

HIGH-ORDER, COMPACT, AND SYMMETRIC FINITE DIFFERENCE METHODS FOR A d -DIMENSIONAL HYPERCUBE *

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Abstract. This paper presents compact, symmetric, and high-order finite difference methods (FDMs) for the variable Poisson equation on a d -dimensional hypercube. Our scheme produces a symmetric linear system: an important property that does not immediately hold for a high-order FDM. Since the model problem is coercive, the linear system is in fact symmetric positive definite, and consequently many fast solvers are applicable. Furthermore, the symmetry combined with the minimum support of the stencil keeps the storage requirement minimal. Theoretically speaking, we prove that a compact, symmetric 1D FDM on a uniform grid can achieve arbitrary consistency order. On the other hand, in the d -dimensional setting, where $d \geq 2$, the maximum consistency order that a compact, symmetric FDM on a uniform grid can achieve is 4. If $d = 2$ and the diffusion coefficient satisfies a certain derivative condition, the maximum consistency order is 6. Moreover, the finite compact, symmetric, 4th-order FDMs for $d \geq 3$, can be conveniently expressed as a linear combination of two types of FDMs: one that depends on partial derivatives along one axis, and the other along two axes. All finite difference stencils are explicitly provided for ease of reproducibility.

Key words. Compact symmetric finite difference methods, high-order schemes, elliptic PDE with variable coefficients, symmetric linear systems

MSC codes. 65N06, 35J25

1. Introduction. In this paper, we are concerned with the construction of high-order compact finite difference methods (FDMs) for the following variable Poisson equation on a d -dimensional hypercube:

$$(1.1) \quad \begin{cases} \mathcal{L}u := -\nabla \cdot (a \nabla u) = f & \text{in } \Omega, \\ u = g & \text{on } \partial\Omega, \end{cases}$$

where $\Omega = (0,1)^d$, a, f, g are sufficiently smooth functions, $a(\mathbf{x}) > 0$ for all $\mathbf{x} \in \Omega$, and $d \in \mathbb{N}$. The above Poisson equation with a variable diffusion coefficient, a , is known to model many physical phenomena such as fluid flow in heterogeneous media [1], steady-state heat conduction in media where the thermal conductivity varies, electrostatic potential from a charge distribution [6], and semiconductors [13]. Over the years, various numerical methods have been proposed to solve it, including the finite difference method (FDM) [10, 12].

Whenever possible, it is preferable to use a high-order scheme for numerically solving (1.1), since the linear system required to achieve a certain accuracy is smaller than that of a low-order scheme and the error decays faster as we refine the grid. At the same time, having a scheme that produces a symmetric linear system is also beneficial as it reduces the storage requirement and allows us to use many available fast solvers given that the model problem in (1.1) is also coercive. We automatically obtain a symmetric (positive definite) linear system if we discretize (1.1) using a standard finite element or Galerkin method (due to the inner products in its weak

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formulation), but not necessarily from FDMs. Although a compact, symmetric, and 2nd-order FDM is well-known (see [12] for example), it is surprising that no work exists on its high-order counterpart—at least to the best of our knowledge.

One way to increase the order of the scheme is by enlarging the stencil size, but this inevitably increases the number of nonzero entries in the linear system. Furthermore, extra boundary stencils must be constructed separately near the boundary of the domain, which is inconvenient. Therefore, it is natural to consider a compact FDM, where each stencil has a 1-ring (minimum support), since the boundary stencils for the Dirichlet boundary condition in (1.1) are simply subsets of the interior stencils.

Many studies have focused on the maximum order attainable by a compact FDM. In the d -dimensional setting with $d \geq 1$, this corresponds to a 3^d -point stencil. In 1D, one can achieve a compact and arbitrarily high-order FDM for (1.1) with piecewise smooth a [7], but the finite difference stencil is not symmetric (i.e., the resulting linear system is not symmetric). This result generalizes the 1D result of [14] for (1.1) with $a = 1$. In 2D, the maximum order attainable by a compact FDM is 6. This fact was discovered by [2, 3, 14] for $a = 1$, [4] for a smooth variable a on a rectangular domain, and [8] for a smooth variable a on a curved domain. The authors of [16, 18] also proposed 6th-order 2D FDMs for (1.1) with $a = 1$. Although compact, the finite difference stencils proposed by [4, 8] are not symmetric. If a quasi-uniform or non-uniform grid is used, then the maximum order attainable becomes 4 and 3 respectively for $a = 1$ [2]. In 3D, [2, 5, 15, 17] presented various 6th-order FDMs for $a = 1$. In fact, the author of [2] proved stronger results, which state that the maximum order attainable by a compact symmetric FDM for solving the Poisson equation ($a = 1$) with a periodic boundary condition is 6 for all $d \geq 2$, and that for any dimension d , there exists an arbitrarily high-order FDM for (1.1) with $a = 1$, but it is not compact. These FDMs normally involve derivatives of the diffusion coefficient a and the source term f , but they can be replaced by their function values, as discussed in [4, 5, 8, 16].

Given the importance of such FDMs and the current state of the literature, we aim to investigate the maximum order attainable by a compact symmetric FDM for solving (1.1) with a smooth variable a in the d -dimensional setting. To the best of our knowledge, this issue has not been addressed in the literature and this is precisely where our contributions lie.

1.1. Main contributions. We develop high-order, compact, and symmetric finite difference schemes on a uniform grid for (1.1). In the one-dimensional setting, we show that the maximum order attainable by such compact symmetric finite difference schemes can be as high as we wish. Meanwhile, in the d -dimensional setting, where $d \geq 2$, we prove that the maximum order attainable by a non-symmetric compact finite difference scheme is 6. If we further require our finite difference stencils to be symmetric (so that the resulting linear system is symmetric), then the maximum order attainable is 4. In the 2D setting, we can still obtain a compact, symmetric, 6th-order finite difference scheme if the coefficient a in (1.1) satisfies a certain derivative condition. Our technique recovers all such schemes derived from Taylor expansions. Some remaining free parameters in these schemes can be optimized to reduce the magnitude of the leading truncation error term. A dimensional reduction strategy is employed to transform the analysis of a higher-dimensional problem into a 2D one, thereby enabling the application of 2D results, which are readily verifiable using symbolic computation. What is more interesting is that, in the d -dimensional setting, these compact symmetric finite difference schemes can be written as a linear combination of two types of schemes: one involves partial derivatives along a single axis of the

data in (1.1), while the other involves partial derivatives along two axes. For ease of reproducibility, the constructed finite difference stencils are explicitly given. Finally, we demonstrate the computational benefits of using compact, symmetric, high-order finite difference schemes in obtaining fast accurate solutions through several examples.

1.2. Organization. For readers' convenience, we list the notations and definitions in Section 2. Section 3 discusses the construction of compact, symmetric, and arbitrarily high-order FDMs in the one-dimensional setting. Section 4 presents compact, symmetric, and 4th-order FDMs in the d -dimensional setting, where $d \geq 2$. To verify our theoretical findings, we provide some numerical experiments in Section 5. We discuss the derivation details of the FDMs in Section 4 and prove that there is a limit to the consistency order achievable by a compact FDM in Section 6. Finally, we present our concluding remarks in Section 7.

2. Notations and definitions. For the sake of clarity, we list the notations and definitions that we use throughout the paper:

- $\mathbb{N}_0$ stands for the set all nonnegative integers $\mathbb{N} \cup \{0\}$.
- The standard unit vector basis of $\mathbb{R}^d$ is denoted by $\vec{e}_j$ with $1 \leq j \leq d$, while d -dimensional zero vector is denoted by $\vec{0}$. The symbol $\rightarrow$ on top of a variable indicates that it is a d -dimensional real vector.
- Let $\mathbf{k} \in \mathbb{N}_0^d$ such that $\mathbf{k} := (k_1, \dots, k_d)$. The sum of the components of a multi-index $\mathbf{k}$ is given by $|\mathbf{k}| := \sum_{j=1}^d k_j$. For $\ell \in \mathbb{N}_0^d$, we say that $\mathbf{k} \leq \ell$ if $k_j \leq \ell_j$ for all $1 \leq j \leq d$. Meanwhile, if $\vec{0} \leq \ell \leq \mathbf{k}$, the binomial coefficient is defined as $\binom{\mathbf{k}}{\ell} := \prod_{j=1}^d \binom{k_j}{\ell_j}$.
- For a smooth function v , $\partial^{\mathbf{k}}v$ stands for its $\mathbf{k}$ -th partial derivative.
- We use $\mathbf{c}^* \in \Omega$ to denote the center (base) point of a finite difference stencil.
- The notation $\mathcal{O}(h^M)$ with various subscripts refers to a function that is bounded by Ch^M as $h \rightarrow 0^+$, where the constant C only depends on the expressions and their derivatives in the subscript, and C remains bounded if its dependencies are bounded.
- $\delta(k)$, $k \in \mathbb{Z}$, is the sequence such that $\delta(0) := 1$ and $\delta(k) := 0$ for $k \neq 0$.

Next, we formally define what it means for a finite difference scheme to be compact, symmetric, and M th-order consistent. Throughout this paper, unless otherwise stated, we assume that we have a uniform grid on the domain $\Omega := (0, 1)^d$ with mesh size $h = N^{-1}$, $N \in \mathbb{N}$, and define $\Omega_h := \Omega \cap (h\mathbb{Z}^d)$.

DEFINITION 2.1. Consider a finite difference scheme $\mathcal{L}_h u_h = f_h$ for (1.1) on Ω_h , where u_h and f_h are grid functions on Ω_h (i.e., $u_h, f_h : \Omega_h \rightarrow \mathbb{R}$), f_h depends on a , f , g , as well as their derivatives, and the discretization operator $\mathcal{L}_h$ has the form

$$(2.1) \quad \mathcal{L}_h u_h(\mathbf{c}^*) = \sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) u_h(\mathbf{c}^* + ph) \quad \text{for all } \mathbf{c}^* \in \Omega_h,$$

where $C_p(\mathbf{c}^*) \in \mathbb{R}$ and $\mathcal{S} = \{-1, 0, 1\}^d$. Such a scheme is called compact.

(a) The finite difference scheme $\mathcal{L}_h u_h = f_h$ is also symmetric if

$$(2.2) \quad C_p(\mathbf{c}^*) = C_{-p}(\mathbf{c}^* + ph) \quad \forall \mathbf{c}^* \in \Omega_h, p \in \mathcal{S}.$$

(b) Suppose f_h has a magnitude of $\Lambda(h) > 0$; i.e., $\Lambda(h)$ depends only on h and $\{f_h/\Lambda(h) : h > 0\}$ is bounded away from 0 and ∞ except when $f, g = 0$. The finite difference scheme $\mathcal{L}_h u_h = f_h$ is also M th-order consistent for some

$M \in \mathbb{N}$ if

$$(2.3) \quad \sup_{\mathbf{c}^* \in \Omega_h} |\mathcal{L}_h u(\mathbf{c}^*) - f_h(\mathbf{c}^*)| = \mathcal{O}(\Lambda(h)h^M), \quad \forall u \in C^\infty(\overline{\Omega}),$$

where f_h is viewed as the result of a well-defined mapping on u .

