}{h} \begin{bmatrix}
0 & 0 & 0 \\
0 & -2 & 0 \\
0 & 0 & 0
\end{bmatrix}.
\]

\[
(6.10)
\]

Note that the discretization of the Neumann boundary condition is the same as the ghost point method, but the right hand side \(f_{ij,k}\) has been adjusted.

**Theorem 6.1.** Let \(U_{ij,k}\) be the finite difference solution obtained from the fourth order scheme with the set of the solution of the finite difference coefficients given above. Then, the algorithm is exact if the solution is any fourth order polynomials when \(K = \sigma = 0\). For general solutions \(u(x, y) \in C^6(\mathcal{R})\), we have the following error estimate,

\[
\|u(x_i, y_j, z_k) - U_{ij,k}\|_{\infty} \leq C h^4.
\]

\[
(6.11)
\]

**Example 3.** A three dimensional example:

\[
u(x, y, z) = \sin(k_1 x) \sin(k_2 y) \sin(k_3 z), \quad (x, y, z) \in (0, 1)^3,
\]

\[
f(x, y, z) = - (k_1^2 + k_2^2 + k_3^2) \sin(k_1 x) \sin(k_2 y) \sin(k_3 z), \quad (x, y, z) \in (0, 1)^3,
\]

\[
\left(\frac{\partial u}{\partial n} + \sigma u\right)_{x=0} = \left( -k_1 \cos(k_1 x) + \sigma \sin(k_1 x) \right) \sin(k_2 y) \sin(k_3 z), \quad (y, z) \in (0, 1)^2.
\]

In Table 7, we show a grid refinement analysis with \(k_1 = 1, k_2 = 2, k_3 = 10\) and \(\sigma = 2\). Note that, the total degree of freedom of the finite difference equations when \(N = 128\) is 2,064,512, more than two millions. We adopt an extrapolation cascading multigrid method with the conjugate gradient (CG) smoother (or BiCGStab if \(A_h\) is non-symmetric) from [21] to solve the sparse linear system. The CPU time is recorded on a Laptop with an Intel(R) Core(TM) i7-8565U CPU @ 1.80GHz and 8.0 GB RAM. We can see clearly a fourth order convergence.
A grid refinement analysis for the 3D example with a Robin BC at $x = 0$. Fourth order convergence can be seen clearly. An extrapolation cascadic multigrid method with the conjugate gradient (CG) smoother [21] is used to solve the linear systems.

| $N$  | $\|E\|_\infty$  | order | CPU  |
|------|----------------|-------|------|
| 8    | 5.9285e-03     | <0.01 s |      |
| 16   | 3.8247e-04     | 0.02 s  |      |
| 32   | 2.3691e-05     | 0.13 s  |      |
| 64   | 1.4883e-05     | 1.32 s  |      |
| 128  | 9.2985e-08     | 11.00 s |      |

7. Conclusions and discussions. In this paper, we have solved an important problem in computational mathematics, that is, whether there exist fourth order compact schemes for Poisson, Helmholtz, and diffusion-advection equations with flux type boundary conditions. The answer is yes if we can extend the source term $f$ to one grid line (surface in 3D) with a quadratic extension that is third order accurate. Without the $f$-extension, then we probably can only achieve super-third convergence in which the HOC methods have been developed in this paper. Using a brand new approach, we have developed new fourth order compact schemes in both 2D and 3D that can guarantee the consistence, stability, so the convergence.

The new idea and methodology have also been applied to anisotropic diffusion and advection equations with Dirichlet, Neumann, or Robin BCs with constant coefficients. Fourth order convergence has been proved for Dirichlet boundary conditions while super-third convergence has been proved for flux boundary conditions. So it is still an open question to develop fourth order compact schemes for anisotropic diffusion and advection equations with flux boundary conditions. Technically, the new idea can be applied to BVP of elliptic PDEs with variable coefficients but are not recommended due to the computational cost. This is because for variable coefficient PDEs, the coefficient matrix for the finite difference and weight coefficients would be different at every grid point. We need to solve $O(N^2)$ such systems of equations with the sign constraint for 2D problems. Thus, the computational cost would be overwhelming. We also need the first, second order partial derivatives of the variable coefficients. For constant coefficient PDE, the coefficients of the finite difference equations are just needed to be computed once for all.