Condition (2.3) means the scheme produces a relative error of order h^M , instead of an absolute error. This prevents the trivial multiplication of $o(1)$ factors in the stencil coefficients $C_p(\mathbf{c}^*)$. The use of relative error is also crucial in proving the convergence of the numerical solution of the FDMs, which we shall deal with in subsequent works.

3. Construction of compact, symmetric, and arbitrary high-order 1D FDMs. We begin the discussion of the construction of compact, symmetric, and high-order FDMs by considering the 1D case. Note that $\mathcal{S} = \{-1, 0, 1\}$. The center point of a 1D finite difference stencil is a scalar, and thus we denote it by c^* . The following theorem shows that a 1D compact, symmetric FDM can achieve arbitrarily high consistency order.

THEOREM 3.1. *Let M be a positive integer, $0 < h < 1$, and $c^* \in (0, 1)$ with $(c^* - h, c^* + h) \subset (0, 1)$. Assume that a and f are functions that are M and $M-1$ times differentiable respectively. There is a compact, symmetric, and M th-order consistent finite difference scheme for (1.1) given by*

$$\begin{aligned} \mathcal{L}_h u(c^*) &:= C_{-1}(h)u(c^* - h) + C_0(h)u(c^*) + C_1(h)u(c^* + h) \\ &= \sum_{\ell=0}^{M-1} d_\ell(h)h^{\ell+2}f^{(\ell)}(c^*) + \mathcal{O}_{a,f}(h^{M+2}), \end{aligned}$$

where C_{-1} , C_0 , C_1 , and d_ℓ are defined as

$$(3.1) \quad \begin{aligned} C_1(h) &= \mathcal{E}^M(c^* + \frac{h}{2}), \quad C_{-1}(h) = C_1(-h), \quad C_0(h) = -C_1(h) - C_{-1}(h), \quad \text{and} \\ d_\ell(h) &= \frac{2((-1)^{\ell+1} - 1)}{2^{\ell+2}(\ell+1)!} + \sum_{k=0}^{\ell} \frac{C_{-1}(h)(-1)^{\ell-k+1}\mathcal{G}_k(c^* - \frac{h}{2}) + C_1(h)\mathcal{G}_k(c^* + \frac{h}{2})}{2^{\ell+2}(\ell-k)!}, \end{aligned}$$

such that

$$(3.2) \quad \begin{aligned} \mathcal{E}^M(\cdot) &:= 2a(\cdot) \left(2 + \sum_{j=2}^{M+1} \frac{E_{j,1}(\cdot)}{j!} \left(\frac{h}{2} \right)^{j-1} (1 + (-1)^{j-1}) \right)^{-1} + \mathcal{O}_a(h^{M+1}), \\ \mathcal{G}_k(\cdot) &:= \sum_{j=k+2}^{M+1} \frac{F_{j,k}(\cdot)}{j!} \left(\frac{h}{2} \right)^{j-k-2} (1 + (-1)^{j-1}), \end{aligned}$$

and the quantities $E_{j,1}$, $F_{j,k}$ can be computed using these recursion relations

$$\begin{aligned} E_{2,1} &= -\frac{a'}{a}, \quad E_{j+1,1} = E'_{j,1} - \frac{a'}{a}E_{j,1}, \\ F_{2,0} &= \frac{1}{a}, \quad F_{j,-1} = \frac{E_{j,1}}{a}, \quad F_{j+1,k} = F'_{j,k} + F_{j,k-1}. \end{aligned}$$

Proof. We recall a few basic facts. By [7, Proposition 3.1], for any $b^* \in [0, 1]$,

$$(3.3) \quad \begin{aligned} u(b^* + h) &= u(b^*) + u'(b^*)h \left(1 + \sum_{j=2}^{M+1} \frac{E_{j,1}(b^*)}{j!} h^{j-1} \right) \\ &\quad + \sum_{\ell=0}^{M-1} h^{\ell+2} f^{(\ell)}(b^*) \left(\sum_{j=\ell+2}^{M+1} \frac{F_{j,\ell}(b^*)}{j!} h^{j-\ell-2} \right) + \mathcal{O}_{a,f}(h^{M+2}), \end{aligned}$$

where the quantities $E_{j,1}$, $F_{j,k}$ are computed using the above recursions. Furthermore, if we define $v := au'$, take the Taylor expansion of $v(b^* + h)$ about the point b^* , and use the fact that $-(au')' = f$, we have

$$(3.4) \quad \begin{aligned} a(b^* + h)u'(b^* + h) &= a(b^*)u'(b^*) + \sum_{j=1}^M \frac{(au')^{(j)}(b^*)}{j!} h^j + \mathcal{O}_{a,f}(h^{M+1}) \\ &= a(b^*)u'(b^*) - \sum_{j=1}^M \frac{f^{(j-1)}(b^*)}{j!} h^j + \mathcal{O}_{a,f}(h^{M+1}). \end{aligned}$$

Now, we expand $u(c^*) - u(c^* - h)$ about the point $c^* - h/2$ by using (3.3). More specifically, to expand $u(c^*)$, we let $b^* = c^* - h/2$ and replace h with $h/2$ in (3.3). On the other hand, to expand $u(c^* - h)$, we let $b^* = c^* - h/2$ and replace h with $-h/2$ in (3.3). We do a similar expansion for $u(c^* + h) - u(c^*)$ about the point $c^* + h/2$ to get the following results

$$\begin{aligned} u(c^*) - u(c^* - h) &= u'(c^* - \frac{h}{2}) \left(2 + \sum_{j=2}^{M+1} \frac{E_{j,1}(c^* - h/2)}{j!} (\frac{h}{2})^{j-1} (1 + (-1)^{j-1}) \right) \frac{h}{2} \\ &\quad + \sum_{\ell=0}^{M-1} f^{(\ell)}(c^* - \frac{h}{2}) \mathcal{G}_\ell(c^* - \frac{h}{2}) (\frac{h}{2})^{\ell+2} + \mathcal{O}_{a,f}(h^{M+2}), \\ u(c^* + h) - u(c^*) &= u'(c^* + \frac{h}{2}) \left(2 + \sum_{j=2}^{M+1} \frac{E_{j,1}(c^* + h/2)}{j!} (\frac{h}{2})^{j-1} (1 + (-1)^{j-1}) \right) \frac{h}{2} \\ &\quad + \sum_{\ell=0}^{M-1} f^{(\ell)}(c^* + \frac{h}{2}) \mathcal{G}_\ell(c^* + \frac{h}{2}) (\frac{h}{2})^{\ell+2} + \mathcal{O}_{a,f}(h^{M+2}), \end{aligned}$$

where $\mathcal{G}_\ell$ is defined in (3.2). Using C_{-1}, C_0, C_1 in (3.1), we have

$$\begin{aligned} &C_{-1}(h)u(c^* - h) + C_0(h)u(c^*) + C_1(h)u(c^* + h) \\ &= -C_{-1}(h)(u(c^*) - u(c^* - h)) + C_1(h)(u(c^* + h) - u(c^*)) \\ &= -a(c^* - \frac{h}{2})u'(c^* - \frac{h}{2})h - C_{-1}(h) \sum_{\ell=0}^{M-1} f^{(\ell)}(c^* - \frac{h}{2}) \mathcal{G}_\ell(c^* - \frac{h}{2}) (\frac{h}{2})^{\ell+2} \\ &\quad + a(c^* + \frac{h}{2})u'(c^* + \frac{h}{2})h + C_1(h) \sum_{\ell=0}^{M-1} f^{(\ell)}(c^* + \frac{h}{2}) \mathcal{G}_\ell(c^* + \frac{h}{2}) (\frac{h}{2})^{\ell+2} \\ &\quad + \mathcal{O}_{a,f}(h^{M+2}) \end{aligned}$$

$$\begin{aligned}
&= 2 \sum_{j=1}^M \frac{f^{(j-1)}(c^*)}{j!} ((-1)^j - 1) \left(\frac{h}{2}\right)^{j+1} - C_{-1}(h) \sum_{\ell=0}^{M-1} f^{(\ell)}(c^* - \frac{h}{2}) \mathcal{G}_\ell(c^* - \frac{h}{2}) \left(\frac{h}{2}\right)^{\ell+2} \\
&\quad + C_1(h) \sum_{\ell=0}^{M-1} f^{(\ell)}(c^* + \frac{h}{2}) \mathcal{G}_\ell(c^* + \frac{h}{2}) \left(\frac{h}{2}\right)^{\ell+2} + \mathcal{O}_{a,f}(h^{M+2}) \\
&= \sum_{\ell=0}^{M-1} \sum_{j=0}^{M-1-\ell} \frac{f^{(\ell+j)}(c^*)}{j!} \left(-C_{-1}(h)(-1)^j \mathcal{G}_\ell(c^* - \frac{h}{2}) + C_1(h) \mathcal{G}_\ell(c^* + \frac{h}{2}) \right) \left(\frac{h}{2}\right)^{\ell+j+2} \\
&\quad + 2 \sum_{j=0}^{M-1} \frac{f^{(j)}(c^*)}{(j+1)!} ((-1)^{j+1} - 1) \left(\frac{h}{2}\right)^{j+2} + \mathcal{O}_{a,f}(h^{M+2}) \\
&= \sum_{\ell=0}^{M-1} \frac{f^{(\ell)}(c^*)}{2^{\ell+2}} \left(\frac{2((-1)^{\ell+1} - 1)}{(\ell+1)!} \right. \\
&\quad \left. + \sum_{k=0}^{\ell} \frac{C_{-1}(h)(-1)^{\ell-k+1} \mathcal{G}_k(c^* - \frac{h}{2}) + C_1(h) \mathcal{G}_k(c^* + \frac{h}{2})}{(\ell-k)!} \right) h^{\ell+2} + \mathcal{O}_{a,f}(h^{M+2}),
\end{aligned}$$

where we expanded $f^{(\ell)}(c^* - \frac{h}{2})$ and $f^{(\ell)}(c^* + \frac{h}{2})$ about the point c^* to arrive at the second last line, and rearrange the indices to obtain the final line. The above calculation implies that

$$C_{-1}(h)u(c^* - h) + C_0(h)u(c^*) + C_1(h)u(c^* + h) = \sum_{\ell=0}^{M-1} d_\ell(h)h^{\ell+2}f^{(\ell)}(c^*) + \mathcal{O}_{a,f}(h^{M+2}),$$

where $d_\ell(h)$ is defined in (3.1). Finally, setting $f_h(c^*) = \sum_{\ell=0}^{M-1} d_\ell(h)h^{\ell+2}f^{(\ell)}(c^*)$, we have $f_h(c^*) = d_0(0)h^2f(c^*) + \mathcal{O}_{a,f}(h^3) = -f(c^*)h^2 + \frac{1}{4}(C_1(0) - C_{-1}(0))\mathcal{G}_0(c^*)f(c^*)h^2 + \mathcal{O}_{a,f}(h^3) = -f(c^*)h^2 + \mathcal{O}_{a,f}(h^3)$. Therefore, the finite difference scheme $\mathcal{L}_h u_h = f_h$ is M th-order consistent in the sense of (2.3) with $\Lambda(h) = -h^2$. The proof is completed. $\square$

Given the previous theorem, a compact, symmetric, and 12th-order 1D finite difference scheme for (1.1) can be obtained by taking

$$\begin{aligned}
\mathcal{E}^{12}(c^* + \frac{h}{2}) &= a(c^* + \frac{h}{2}) + w_1(c^* + \frac{h}{2})h^2 + w_2(c^* + \frac{h}{2})h^4 + w_3(c^* + \frac{h}{2})h^6 \\
&\quad + w_4(c^* + \frac{h}{2})h^8 + w_5(c^* + \frac{h}{2})h^{10},
\end{aligned}$$

where

$$\begin{aligned}
w_1(x) &:= q_1 \frac{(a^{(1)}(x))^2}{a(x)} + q_2 a^{(2)}(x), \\
w_2(x) &:= q_3 \frac{(a^{(1)}(x))^4}{(a(x))^3} + q_4 \frac{a^{(2)}(x)(a^{(1)}(x))^2}{(a(x))^2} + q_5 \frac{(a^{(2)}(x))^2}{a(x)} + q_6 \frac{a^{(3)}(x)a^{(1)}(x)}{a(x)} + q_7 a^{(4)}(x), \\
w_3(x) &:= q_8 \frac{(a^{(1)}(x))^6}{(a(x))^5} + q_9 \frac{a^{(2)}(x)(a^{(1)}(x))^4}{(a(x))^4} + q_{10} \frac{(a^{(2)}(x))^2(a^{(1)}(x))^2}{(a(x))^3} + q_{11} \frac{(a^{(2)}(x))^3}{(a(x))^2} \\
&\quad + q_{12} \frac{a^{(3)}(x)(a^{(1)}(x))^3}{(a(x))^3} + q_{13} \frac{a^{(3)}(x)a^{(2)}(x)a^{(1)}(x)}{(a(x))^2} + q_{14} \frac{(a^{(3)}(x))^2}{a(x)} \\
&\quad + q_{15} \frac{a^{(4)}(x)(a^{(1)}(x))^2}{(a(x))^2} + q_{16} \frac{a^{(4)}(x)a^{(2)}(x)}{a(x)} + q_{17} \frac{a^{(5)}(x)a^{(1)}(x)}{a(x)} + q_{18} a^{(6)}(x), \\
w_4(x) &:= q_{19} \frac{(a^{(1)}(x))^8}{(a(x))^7} + q_{20} \frac{a^{(2)}(x)(a^{(1)}(x))^6}{(a(x))^6} + q_{21} \frac{(a^{(2)}(x))^2(a^{(1)}(x))^4}{(a(x))^5} \\
&\quad + q_{22} \frac{(a^{(2)}(x))^3(a^{(1)}(x))^2}{(a(x))^4} + q_{23} \frac{(a^{(2)}(x))^4}{(a(x))^3} + q_{24} \frac{a^{(3)}(x)(a^{(1)}(x))^5}{(a(x))^5}
\end{aligned}$$

$$\begin{aligned}
& + q_{25} \frac{a^{(3)}(x)a^{(2)}(x)(a^{(1)}(x))^3}{(a(x))^4} + q_{26} \frac{a^{(3)}(x)(a^{(2)}(x))^2a^{(1)}(x)}{(a(x))^3} + q_{27} \frac{(a^{(3)}(x))^2(a^{(1)}(x))^2}{(a(x))^3} \\
& + q_{28} \frac{(a^{(3)}(x))^2a^{(2)}(x)}{(a(x))^2} + q_{29} \frac{a^{(4)}(x)(a^{(1)}(x))^4}{(a(x))^4} + q_{30} \frac{a^{(4)}(x)a^{(2)}(x)(a^{(1)}(x))^2}{(a(x))^3} \\
& + q_{31} \frac{a^{(4)}(x)(a^{(2)}(x))^2}{(a(x))^2} + q_{32} \frac{a^{(4)}(x)a^{(3)}(x)a^{(1)}(x)}{(a(x))^2} + q_{33} \frac{(a^{(4)}(x))^2}{a(x)} \\
& + q_{34} \frac{a^{(5)}(x)(a^{(1)}(x))^3}{(a(x))^3} + q_{35} \frac{a^{(5)}(x)a^{(2)}(x)a^{(1)}(x)}{(a(x))^2} + q_{36} \frac{a^{(5)}(x)a^{(3)}(x)}{a(x)} \\
& + q_{37} \frac{a^{(6)}(x)(a^{(1)}(x))^2}{(a(x))^2} + q_{38} \frac{a^{(6)}(x)a^{(2)}(x)}{a(x)} + q_{39} \frac{a^{(7)}(x)a^{(1)}(x)}{a(x)} + q_{40} a^{(8)}(x), \\
w_5(x) := & q_{41} \frac{(a^{(1)}(x))^{10}}{(a(x))^9} + q_{42} \frac{a^{(2)}(x)(a^{(1)}(x))^8}{(a(x))^8} + q_{43} \frac{(a^{(2)}(x))^2(a^{(1)}(x))^6}{(a(x))^7} \\
& + q_{44} \frac{(a^{(2)}(x))^3(a^{(1)}(x))^4}{(a(x))^6} + q_{45} \frac{(a^{(2)}(x))^4(a^{(1)}(x))^2}{(a(x))^5} + q_{46} \frac{(a^{(2)}(x))^5}{(a(x))^4} \\
& + q_{47} \frac{a^{(3)}(x)(a^{(1)}(x))^7}{(a(x))^7} + q_{48} \frac{a^{(3)}(x)a^{(2)}(x)(a^{(1)}(x))^5}{(a(x))^6} + q_{49} \frac{a^{(3)}(x)(a^{(2)}(x))^2(a^{(1)}(x))^3}{(a(x))^5} \\
& + q_{50} \frac{a^{(3)}(x)(a^{(2)}(x))^3a^{(1)}(x)}{(a(x))^4} + q_{51} \frac{(a^{(3)}(x))^2(a^{(1)}(x))^4}{(a(x))^5} + q_{52} \frac{(a^{(3)}(x))^2a^{(2)}(x)(a^{(1)}(x))^2}{(a(x))^4} \\
& + q_{53} \frac{(a^{(3)}(x))^2(a^{(2)}(x))^2}{(a(x))^3} + q_{54} \frac{(a^{(3)}(x))^3a^{(1)}(x)}{(a(x))^3} + q_{55} \frac{a^{(4)}(x)(a^{(1)}(x))^6}{(a(x))^6} \\
& + q_{56} \frac{a^{(4)}(x)a^{(2)}(x)(a^{(1)}(x))^4}{(a(x))^5} + q_{57} \frac{a^{(4)}(x)(a^{(2)}(x))^2(a^{(1)}(x))^2}{(a(x))^4} + q_{58} \frac{a^{(4)}(x)(a^{(2)}(x))^3}{(a(x))^3} \\
& + q_{59} \frac{a^{(4)}(x)a^{(3)}(x)(a^{(1)}(x))^3}{(a(x))^4} + q_{60} \frac{a^{(4)}(x)a^{(3)}(x)a^{(2)}(x)a^{(1)}(x)}{(a(x))^3} \\
& + q_{61} \frac{a^{(4)}(x)(a^{(3)}(x))^2}{(a(x))^2} + q_{62} \frac{(a^{(4)}(x))^2(a^{(1)}(x))^2}{(a(x))^3} + q_{63} \frac{(a^{(4)}(x))^2a^{(2)}(x)}{(a(x))^2} \\
& + q_{64} \frac{a^{(5)}(x)(a^{(1)}(x))^5}{(a(x))^5} + q_{65} \frac{a^{(5)}(x)a^{(2)}(x)(a^{(1)}(x))^3}{(a(x))^4} + q_{66} \frac{a^{(5)}(x)(a^{(2)}(x))^2a^{(1)}(x)}{(a(x))^3} \\
& + q_{67} \frac{a^{(5)}(x)a^{(3)}(x)(a^{(1)}(x))^2}{(a(x))^3} + q_{68} \frac{a^{(5)}(x)a^{(3)}(x)a^{(2)}(x)}{(a(x))^2} + q_{69} \frac{a^{(5)}(x)a^{(4)}(x)a^{(1)}(x)}{(a(x))^2} \\
& + q_{70} \frac{(a^{(5)}(x))^2}{a(x)} + q_{71} \frac{a^{(6)}(x)(a^{(1)}(x))^4}{(a(x))^4} + q_{72} \frac{a^{(6)}(x)a^{(2)}(x)(a^{(1)}(x))^2}{(a(x))^3} \\
& + q_{73} \frac{a^{(6)}(x)(a^{(2)}(x))^2}{(a(x))^2} + q_{74} \frac{a^{(6)}(x)a^{(3)}(x)a^{(1)}(x)}{(a(x))^2} + q_{75} \frac{a^{(6)}(x)a^{(4)}(x)}{a(x)} \\
& + q_{76} \frac{a^{(7)}(x)(a^{(1)}(x))^3}{(a(x))^3} + q_{77} \frac{a^{(7)}(x)a^{(2)}(x)a^{(1)}(x)}{(a(x))^2} + q_{78} \frac{a^{(7)}(x)a^{(3)}(x)}{a(x)} \\
& + q_{79} \frac{a^{(8)}(x)(a^{(1)}(x))^2}{(a(x))^2} + q_{80} \frac{a^{(8)}(x)a^{(2)}(x)}{a(x)} + q_{81} \frac{a^{(9)}(x)a^{(1)}(x)}{a(x)} + q_{82} a^{(10)}(x),
\end{aligned}$$