While the developed methods are for rectangular domains, we think the methods still can work for polygonal domain such as an L-shaped domain as long as all boundary segments are parallel to one of the axes. For general curved boundary, we can derive third order accurate compact schemes using the augmented approach developed in [22]. But we are not sure about fourth order compact schemes and think it will be very challenging for developing such schemes.

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Appendix A. High order PDE relations for general elliptic PDEs with constant coefficients.

To derive the fourth order compact finite difference scheme for an anisotropic diffusion and advection equations,

\[ A_{11}u_{xx} + 2A_{12}u_{xy} + A_{22}u_{yy} + au_x + bu_y + Ku = f, \]  

with a Dirichlet or Robin boundary conditions, we need more PDE relations in order to derive high order compact schemes.

**Lemma A.1.** Let \( u(x, y) \in C^5(\mathbb{R}) \) be the solution to \((A.1)\), then the following relations are true.

\[
\begin{align*}
A_{11}u_{xx} + 2A_{12}u_{xy} + A_{22}u_{yy} + au_x + bu_y + Ku &= f, \\
A_{11}u_{xx} + 2A_{12}u_{xy} + A_{22}u_{yy} + au_x + bu_y + Ku &= f, \\
A_{11}u_{xx} + 2A_{12}u_{xy} + A_{22}u_{yy} + au_x + bu_y + Ku &= f, \\
A_{11}u_{xx} + 2A_{12}u_{xy} + A_{22}u_{yy} + au_x + bu_y + Ku &= f, \\
A_{11}u_{xx} + 2A_{12}u_{xy} + A_{22}u_{yy} + au_x + bu_y + Ku &= f, \\
A_{11}u_{xx} + 2A_{12}u_{xy} + A_{22}u_{yy} + au_x + bu_y + Ku &= f.
\end{align*}
\]

A.1. The linear system of equations of the FD coefficients at interior grid points for diffusion and advection equations. The finite difference coefficients \( \alpha_{ij, jk} \) and \( \beta_{ij, jk} \) for interior grid points are determined from the following system of equations. The first six equations (required for all quadratic
polynomials) are,

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} - K = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{i_k} - K \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{j_k} - K \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{j_k} = 0
\]

(A.2)

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^2}{2} \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( A_{11} + \frac{h_{i_k}^2}{2} K + ah_{i_k} \right) = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{j_k}^2}{2} \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( A_{22} + \frac{h_{j_k}^2}{2} K + bh_{j_k} \right) = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{i_k} h_{j_k} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( 2A_{12} + h_{i_k} h_{j_k} K + bh_{i_k} + ah_{j_k} \right) = 0.
\]

The next four equations (required for cubic polynomials) are

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^3}{3!} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} \left( A_{11} + a \frac{h_{i_k}}{2} \right) = 0
\]

(A.3)

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{j_k}^2}{2} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( A_{11} h_{j_k} + 2A_{12} h_{i_k} + a h_{i_k} h_{j_k} + b \frac{h_{j_k}^2}{2} \right) = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k} h_{j_k}^2}{2} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( A_{22} h_{i_k} + 2A_{12} h_{j_k} + a \frac{h_{j_k}^2}{2} + b h_{i_k} h_{j_k} \right) = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^3}{3!} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} \left( A_{22} + b \frac{h_{j_k}}{2} \right) = 0.
\]

The next five equations (required for quartic polynomials) are

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^4}{4!} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{i_k} \frac{h_{i_k}^2}{2} A_{11} = 0
\]

(A.4)

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k} h_{j_k}^3}{3!} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( h_{i_k} h_{j_k} A_{11} + h_{i_k}^2 A_{12} \right) = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{6h_{i_k}^2 h_{j_k}^2}{4!} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( \frac{h_{i_k}^2}{2} A_{11} + 2h_{i_k} h_{j_k} A_{12} + \frac{h_{j_k}^2}{2} A_{22} \right) = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k} h_{j_k}^3}{3!} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} \left( h_{i_k} h_{j_k} A_{22} + h_{j_k}^2 A_{12} \right) = 0
\]

\[
\sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^4}{4!} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{j_k} \frac{h_{j_k}^2}{2} A_{22} = 0.
\]