whose coefficients take the following values

$$\begin{aligned}
q_1 &= \frac{-1}{12}, \quad q_2 = \frac{1}{24}, \quad q_3 = \frac{-1}{180}, \quad q_4 = \frac{17}{1440}, \quad q_5 = \frac{-1}{720}, \quad q_6 = \frac{-1}{240}, \quad q_7 = \frac{1}{1920}, \\
q_8 &= \frac{-11}{15120}, \quad q_9 = \frac{23}{10080}, \quad q_{10} = \frac{-137}{80640}, \quad q_{11} = \frac{11}{120960}, \quad q_{12} = \frac{-1}{1260}, \quad q_{13} = \frac{31}{40320}, \\
q_{14} &= \frac{-1}{16128}, \quad q_{15} = \frac{31}{161280}, \quad q_{16} = \frac{-1}{20160}, \quad q_{17} = \frac{-1}{26880}, \quad q_{18} = \frac{1}{322560}, \\
q_{19} &= \frac{-107}{907200}, \quad q_{20} = \frac{887}{1814400}, \quad q_{21} = \frac{-377}{604800}, \quad q_{22} = \frac{989}{4147200}, \quad q_{23} = \frac{-107}{14515200}, \\
q_{24} &= \frac{-17}{100800}, \quad q_{25} = \frac{13}{37800}, \quad q_{26} = \frac{-193}{1612800}, \quad q_{27} = \frac{-1}{22400}, \quad q_{28} = \frac{5}{387072}, \\
q_{29} &= \frac{101}{2419200}, \quad q_{30} = \frac{-197}{3225600}, \quad q_{31} = \frac{17}{3225600}, \quad q_{32} = \frac{19}{1382400}, \quad q_{33} = \frac{-1}{2073600}, \\
q_{34} &= \frac{-1}{120960}, \quad q_{35} = \frac{1}{129024}, \quad q_{36} = \frac{-1}{829440}, \quad q_{37} = \frac{1}{774144}, \quad q_{38} = \frac{-1}{2903040}, \\
q_{39} &= \frac{-1}{5806080}, \quad q_{40} = \frac{1}{92897280}, \quad q_{41} = \frac{-2549}{119750400}, \quad q_{42} = \frac{26263}{239500800}, \\
q_{43} &= \frac{-94043}{479001600}, \quad q_{44} = \frac{67339}{479001600}, \quad q_{45} = \frac{-35971}{1094860800}, \quad q_{46} = \frac{2549}{3832012800}, \\
q_{47} &= \frac{-751}{19958400}, \quad q_{48} = \frac{1319}{11404800}, \quad q_{49} = \frac{-1921}{19958400}, \quad q_{50} = \frac{22313}{1277337600}, \\
q_{51} &= \frac{-379}{22809600}, \quad q_{52} = \frac{39}{1971200}, \quad q_{53} = \frac{-1087}{510935040}, \quad q_{54} = \frac{-1}{887040}, \quad q_{55} = \frac{37}{3942400}, \\
q_{56} &= \frac{-541}{22809600}, \quad q_{57} = \frac{7643}{567705600}, \quad q_{58} = \frac{-751}{1277337600}, \quad q_{59} = \frac{521}{79833600},
\end{aligned}$$

$$\begin{aligned}
q_{60} &= \frac{-5743}{1277337600}, & q_{61} &= \frac{83}{340623360}, & q_{62} &= \frac{-17669}{30656102400}, & q_{63} &= \frac{101}{958003200}, \\
q_{64} &= \frac{-299}{159667200}, & q_{65} &= \frac{601}{159667200}, & q_{66} &= \frac{-1087}{851558400}, & q_{67} &= \frac{-29}{29937600}, \\
q_{68} &= \frac{59}{218972160}, & q_{69} &= \frac{83}{567705600}, & q_{70} &= \frac{-1}{162201600}, & q_{71} &= \frac{193}{638668800}, \\
q_{72} &= \frac{-3349}{7664025600}, & q_{73} &= \frac{299}{7664025600}, & q_{74} &= \frac{83}{851558400}, & q_{75} &= \frac{-1}{141926400}, \\
q_{76} &= \frac{-1}{23950080}, & q_{77} &= \frac{59}{1532805120}, & q_{78} &= \frac{-1}{170311680}, & q_{79} &= \frac{59}{12262440960}, \\
q_{80} &= \frac{-1}{766402560}, & q_{81} &= \frac{-1}{2043740160}, & q_{82} &= \frac{1}{40874803200}.
\end{aligned}$$

Other $2n$ -th order schemes with $1 \leq n \leq 5$ can be recovered by simply neglecting all terms involving h^{2k} with $k \geq n$ in $\mathcal{E}^{12}(c^* + \frac{h}{2})$.

4. Compact, symmetric, and fourth-order d -dimensional FDMs, $d \geq 2$.

In this section, we state the main result of this paper, which is given by the following theorem, and present compact, symmetric, and 4th-order finite difference schemes for (1.1). To improve readability, we provide all the derivation details in Section 6.

THEOREM 4.1. *Let $M \in \mathbb{N}$ and $h > 0$. Assume that a , f , and g are sufficiently smooth functions. Consider the compact finite difference scheme $\mathcal{L}_h u_h = f_h$ for (1.1) on Ω_h given by $\mathcal{L}_h u(\mathbf{c}^*) := \sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) u(\mathbf{c}^* + ph)$ with $\mathbf{c}^* \in \Omega_h$, $C_p(\mathbf{c}^*) := \sum_{k=0}^{M+1} c_{p,k} h^k + \mathcal{O}_a(h^{M+2})$, $c_{p,k} = \mathcal{O}_a(1)$ for $p \in \mathcal{S}$, and f_h is a grid function on Ω_h that depends on a , f , their derivatives, and g . Then, the following statements hold:*

- (a) *For any $d \geq 2$, the consistency order of such a compact scheme is at most 6.*
- (b) *For any $d \geq 2$, if $\frac{|\nabla a|^2}{a^2} - \frac{2\Delta a}{a}$ is not constant on Ω , then the maximum consistency order of such a compact scheme, which is also symmetric, is 4.*
- (c) *If $d = 2$ and $\frac{|\nabla a|^2}{a^2} - \frac{2\Delta a}{a}$ is constant, then such a compact scheme, which is also symmetric and 6th-order consistent, exists.*

Proof. The explicit constructions of 4th and 6th-order consistent finite difference schemes for items (b) and (c) are provided in Sections 4.1 and 4.2. For the restrictions on the maximum consistency order, items (a) and (b) are proved in Lemmas 6.3 and 6.4 respectively. $\square$

4.1. The 2D and 3D cases. We provide the main steps for constructing a finite difference scheme satisfying the form described in Theorem 4.1. See Section 6 for an in-depth discussion. One key observation that we utilize is

$$(4.1) \quad u(\mathbf{c}^* + ph) = \sum_{\ell \in \Pi_{M+1}} \sum_{k=|\ell|}^{M+1} A_\ell^k(p) h^k \cdot \partial^\ell u(\mathbf{c}^*) + F(p) + \mathcal{O}_{a,u}(h^{M+2}), \quad \forall \mathbf{c}^* \in \Omega_h,$$

where $A_\ell^k(p)$, $F(p)$ are explicitly known quantities obtained from Taylor expansions that depend on a and its partial derivatives at $\mathbf{c}^*$, $F(p)$ also depends on f and its partial derivatives at $\mathbf{c}^*$, and

$$(4.2) \quad \Pi_M := \{\ell \in \mathbb{N}_0^d : \ell_1 \leq 1, |\ell| \leq M\}, \quad M \in \mathbb{N}_0 \quad \text{with} \quad \ell := (\ell_1, \dots, \ell_d).$$

All the coefficients $c_{p,k}$ in Theorem 4.1 can be determined by solving a linear system, which has special cascade structures and involves the quantities $A_\ell^k(p)$ in (4.1). Moreover, with the aid of symbolic computation, we observe that there are free parameters available. As a result, for all $\mathbf{c}^* \in \Omega_h$, we can write

$$C_p(\mathbf{c}^*) = \sum_{m=-1}^M \sum_{k=1}^{K_m} \kappa_{m,k} C_p^{[m],k}(\mathbf{c}^*) h^{M-m}, \quad \forall p \in \mathcal{S},$$

where K_m is the number of available basis stencil coefficients obtained via symbolic computation, $\kappa_{m,k}$ are some constants for all $\mathbf{c}^* \in \Omega_h$, $C_p^{[m],k}(\mathbf{c}^*)$ are basis stencil coefficients, and $\mathcal{S} = \{-1, 0, 1\}^d$ with $d = 2, 3$. Furthermore, we can compute the right-hand basis grid functions, $f_h^{[m],k}(\mathbf{c}^*)$, which are defined as

$$f_h^{[m],k}(\mathbf{c}^*) := \sum_{p \in \mathcal{S}} C_p^{[m],k}(\mathbf{c}^*) F(p), \quad \forall \mathbf{c}^* \in \Omega_h,$$

where $F(p)$ comes from Taylor expansions done in (4.1).

Now, the M th-order compact finite difference schemes take the following form

$$(4.3) \quad \begin{aligned} \sum_{p \in \mathcal{S}} \sum_{m=-1}^M \sum_{k=1}^{K_m} \kappa_{m,k} C_p^{[m],k}(\mathbf{c}^*) h^{M-m} u(\mathbf{c}^* + ph) \\ = \sum_{m=-1}^M \sum_{k=1}^{K_m} \kappa_{m,k} f_h^{[m],k}(\mathbf{c}^*) h^{M-m} + \mathcal{O}_{a,u}(h^{M+2}), \quad \forall \mathbf{c}^* \in \Omega_h. \end{aligned}$$

By (2.2), to guarantee that the linear system produced by the discretization is symmetric, we further enforce the following conditions on the stencil coefficients in (4.3)

$$(4.4) \quad \sum_{m=-1}^M \sum_{k=1}^{K_m} \kappa_{m,k} C_p^{[m],k}(\mathbf{c}^*) h^{M-m} = \sum_{m=-1}^M \sum_{k=1}^{K_m} \kappa_{m,k} C_{-p}^{[m],k}(\mathbf{c}^* + ph) h^{M-m},$$

for all $\mathbf{c}^* \in \Omega_h$ and $p \in \mathcal{S}$. As we shall see soon, each $C_p^{[m],k}$ is a function evaluated at the point $\mathbf{c}^* + ph/2$.

Next, we shall present the explicit forms of all possible $C_p^{[m],k}(\mathbf{c}^*)$ for $p \in \mathcal{S} \setminus \{\vec{0}\}$ with $C_{\vec{0}}^{[m],k}(\mathbf{c}^*)$ being uniquely determined by $C_{\vec{0}}^{[m],k}(\mathbf{c}^*) = -\sum_{p \in \mathcal{S} \setminus \{\vec{0}\}} C_p^{[m],k}(\mathbf{c}^*)$ according to Lemma 6.1(b), and all possible $f_h^{[m],k}(\mathbf{c}^*)$. Afterwards, we shall discuss some restrictions on $\kappa_{m,k}$. In what follows, we define $\tilde{a} := -\ln a$ and $\tilde{f} := -f/a$.

For $d = 2$, we have $\mathcal{S} = \{(0, 0), \pm(1, 0), \pm(0, 1), \pm(1, 1), \pm(1, -1)\}$, and

$$(4.5) \quad \begin{aligned} K_{-1} = 8, \quad K_0 = 6, \quad K_1 = 4, \quad K_2 = 2, \quad K_3 = K_4 = K_5 = K_6 = 1, \\ K_M = 0 \quad \forall M \geq 7. \end{aligned}$$

The basis stencil coefficients can be written as

$$(4.6) \quad C_p^{[m],k}(\mathbf{c}^*) = \begin{cases} (a\Phi^H \pm a\tilde{\Phi}^H)(\mathbf{c}^* + ph/2), & p = \pm(1, 0), \\ (a\Phi^V \pm a\tilde{\Phi}^V)(\mathbf{c}^* + ph/2), & p = \pm(0, 1), \\ (a\Phi^D \pm a\tilde{\Phi}^D)(\mathbf{c}^* + ph/2), & p = \pm(1, 1), \\ (a\Phi^A \pm a\tilde{\Phi}^A)(\mathbf{c}^* + ph/2), & p = \pm(1, -1), \end{cases}$$

where superscripts ‘‘H’’ (horizontal), ‘‘V’’ (vertical), ‘‘D’’ (diagonal), and ‘‘A’’ (antidiagonal) emphasize the stencil’s location. The sign in between Φ and $\tilde{\Phi}$ matches the sign of p . For example, if $p = (1, 0)$, then $C_p^{[m],k}(\mathbf{c}^*) = (a\Phi^H + a\tilde{\Phi}^H)(\mathbf{c}^* + ph/2)$.

Below, we list the values that these Φ and $\tilde{\Phi}$ with various superscripts as well as the right-hand basis grid functions take depending on m and k :

$$(\Phi^H, \Phi^V, \Phi^D, \Phi^A, \tilde{\Phi}^H, \tilde{\Phi}^V, \tilde{\Phi}^D, \tilde{\Phi}^A, f_h^{[m],k})$$

$$= \begin{cases} -\vec{e}_k, & \text{if } m = -1, 0, \text{ and } k = 1, \dots, 4, \\ \vec{e}_k, & \text{if } m = -1, \text{ and } k = 5, \dots, 8, \\ 2\vec{e}_5 - \vec{e}_7 + \vec{e}_8, & \text{if } m = 0, k = 5; \text{ or, } m = 1, k = 3, \\ 2\vec{e}_6 - \vec{e}_7 - \vec{e}_8, & \text{if } m = 0, k = 6; \text{ or, } m = 1, k = 4, \\ -\vec{e}_{2k-1} - \vec{e}_{2k} + kh^2 f \vec{e}_9, & \text{if } m = 1, 2, \text{ and } k = 1, 2, \end{cases}$$

where $\vec{e}_k$, $k = 1, \dots, 9$ are the standard unit vector basis of $\mathbb{R}^9$.

If $m = 3, 4$ and $k = 1$, then

$$\begin{aligned} \Phi^H &= -4 + \frac{1}{4}h^2 (|\nabla \tilde{a}|^2 + \tilde{a}_{xx} - \tilde{a}_{yy}), & \Phi^V &= -4 + \frac{1}{4}h^2 (|\nabla \tilde{a}|^2 - \tilde{a}_{xx} + \tilde{a}_{yy}), \\ \Phi^D &= -1 + \frac{1}{4}h^2 \tilde{a}_{xy}, & \Phi^A &= -1 - \frac{1}{4}h^2 \tilde{a}_{xy}, \\ \tilde{\Phi}^H &= \tilde{\Phi}^V = \tilde{\Phi}^D = \tilde{\Phi}^A = 0, & f_h^{[m],k} &= -a \left(6h^2 \tilde{f} + \frac{1}{2}h^4 \left(\Delta \tilde{f} - \nabla \tilde{a} \cdot \nabla \tilde{f} \right) \right). \end{aligned}$$

Finally, if $m = 5, 6$ and $k = 1$, then

$$\begin{aligned} \Phi^H &= -4 + h^2 \left(-\frac{11}{60}(\eta_1 + \eta_2) + \frac{1}{2}\tilde{a}_{xx} \right) + \frac{1}{960}h^4 \left(-8|\nabla \tilde{a}|^4 + 26\nabla \tilde{a} \cdot \nabla \Delta \tilde{a} \right. \\ &\quad \left. - 16\Delta^2 \tilde{a} + 14(\Delta \tilde{a})^2 + 7|\nabla \tilde{a}|^2 \Delta \tilde{a} + 10\tilde{a}_{xxyy} - 22\tilde{a}_{xx}\tilde{a}_{yy} + 5\Delta \tilde{a}\eta_5 - 7\Delta\eta_5 \right. \\ &\quad \left. - 11|\nabla \tilde{a}|^2 \eta_5 - 2\nabla \tilde{a} \cdot \nabla \eta_5 \right), \\ \Phi^V &= -4 + h^2 \left(-\frac{11}{60}(\eta_1 + \eta_2) + \frac{1}{2}\tilde{a}_{yy} \right) + \frac{1}{960}h^4 \left(-8|\nabla \tilde{a}|^4 + 26\nabla \tilde{a} \cdot \nabla \Delta \tilde{a} \right. \\ &\quad \left. - 16\Delta^2 \tilde{a} + 14(\Delta \tilde{a})^2 + 7|\nabla \tilde{a}|^2 \Delta \tilde{a} + 10\tilde{a}_{xxyy} - 22\tilde{a}_{xx}\tilde{a}_{yy} - 5\Delta \tilde{a}\eta_5 + 7\Delta\eta_5 \right. \\ &\quad \left. + 11|\nabla \tilde{a}|^2 \eta_5 + 2\nabla \tilde{a} \cdot \nabla \eta_5 \right), \\ \Phi^D &= -1 + h^2 \left(\frac{1}{120}\eta_4 + \frac{1}{4}\tilde{a}_{xy} \right) + \frac{1}{1440}h^4 (\partial_{xy}(4(\eta_1 + \eta_2) + \eta_4) - 3a_{xy}\eta_4), \\ \Phi^A &= -1 + h^2 \left(\frac{1}{120}\eta_4 - \frac{1}{4}\tilde{a}_{xy} \right) - \frac{1}{1440}h^4 (\partial_{xy}(4(\eta_1 + \eta_2) + \eta_4) - 3a_{xy}\eta_4), \\ \tilde{\Phi}^H &= \frac{1}{40}h^3 \partial_x(\eta_1 + \eta_2) + \frac{1}{960}h^5 (\partial_{xxx}(\eta_1 + \eta_2) - 3\tilde{a}_{xx}\partial_x(\eta_1 + \eta_2)), \\ \tilde{\Phi}^V &= \frac{1}{40}h^3 \partial_y(\eta_1 + \eta_2) + \frac{1}{960}h^5 (\partial_{yyy}(\eta_1 + \eta_2) - 3\tilde{a}_{yy}\partial_y(\eta_1 + \eta_2)), \\ \tilde{\Phi}^D &= \tilde{\Phi}^A = 0, \\ f_h^{[m],k} &= -a \left[6h^2 \tilde{f} + \frac{1}{2}h^4 \left(\Delta \tilde{f} - \nabla \tilde{a} \cdot \nabla \tilde{f} + \frac{1}{10}(\eta_1 + \eta_2)\tilde{f} \right) - \frac{1}{240}h^6 \left(-4(\tilde{f}_{xxx} \right. \right. \\ &\quad \left. \left. + 4\tilde{f}_{xxyy} + \tilde{f}_{yyyy}) + 8(\tilde{a}_x \tilde{f}_{xxx} + 2\tilde{a}_y \tilde{f}_{xxy} + 2\tilde{a}_x \tilde{f}_{xyy} + \tilde{a}_y \tilde{f}_{yyy}) \right. \right. \\ &\quad \left. \left. + ((\eta_1 - \eta_2)(\tilde{f}_{xx} - \tilde{f}_{yy}) + 16\eta_3 \tilde{f}_{xy}) + (\tilde{a}_x(3\eta_1 + \eta_2) - 2\partial_x(\eta_1 - \eta_2))\tilde{f}_x \right. \right. \\ &\quad \left. \left. + (\tilde{a}_y(\eta_1 + 3\eta_2) + 2\partial_y(\eta_1 - \eta_2))\tilde{f}_y + \left(\frac{1}{4}(\eta_1^2 + \eta_2^2) + \tilde{a}_x \partial_x(2\eta_1 + \eta_2) \right. \right. \right. \\ &\quad \left. \left. \left. + \tilde{a}_y \partial_y(\eta_1 + 2\eta_2) - \partial_{xx}(2\eta_1 + \eta_2) - \partial_{yy}(\eta_1 + 2\eta_2) \right) \tilde{f} \right) \right], \end{aligned}$$

where $\eta_1 = 2\tilde{a}_{xx} - \tilde{a}_x^2$, $\eta_2 = 2\tilde{a}_{yy} - \tilde{a}_y^2$, $\eta_3 = 2\tilde{a}_{xy} - \tilde{a}_x \tilde{a}_y$, $\eta_4 = \Delta \tilde{a} + 7|\nabla \tilde{a}|^2$, $\eta_5 = \tilde{a}_{xx} - \tilde{a}_{yy}$.

A few observations are in order. The basis stencil coefficients $C_p^{[m],k}(\mathbf{c}^*)$ are symmetric if $\tilde{\Phi}^H, \tilde{\Phi}^V, \tilde{\Phi}^D$, and $\tilde{\Phi}^A$ are all equal to zeros. On the other hand, the basis stencil coefficients $C_p^{[m],k}(\mathbf{c}^*)$ are anti-symmetric if Φ^H, Φ^V, Φ^D , and Φ^A are all equal to zeros; i.e., $C_p^{[m],k}(\mathbf{c}^*) = -C_{-p}^{[m],k}(\mathbf{c}^* + ph)$ for all $\mathbf{c}^* \in \Omega_h$ and $p \in \mathcal{S}$. The basis stencil coefficients $C_p^{[5],1}, C_p^{[6],1}$ are neither symmetric nor anti-symmetric, but they can be decomposed into symmetric and anti-symmetric parts by taking even and odd powers of h . The free parameters $\kappa_{m,k}$ in (4.6) can be chosen to help us satisfy (4.4) given the symmetric/anti-symmetric property of the basis stencil coefficients. One natural choice is to set $\kappa_{m,k} = 0$ for all basis stencil coefficients that are not symmetric (this also includes the anti-symmetric ones). At the same time, this freedom allows us to potentially minimize the leading truncation error term, which is expected to produce a smaller error for a given grid size.