A.2. The linear system of equations of the FD coefficients at a flux boundary grid points for diffusion and advection equations. For a flux Robin condition. The linear system of equations for the FD coefficients has similar form as above but the summation \( \sum_{i_k=-1}^{1} \) changes to \( \sum_{i_k=0}^{1} \) in all equations involving \( \alpha_{i_k,j_k} \) terms. The first-third, fifth-sixth, nine-tenth, fourteenth, and sixteenth equations will need
to be changed to
(A.5)

\[ \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{i_k} - K - \sigma \sum_{j_k=-1}^{1} \gamma_{j_k} = 0 \]

\[ \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{i_k} - K + \beta_{i_k,j_k} h_{i_k} + \gamma_{j_k} A_{11} = 0 \]

\[ \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{j_k} - K + \beta_{i_k,j_k} h_{j_k} - \gamma_{j_k} (\sigma h_{j_k} - A_{12}) = 0 \]

\[ \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{j_k}^2}{2} - \beta_{i_k,j_k} \left( A_{22} + \frac{h_{j_k}^2}{2} K + bh_{j_k} \right) - \sigma \sum_{j_k=-1}^{1} \gamma_{j_k} \left( \frac{h_{j_k}^2}{2} - A_{12} h_{j_k} \right) = 0 \]

\[ \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} h_{i_k} h_{j_k} = \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} (2A_{12} + h_{i_k} h_{j_k} K + bh_{i_k} + ah_{j_k}) + \gamma_{j_k} A_{11} h_{j_k} = 0 \]

\[ \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{j_k}^3}{3!} - \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \beta_{i_k,j_k} h_{j_k} \left( A_{22} + b \frac{h_{j_k}}{2} \right) - \sigma \sum_{j_k=-1}^{1} \gamma_{j_k} \frac{h_{j_k}^3}{3!} = 0 \]

\[ \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^2}{2} - \beta_{i_k,j_k} \left( A_{22} h_{i_k} + 2A_{12} h_{j_k} + a \frac{h_{j_k}^2}{2} + bh_{i_k} h_{j_k} \right) \]

\[ - \sum_{j_k=-1}^{1} \gamma_{j_k} \left( A_{12} \frac{h_{j_k}^3}{3!} - A_{12} \frac{h_{j_k}^2}{2} \right) = 0 \]

\[ \sum_{i_k=-1}^{1} \sum_{j_k=0}^{1} \alpha_{i_k,j_k} \frac{h_{i_k}^3}{3!} - \sum_{i_k=-1}^{1} \sum_{j_k=0}^{1} \beta_{i_k,j_k} (h_{i_k} h_{j_k} A_{22} + h_{j_k}^2 A_{12}) + \gamma_{j_k} A_{11} \frac{h_{j_k}^3}{3!} = 0 \]

\[ \sum_{i_k=-1}^{1} \sum_{j_k=-1}^{1} \alpha_{i_k,j_k} \frac{h_{j_k}^4}{4!} - \beta_{i_k,j_k} \left( \frac{h_{j_k}^2}{2} A_{22} + \gamma_{j_k} A_{12} \frac{h_{j_k}^3}{3!} \right) = 0. \]

A.3. Finite difference coefficients of $U_{ij}$ for diffusion and advection equations.

A.4. Combination coefficients of $f_{ij}$ terms for diffusion and advection equations.
Fig. 9. Finite difference coefficients for diffusion-advection equations at interior grid points computed with Maple. Note that the sign property holds when \( h \) or \( a \) and \( b \) are sufficient small.