For a general a , we can take $M \leq 4$ in (4.6) to ensure that the resulting finite difference scheme is symmetric. Meanwhile, if we further assume that $2\Delta\tilde{a} - |\nabla\tilde{a}|^2$ is constant, then we can take $M \leq 6$ in (4.6) to guarantee the symmetry. Under this assumption, the basis stencil coefficients become symmetric, since $\tilde{\Phi}^A, \tilde{\Phi}^D$ are already zeros to begin with, and $\tilde{\Phi}^H, \tilde{\Phi}^V$ are now also zeros for $M = 5, 6$. In particular, if a is constant in (1.1) and $M = 6$, we recover the 6th-order 2D finite difference scheme, which is widely known in the literature [3, 11, 17, 18]. If symmetry is not required, we can take $M \leq 6$ in (4.6) and no restriction (except for item (c) in Lemma 6.1) is imposed on $\kappa_{m,k}$ in (4.6).

For $d = 3$, we have

$$\begin{aligned} \mathcal{S} = \{ & (0, 0, 0), \pm(1, 0, 0), \pm(0, 1, 0), \pm(0, 0, 1), \pm(1, 1, 0), \pm(1, -1, 0), \\ & \pm(1, 0, 1), \pm(1, 0, -1), \pm(0, 1, 1), \pm(0, 1, -1), \pm(1, 1, 1), \pm(-1, 1, 1), \\ & \pm(1, -1, 1), \pm(1, 1, -1) \}, \end{aligned}$$

and the number of available basis stencil coefficients are

$$(4.7) \quad \begin{aligned} K_{-1} &= 26, \quad K_0 = 23, \quad K_1 = 18, \quad K_2 = 11, \quad K_3 = 5, \quad K_4 = 2, \\ K_5 &= K_6 = 1, \quad K_M = 0 \quad \forall M \geq 7; \end{aligned}$$

meanwhile, if we further exclude 8 corner points from $\mathcal{S}$, then we have

$$(4.8) \quad \begin{aligned} K_{-1} &= 18, \quad K_0 = 15, \quad K_1 = 10, \quad K_2 = 4, \quad K_3 = K_4 = 1, \quad K_5 = K_6 = 0, \\ K_M &= 0 \quad \forall M \geq 7, \end{aligned}$$

and no additional points can be removed from $\mathcal{S}$ while keeping $K_4 > 0$. Similar to (4.6), the stencil coefficients can be written as

$$(4.9) \quad C_p^{[m],k}(\mathbf{c}^*) = \begin{cases} (a\Phi^F \pm a\tilde{\Phi}^F)(\mathbf{c}^* + ph/2), & p = \pm(1, 0, 0), \\ (a\Phi^R \pm a\tilde{\Phi}^R)(\mathbf{c}^* + ph/2), & p = \pm(0, 1, 0), \\ (a\Phi^U \pm a\tilde{\Phi}^U)(\mathbf{c}^* + ph/2), & p = \pm(0, 0, 1), \\ (a\Phi^{FR} \pm a\tilde{\Phi}^{FR})(\mathbf{c}^* + ph/2), & p = \pm(1, 1, 0), \\ (a\Phi^{BR} \pm a\tilde{\Phi}^{BR})(\mathbf{c}^* + ph/2), & p = \pm(-1, 1, 0), \\ (a\Phi^{FU} \pm a\tilde{\Phi}^{FU})(\mathbf{c}^* + ph/2), & p = \pm(1, 0, 1), \\ (a\Phi^{BU} \pm a\tilde{\Phi}^{BU})(\mathbf{c}^* + ph/2), & p = \pm(-1, 0, 1), \end{cases}$$

$$\begin{cases} (a\Phi^{\text{RU}} \pm a\tilde{\Phi}^{\text{RU}})(\mathbf{c}^* + ph/2), & p = \pm(0, 1, 1), \\ (a\Phi^{\text{LU}} \pm a\tilde{\Phi}^{\text{LU}})(\mathbf{c}^* + ph/2), & p = \pm(0, -1, 1), \\ (a\Phi^{\text{FRU}} \pm a\tilde{\Phi}^{\text{FRU}})(\mathbf{c}^* + ph/2), & p = \pm(1, 1, 1), \\ (a\Phi^{\text{FRD}} \pm a\tilde{\Phi}^{\text{FRD}})(\mathbf{c}^* + ph/2), & p = \pm(1, 1, -1), \\ (a\Phi^{\text{FLU}} \pm a\tilde{\Phi}^{\text{FLU}})(\mathbf{c}^* + ph/2), & p = \pm(1, -1, 1), \\ (a\Phi^{\text{BRU}} \pm a\tilde{\Phi}^{\text{BRU}})(\mathbf{c}^* + ph/2), & p = \pm(-1, 1, 1), \end{cases}$$

where superscripts “F” (front), “B” (back), “R” (right), “L” (left), “U” (up), “D” (down), or their combinations indicates the stencil’s location. Below, we list the values that these Φ and $\tilde{\Phi}$ with various superscripts as well as the right-hand basis grid functions take depending on m and k :

$$\begin{aligned} & (\Phi^{\text{F}}, \Phi^{\text{R}}, \Phi^{\text{U}}, \Phi^{\text{FR}}, \Phi^{\text{BR}}, \Phi^{\text{FU}}, \Phi^{\text{BU}}, \Phi^{\text{RU}}, \Phi^{\text{LU}}, \Phi^{\text{FRU}}, \Phi^{\text{FRD}}, \Phi^{\text{FLU}}, \Phi^{\text{BRU}}, \\ & \tilde{\Phi}^{\text{F}}, \tilde{\Phi}^{\text{R}}, \tilde{\Phi}^{\text{U}}, \tilde{\Phi}^{\text{FR}}, \tilde{\Phi}^{\text{BR}}, \tilde{\Phi}^{\text{FU}}, \tilde{\Phi}^{\text{BU}}, \tilde{\Phi}^{\text{RU}}, \tilde{\Phi}^{\text{LU}}, \tilde{\Phi}^{\text{FRU}}, \tilde{\Phi}^{\text{FRD}}, \tilde{\Phi}^{\text{FLU}}, \tilde{\Phi}^{\text{BRU}}, f_h^{[m],k}) \\ & = \begin{cases} -\vec{e}_k, & \text{if } m = -1, 0, \text{ and } k = 1, \dots, 13, \\ -\vec{e}_k, & \text{if } m = -1, \text{ and } k = 14, \dots, 26, \\ \vec{e}_{14} + \vec{e}_{15} - \vec{e}_{17}, & \text{if } m = 0, k = 14; \text{ or, } m = 1, k = 9, \\ -\vec{e}_{14} + \vec{e}_{15} - \vec{e}_{18}, & \text{if } m = 0, k = 15; \text{ or, } m = 1, k = 10, \\ \vec{e}_{14} + \vec{e}_{16} - \vec{e}_{19}, & \text{if } m = 0, k = 16; \text{ or, } m = 1, k = 11, \\ -\vec{e}_{14} + \vec{e}_{16} - \vec{e}_{20}, & \text{if } m = 0, k = 17; \text{ or, } m = 1, k = 12, \\ \vec{e}_{15} + \vec{e}_{16} - \vec{e}_{21}, & \text{if } m = 0, k = 18; \text{ or, } m = 1, k = 13, \\ -\vec{e}_{15} + \vec{e}_{16} - \vec{e}_{22}, & \text{if } m = 0, k = 19; \text{ or, } m = 1, k = 14, \\ \vec{e}_{14} + \vec{e}_{15} + \vec{e}_{16} - \vec{e}_{23}, & \text{if } m = 0, k = 20; \text{ or, } m = 1, k = 15, \\ \vec{e}_{14} + \vec{e}_{15} - \vec{e}_{16} - \vec{e}_{24}, & \text{if } m = 0, k = 21; \text{ or, } m = 1, k = 16, \\ \vec{e}_{14} - \vec{e}_{15} + \vec{e}_{16} - \vec{e}_{25}, & \text{if } m = 0, k = 22; \text{ or, } m = 1, k = 17, \\ -\vec{e}_{14} + \vec{e}_{15} + \vec{e}_{16} - \vec{e}_{26}, & \text{if } m = 0, k = 21; \text{ or, } m = 1, k = 16, \\ -\vec{e}_1 - \vec{e}_2 - \vec{e}_3 + h^2 f \vec{e}_{27}, & \text{if } m = 1, 2, \text{ and } k = 1, \\ -2\vec{e}_{k-1} - \vec{e}_{2k} - \vec{e}_{2k+1} + 2h^2 f \vec{e}_{27}, & \text{if } m = 1, 2, \text{ and } k = 2, 3, 4, \\ -\vec{e}_5 - \vec{e}_7 - \vec{e}_9 - \vec{e}_{10} + 3h^2 f \vec{e}_{27}, & \text{if } m = 1, 2, \text{ and } k = 5, \\ -\vec{e}_5 - \vec{e}_6 - \vec{e}_8 - \vec{e}_{11} + 3h^2 f \vec{e}_{27}, & \text{if } m = 1, 2, \text{ and } k = 6, \\ -\vec{e}_4 - \vec{e}_7 - \vec{e}_8 - \vec{e}_{12} + 3h^2 f \vec{e}_{27}, & \text{if } m = 1, 2, \text{ and } k = 7, \\ -\vec{e}_4 - \vec{e}_6 - \vec{e}_9 - \vec{e}_{13} + 3h^2 f \vec{e}_{27}, & \text{if } m = 1, 2, \text{ and } k = 8, \\ -4\vec{e}_{14} + 2(\vec{e}_{17} - \vec{e}_{18} + \vec{e}_{19} - \vec{e}_{20}) & \text{if } m = 2, k = 9; \text{ or, } m = 3, k = 3, \\ -\vec{e}_{23} - \vec{e}_{24} - \vec{e}_{25} + \vec{e}_{26}, & \\ -4\vec{e}_{15} + 2(\vec{e}_{17} + \vec{e}_{18} + \vec{e}_{21} - \vec{e}_{22}) & \text{if } m = 2, k = 10; \text{ or, } m = 3, k = 4, \\ -\vec{e}_{23} - \vec{e}_{24} + \vec{e}_{25} - \vec{e}_{26}, & \\ -4\vec{e}_{16} + 2(\vec{e}_{19} + \vec{e}_{20} + \vec{e}_{21} + \vec{e}_{22}) & \text{if } m = 2, k = 11; \text{ or, } m = 3, k = 5, \\ -\vec{e}_{23} + \vec{e}_{24} - \vec{e}_{25} - \vec{e}_{26}, & \end{cases} \end{aligned}$$

where $\vec{e}_k$, $k = 1, \dots, 27$ are the standard unit vector basis of $\mathbb{R}^{27}$.

If $m = 3, 4$ and $k = 1$, then

$$\begin{aligned}
\Phi^F &= -2 + \frac{1}{4}h^2 (|\nabla \tilde{a}|^2 + \tilde{a}_{xx} - \tilde{a}_{yy} - \tilde{a}_{zz}), \\
\Phi^R &= -2 + \frac{1}{4}h^2 (|\nabla \tilde{a}|^2 - \tilde{a}_{xx} + \tilde{a}_{yy} - \tilde{a}_{zz}), \\
\Phi^U &= -2 + \frac{1}{4}h^2 (|\nabla \tilde{a}|^2 - \tilde{a}_{xx} - \tilde{a}_{yy} + \tilde{a}_{zz}), \\
\Phi^{FR} &= -1 + \frac{1}{4}h^2 \tilde{a}_{xy}, \quad \Phi^{FU} = -1 + \frac{1}{4}h^2 \tilde{a}_{xz}, \quad \Phi^{RU} = -1 + \frac{1}{4}h^2 \tilde{a}_{yz}, \\
\Phi^{BR} &= -1 - \frac{1}{4}h^2 \tilde{a}_{xy}, \quad \Phi^{BU} = -1 - \frac{1}{4}h^2 \tilde{a}_{xz}, \quad \Phi^{LU} = -1 - \frac{1}{4}h^2 \tilde{a}_{yz}, \\
f_h^{[m],k} &= -a \left(6h^2 \tilde{f} + \frac{1}{2}h^4 \left(\Delta \tilde{f} - \nabla \tilde{a} \cdot \nabla \tilde{f} \right) \right),
\end{aligned}$$

and $\Phi^{FRU}, \Phi^{FRD}, \Phi^{FLU}, \Phi^{BRU}, \tilde{\Phi}^F, \tilde{\Phi}^R, \tilde{\Phi}^U, \tilde{\Phi}^{FR}, \tilde{\Phi}^{BR}, \tilde{\Phi}^{FU}, \tilde{\Phi}^{BU}, \tilde{\Phi}^{RU}, \tilde{\Phi}^{LU}, \tilde{\Phi}^{FRU}, \tilde{\Phi}^{FRD}, \tilde{\Phi}^{FLU}, \tilde{\Phi}^{BRU}$ are all zeros.

Finally, if $m = 3, 4$ and $k = 2$, then

$$\begin{aligned}
\Phi^F &= -8 + h^2 \tilde{a}_{xx}, \quad \Phi^R = -8 + h^2 \tilde{a}_{yy}, \quad \Phi^U = -8 + h^2 \tilde{a}_{zz}, \\
\tilde{\Phi}^F &= \frac{1}{4}h^3 \partial_x (|\nabla \tilde{a}|^2 - \Delta \tilde{a}), \quad \tilde{\Phi}^R = \frac{1}{4}h^3 \partial_y (|\nabla \tilde{a}|^2 - \Delta \tilde{a}), \quad \tilde{\Phi}^U = \frac{1}{4}h^3 \partial_z (|\nabla \tilde{a}|^2 - \Delta \tilde{a}), \\
\Phi^{FRU} &= -1 + \frac{1}{4}h^2 (\tilde{a}_{xy} + \tilde{a}_{xz} + \tilde{a}_{yz}), \quad \Phi^{FRD} = -1 + \frac{1}{4}h^2 (\tilde{a}_{xy} - \tilde{a}_{xz} - \tilde{a}_{yz}), \\
\Phi^{FLU} &= -1 + \frac{1}{4}h^2 (-\tilde{a}_{xy} + \tilde{a}_{xz} - \tilde{a}_{yz}), \quad \Phi^{BRU} = -1 + \frac{1}{4}h^2 (-\tilde{a}_{xy} - \tilde{a}_{xz} + \tilde{a}_{yz}), \\
f_h^{[m],k} &= -a \left(12h^2 \tilde{f} + h^4 \left(\frac{1}{2} (\Delta \tilde{f} - \nabla \tilde{a} \cdot \nabla \tilde{f}) + (|\nabla \tilde{a}|^2 - \Delta \tilde{a}) \tilde{f} \right) \right),
\end{aligned}$$

and $\Phi^{FR}, \Phi^{BR}, \Phi^{FU}, \Phi^{BU}, \Phi^{RU}, \Phi^{LU}, \tilde{\Phi}^{FR}, \tilde{\Phi}^{BR}, \tilde{\Phi}^{FU}, \tilde{\Phi}^{BU}, \tilde{\Phi}^{RU}, \tilde{\Phi}^{LU}, \tilde{\Phi}^{FRU}, \tilde{\Phi}^{FRD}, \tilde{\Phi}^{FLU}, \tilde{\Phi}^{BRU}$ are all zeros.

Same as before, the basis stencil coefficients $C_p^{[m],k}(\mathbf{c}^*)$ are symmetric if all $\tilde{\Phi}$ are zeros. Meanwhile, if all Φ are zeros, then the basis stencil coefficients $C_p^{[m],k}(\mathbf{c}^*)$ are anti-symmetric. Additionally, the basis stencil coefficient $C_p^{[4],2}$ is neither symmetric nor anti-symmetric, but they can be decomposed into symmetric and anti-symmetric parts by taking even and odd powers of h . Also, identical to the 2D setting, the freedom in the choices of $\kappa_{m,k}$ in (4.6) can be exploited to help us achieve (4.4) and minimize the leading truncation error. For a general a , we can take $M \leq 4$ in (4.6) to ensure that the resulting finite difference scheme is symmetric. If symmetry is not required, we can take $M \leq 6$ in (4.6). For $M = 5, 6$, there is a single basis stencil coefficient, but it is difficult to compute symbolically.

4.2. The general d -dimensional case. In Section 3 and Section 4.1 we have shown that there are compact, symmetric, and 4th-order finite difference schemes in dimensions one and two. In this section, we shall show that such a scheme exists in arbitrary dimensions, and it is constructed simply via a linear combination of the aforementioned lower dimensional schemes. This is possible due to the bilinear structure of the right hand side function f_h in (4.10).

We begin by adapting the lower dimensional schemes into higher dimensions $d \geq 3$, where they become schemes that involve partial derivatives along one and two axes. To this end, we define $\mathcal{L}'_i := \partial^{2\vec{e}_i} - \partial^{\vec{e}_i} \tilde{a} \cdot \partial^{\vec{e}_i}$ and $\tilde{f}_i = \mathcal{L}'_i u$, $1 \leq i \leq d$. Observe that the original PDE in (1.1) can be written into $\sum_{i=1}^d \mathcal{L}'_i u = \tilde{f} = \sum_{i=1}^d \tilde{f}_i$.

Let $\mathcal{S} = \{-1, 0, 1\}^d$ as usual. Then, the scheme along the i -th direction is given by $\sum_{p \in \mathcal{S}} C_{p,i}(\mathbf{c}^*) u(\mathbf{c}^* + ph) = f_{h,i}(\mathbf{c}^*)$, where

$$C_{p,i}(\mathbf{c}^*) = \begin{cases} a(-1 + \frac{1}{24}h^2(\partial^{2\vec{e}_i}\tilde{a} + (\partial^{\vec{e}_i}\tilde{a})^2))|_{\mathbf{c}^*+ph/2}, & \text{if } p = \pm\vec{e}_i, \\ -(C_{-\vec{e}_i,i}(\mathbf{c}^*) + C_{\vec{e}_i,i}(\mathbf{c}^*)), & \text{if } p = \vec{0}, \\ 0, & \text{otherwise,} \end{cases}$$

$$f_{h,i} = -a(h^2\tilde{f}_i + \frac{1}{12}h^4\mathcal{L}'_i\tilde{f}_i) = -a\left(h^2\tilde{f}_i + \frac{1}{12}h^4(\partial^{2\vec{e}_i}\tilde{f}_i - \partial^{\vec{e}_i}\tilde{a}\partial^{\vec{e}_i}\tilde{f}_i)\right).$$

The scheme along the i -th and j -th direction is given by $\frac{1}{6}$ times the 2D basis coefficient $C_p^{[4],1}$ and the corresponding right-hand basis grid function $f_h^{[4],1}$ in Section 4.1. More explicitly, the scheme along two directions $1 \leq i < j \leq d$ is given by $\sum_{p \in \mathcal{S}} C_{p,i,j}(\mathbf{c}^*) u(\mathbf{c}^* + ph) = f_{h,i,j}(\mathbf{c}^*)$, where

$$C_{p,i,j}(\mathbf{c}^*) = \begin{cases} a(-\frac{2}{3} + \frac{1}{24}h^2((\partial^{\vec{e}_i}\tilde{a})^2 + (\partial^{\vec{e}_j}\tilde{a})^2 + \partial^{2\vec{e}_i}\tilde{a} - \partial^{2\vec{e}_j}\tilde{a}))|_{\mathbf{c}^*+ph/2}, & \text{if } p = \pm\vec{e}_i, \\ a(-\frac{2}{3} + \frac{1}{24}h^2((\partial^{\vec{e}_i}\tilde{a})^2 + (\partial^{\vec{e}_j}\tilde{a})^2 - \partial^{2\vec{e}_i}\tilde{a} + \partial^{2\vec{e}_j}\tilde{a}))|_{\mathbf{c}^*+ph/2}, & \text{if } p = \pm\vec{e}_j, \\ a(-\frac{1}{6} + \frac{1}{24}h^2\partial^{\vec{e}_i+\vec{e}_j}\tilde{a})|_{\mathbf{c}^*+ph/2}, & \text{if } p = \pm(\vec{e}_i + \vec{e}_j), \\ a(-\frac{1}{6} - \frac{1}{24}h^2\partial^{\vec{e}_i+\vec{e}_j}\tilde{a})|_{\mathbf{c}^*+ph/2}, & \text{if } p = \pm(\vec{e}_i - \vec{e}_j), \\ -\sum_{p \in \mathcal{S} \setminus \{\vec{0}\}} C_{p,i,j}(\mathbf{c}^*), & \text{if } p = \vec{0}, \\ 0, & \text{otherwise,} \end{cases}$$

$$f_{h,i,j} = -a\left(h^2(\tilde{f}_i + \tilde{f}_j) + \frac{1}{12}h^4(\mathcal{L}'_i + \mathcal{L}'_j)(\tilde{f}_i + \tilde{f}_j)\right).$$

Note that these two schemes are 4th-order consistent to the PDEs $\mathcal{L}'_i u = \tilde{f}_i$ and $(\mathcal{L}'_i + \mathcal{L}'_j)u = \tilde{f}_i + \tilde{f}_j$ respectively.