\[
\begin{align*}
\frac{\partial^2 u}{\partial t^2} + 2 a^2 \frac{\partial^2 u}{\partial x^2} + 2 a^2 \frac{\partial^2 u}{\partial y^2} + a^2 \frac{\partial^2 u}{\partial z^2} - 3 a^2 \frac{\partial u}{\partial x} + 6 a^2 \frac{\partial u}{\partial y} + 42 a^2 \frac{\partial u}{\partial z} + 42 a^2 \frac{\partial^2 u}{\partial x \partial y} + 6 b^2 \frac{\partial^2 u}{\partial x \partial z} - 36 a^2 \frac{\partial^2 u}{\partial y \partial z} - 72 a b \frac{\partial u}{\partial x} - 36 b^2 \frac{\partial u}{\partial x} + 144 a b + 144 b h - 288 h^2 &= 0. \\
12 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right) \\
\frac{\partial^2 b}{\partial t^2} - a^2 b^2 h^2 + 8 a^2 b^2 h^2 + 6 a^2 b^2 h^2 - 50 b^2 h^2 + 36 a^2 b^2 h^2 - 108 b^2 h^2 - 288 b a + 576 \\
6 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right) \\
\frac{\partial^2 a}{\partial t^2} - 2 a^2 b^2 h^2 + 2 a^2 b^2 h^2 - a^2 b^2 h^2 - 3 a^2 h^2 + 4 a^2 b^2 h^2 - 3 a^2 b^2 h^2 - 6 a^2 h^2 + 42 a^2 b^2 h^2 - 42 a^2 b^2 h^2 + 6 b^2 h^2 + 36 a^2 h^2 - 72 a b h^2 + 36 b^2 h^2 - 144 a b + 144 b h + 288 \\
12 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right) \\
\frac{\partial^2 b}{\partial t^2} - a^2 b^2 h^2 - 8 a^2 b^2 h^2 + 4 a^2 b^2 h^2 + 3 a^2 h^2 - 6 a^2 h^2 + 42 a^2 b^2 h^2 - 42 a^2 b^2 h^2 + 6 b^2 h^2 + 36 a^2 h^2 - 72 a b h^2 + 36 b^2 h^2 - 144 a b + 144 b h + 288 \\
6 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right) \\
\frac{\partial^2 a}{\partial t^2} - 2 a^2 b^2 h^2 - 2 a^2 b^2 h^2 - a^2 b^2 h^2 - 3 a^2 h^2 + 4 a^2 b^2 h^2 - 3 a^2 b^2 h^2 - 6 a^2 h^2 + 42 a^2 b^2 h^2 - 42 a^2 b^2 h^2 + 6 b^2 h^2 + 36 a^2 h^2 - 72 a b h^2 + 36 b^2 h^2 - 144 a b + 144 b h + 288 \\
12 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right) \\
\frac{\partial^2 b}{\partial t^2} - a^2 b^2 h^2 - 8 a^2 b^2 h^2 + 4 a^2 b^2 h^2 + 3 a^2 h^2 - 6 a^2 h^2 + 42 a^2 b^2 h^2 - 42 a^2 b^2 h^2 + 6 b^2 h^2 + 36 a^2 h^2 - 72 a b h^2 + 36 b^2 h^2 - 144 a b + 144 b h + 288 \\
6 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right) \\
\frac{\partial^2 a}{\partial t^2} - 2 a^2 b^2 h^2 - 2 a^2 b^2 h^2 - a^2 b^2 h^2 - 3 a^2 h^2 + 4 a^2 b^2 h^2 - 3 a^2 b^2 h^2 - 6 a^2 h^2 + 42 a^2 b^2 h^2 - 42 a^2 b^2 h^2 + 6 b^2 h^2 + 36 a^2 h^2 - 72 a b h^2 + 36 b^2 h^2 - 144 a b + 144 b h + 288 \\
12 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right) \\
\frac{\partial^2 b}{\partial t^2} - a^2 b^2 h^2 - 8 a^2 b^2 h^2 + 4 a^2 b^2 h^2 + 3 a^2 h^2 - 6 a^2 h^2 + 42 a^2 b^2 h^2 - 42 a^2 b^2 h^2 + 6 b^2 h^2 + 36 a^2 h^2 - 72 a b h^2 + 36 b^2 h^2 - 144 a b + 144 b h + 288 \\
6 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right) \\
\frac{\partial^2 a}{\partial t^2} - 2 a^2 b^2 h^2 - 2 a^2 b^2 h^2 - a^2 b^2 h^2 - 3 a^2 h^2 + 4 a^2 b^2 h^2 - 3 a^2 b^2 h^2 - 6 a^2 h^2 + 42 a^2 b^2 h^2 - 42 a^2 b^2 h^2 + 6 b^2 h^2 + 36 a^2 h^2 - 72 a b h^2 + 36 b^2 h^2 - 144 a b + 144 b h + 288 \\
12 h^2 \left( a^2 b^2 h^2 + 12 a^2 b^2 h^2 + 12 b^2 h^2 + 144 \right)
\end{align*}
\]

Fig. 10. Combination coefficients of \( f_{ij} \)'s whose sum equals one for interior diffusion-advection equations computed at interior grid points with Maple.