Let us turn to the d -dimensional scheme. The observation is that, setting

$$(4.10) \quad f_h := -a\left(h^2\tilde{f} + \frac{1}{12}h^4(\Delta\tilde{f} - \nabla\tilde{a} \cdot \nabla\tilde{f})\right),$$

we have

$$\begin{aligned} f_h &= -ah^2 \sum_{i=1}^d \tilde{f}_i - \frac{1}{12}ah^4 \sum_{i=1}^d \sum_{j=1}^d \mathcal{L}'_i \tilde{f}_j \\ &= -a \left[(d-1)h^2 \sum_{i=1}^d \tilde{f}_i + \frac{1}{12}h^4 \left((d-1) \sum_{i=1}^d \mathcal{L}'_i \tilde{f}_i + \sum_{1 \leq i < j \leq d} (\mathcal{L}'_i \tilde{f}_j + \mathcal{L}'_j \tilde{f}_i) \right) \right] \\ &\quad + (d-2)a \left[h^2 \sum_{i=1}^d \tilde{f}_i + \frac{1}{12}h^4 \sum_{i=1}^d \mathcal{L}'_i \tilde{f}_i \right] \\ &= \sum_{1 \leq i < j \leq d} f_{h,i,j} - (d-2) \sum_{i=1}^d f_{h,i}. \end{aligned}$$

Now, for each $p \in \mathcal{S}$, if we set

$$(4.11) \quad C_p(\mathbf{c}^*) = \sum_{1 \leq i < j \leq d} C_{p,i,j}(\mathbf{c}^*) - (d-2) \sum_{i=1}^d C_{p,i}(\mathbf{c}^*),$$

then the finite difference scheme for (1.1) given by $\sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) u(\mathbf{c}^* + ph) = f_h(\mathbf{c}^*)$, where (4.10) and (4.11) hold, is compact and 4th-order consistent. Moreover, this finite difference scheme is symmetric, since it is a linear combination of a scheme involving derivatives along a single axis and another scheme involving derivatives along two axes, both of which are inherently symmetric. Note that $C_p(\mathbf{c}^*) = 0$ except for $p \in \mathcal{S}$ with up to two nonzero coordinates.

When $d = 3$, the scheme in this section coincides with the basis coefficients $C_p^{[4],1}$ and the corresponding right-hand basis grid function. When a is constant, this scheme coincides with the 4th-order ones proposed by [11, 15, 17].

We conclude this section with a final remark concerning the uniform grid assumption, on which our discussion has thus far relied. Similar calculation and analysis can be done for the non-uniform case, where the grid size in each axis is different. However, our calculation suggests that the maximum consistency order for a compact symmetric d -dimensional FDM with $d \geq 2$ on a non-uniform grid is only 2.

5. Numerical experiments. To verify our main theoretical result in the previous section, we present an example for 1D, 2D, and 3D. We use a uniform grid to discretize the domain $\Omega := (l_1, l_2)^d$, where $d = 1, 2, 3$. That is, we take $x_i = l_1 + ih$, $y_j = l_1 + jh$, and $z_k = l_1 + kh$, where $i, j, k = 1, \dots, N-1$ and $h = (l_2 - l_1)/N$, as our grid. In addition, we define the l_∞ -norm of the error as follows for the 3D case

$$\|u_h - u\|_\infty := \max_{1 \leq i, j, k \leq N-1} |(u_h)_{i,j,k} - u(x_i, y_j, z_k)|,$$

where $(u_h)_{i,j,k}$ stands for the approximated solution on the grid point (x_i, y_j, z_k) and u is the exact solution. The errors for the 1D and 2D cases can be similarly computed.

The following is the explicit form of the 2D stencil used in the discretization

$$\sum_{m,n=-1}^1 C_{m,n} (u_h)_{i+m,j+n} = (f_h)_{i,j},$$

where

$$\begin{aligned} C_{\pm 1, \pm 1} &= \frac{a}{6} - \frac{a_x a_y}{24a} h^2 + \frac{1}{48} [4a_{xy} - a_{xx}] h^2, \quad C_{\pm 1, \mp 1} = \frac{a}{6} + \left[\frac{a_x a_y}{24a} - \frac{a_{xx}}{48} \right] h^2, \\ C_{\pm 1, 0} &= \frac{2a}{3} - \frac{a_x^2}{12a} h^2 + \frac{1}{24} [2a_{xx} - 2a_{xy} - a_{yy}] h^2, \\ C_{0, \pm 1} &= \frac{2a}{3} - \frac{a_y^2}{12a} h^2 + \frac{1}{24} [a_{yy} - 2a_{xy}] h^2, \\ C_{0,0} &= - \sum_{\substack{m,n \in \{-1,0,1\}, \\ (m,n) \neq (0,0)}} C_{m,n}, \\ f_h &= -fh^2 + \frac{1}{12a^2} [a(f\Delta a + \nabla a \cdot \nabla f) - a^2 \Delta f - \|\nabla a\|_2^2 f] h^4, \end{aligned}$$

each $C_{m,n}$ with $(m,n) \neq (0,0)$ is evaluated at $(x_i + mh/2, y_j + nh/2)$, and f_h is evaluated at (x_i, y_j) . Meanwhile, the following is the explicit form of the 3D stencil used in the discretization

$$\sum_{m,n,\ell=-1}^1 C_{m,n,\ell} (u_h)_{i+m,j+n,k+\ell} = (f_h)_{i,j,k},$$

where

$$C_{\pm 1,0,0} = \frac{7a}{15}, \quad C_{0,\pm 1,\pm 1} = \frac{a}{10}, \quad C_{\pm 1,\mp 1,\pm 1} = \frac{a}{30} - \frac{a_y^2}{24a} h^2, \quad C_{0,\pm 1,\mp 1} = \frac{a}{10} + \frac{a_y a_z}{12a} h^2,$$

$$\begin{aligned}
C_{\pm 1,0,\mp 1} &= \frac{a}{10} + \frac{a_x a_z}{12a} h^2, \quad C_{\pm 1,\pm 1,\mp 1} = \frac{a}{30} + \frac{1}{24a} [a_y^2 - a_x^2] h^2, \\
C_{0,\pm 1,0} &= \frac{7a}{15} + \frac{a_z}{12a} [a_x - a_y] h^2, \quad C_{\pm 1,\pm 1,\pm 1} = \frac{a}{30} + \frac{1}{24} [a_{yy} + a_{xz} + a_{yz} - a_{xx}] h^2, \\
C_{\pm 1,0,\pm 1} &= \frac{a}{10} + \frac{1}{12a} [a_y^2 - a_x^2] h^2 + \frac{1}{12} [a_{xx} - a_{yy}] h^2, \\
C_{0,0,\pm 1} &= \frac{7a}{15} + \frac{1}{12a} [2a_x^2 - a_y^2 - a_z^2 - a_x a_z - a_y a_z] h^2 \\
&\quad + \frac{1}{24} [a_{yy} + a_{zz} - 3a_{xx} - 2a_{yz}] h^2, \\
C_{\pm 1,\mp 1,0} &= \frac{a}{10} + \frac{1}{24a} [a_x^2 + a_x a_y - a_x a_z] h^2 \\
&\quad + \frac{1}{48} [3a_{yy} - 3a_{xx} - a_{zz} + 2a_{xz} - 2a_{xy} - 2a_{yz}] h^2, \\
C_{\pm 1,\pm 1,0} &= \frac{a}{10} + \frac{1}{24a} [a_x^2 - 2a_y^2 - a_x a_y - a_x a_z] h^2 \\
&\quad + \frac{1}{48} [a_{xx} - a_{yy} - a_{zz} + 2a_{xy} - 2a_{xz} - 2a_{yz}] h^2, \\
C_{\pm 1,\mp 1,\mp 1} &= \frac{a}{30} - \frac{a_x}{24a} h^2 + \frac{1}{24} [a_{xx} + a_{yz} - a_{yy} - a_{xz}] h^2, \\
C_{0,0,0} &= - \sum_{\substack{m,n,\ell \in \{-1,0,1\} \\ (m,n,\ell) \neq (0,0,0)}} C_{m,n,\ell}, \\
f_h &= -f h^2 + \frac{1}{12a^2} [a(f\Delta a + \nabla a \cdot \nabla f) - a^2 \Delta f - \|\nabla a\|_2^2 f] h^4,
\end{aligned}$$

each $C_{m,n,\ell}$ with $(m,n,\ell) \neq (0,0,0)$ is evaluated at $(x_i + mh/2, y_j + nh/2, z_k + \ell h/2)$, and f_h is evaluated at (x_i, y_j, z_k) .

In the actual implementation of the scheme, we may replace the derivatives of a and f in the finite difference stencil with their values. This can be done without degrading the scheme's overall performance. This substitution is done to account for the fact that in practice we may only have access to the samples of a and f , but not to their analytic expressions. The details of such a substitution can be found in [4, Section 2.5] as well as in [8, Section 6.1], and can be generalized to higher dimensions.

EXAMPLE 5.1. Consider the model problem (1.1), where $\Omega := (0,1)^2$,

$$a := \ln(3x^3 + 5x^2 + 4), \quad u := 4^{x^2+2x+3},$$

and f, g are obtained by plugging a, u into (1.1). The numerical results are presented in Table 1. Since we use a compact, symmetric, and 12th-order FDM, the error magnitude is already on the order of 10^{-11} even when the grid size is still relatively large at $h = 2^{-4}$.

EXAMPLE 5.2. Consider the model problem (1.1), where $\Omega := (0,1)^2$,

$$\begin{aligned}
a &:= 4 + \cos(5\pi \tanh(5x - 3)) + \sin(17.5 \tanh(4y - 2)), \\
u &:= e^{\sin(20 \ln(3x^2+2y^2+1))} \cos(20y),
\end{aligned}$$

and f, g are obtained by plugging a, u into (1.1). The numerical results are presented in Table 1 and Figure 1. Note that a is obtained by modifying [9, Example 7.5]. From Figure 1, we observe that a and u both exhibit oscillations. As a result, the mesh size h should be small enough to accurately approximate a and u . Therefore, it is not surprising that we observe a fluctuation in the numerical convergence rates when $h \geq 2^{-6}$, but they stabilize once $h \leq 2^{-7}$.

EXAMPLE 5.3. Consider the model problem (1.1), where $\Omega := (-1,1)^3$,

$$a := 2 + \sin(5x - 3y - 3z), \quad u := \cos(4x) \sin(4y) \cos(5z),$$

Table 1: Numerical results for Theorems 5.1 and 5.2.

Compact, symmetric, and 12th-order 1D FDM			Compact, symmetric, and 4th-order 2D FDM					
Theorem 5.1			Theorem 5.2					
h	$\ u_h - u\ _\infty$	order	h	$\ u_h - u\ _\infty$	order	h	$\ u_h - u\ _\infty$	order
$\frac{1}{2}$	1.1444E-01		$\frac{1}{2^2}$	1.7749E+03		$\frac{1}{2^7}$	2.7205E-04	4.1
$\frac{1}{2^2}$	9.8187E-05	10.2	$\frac{1}{2^3}$	1.9780E+02	3.2	$\frac{1}{2^8}$	1.6633E-05	4.0
$\frac{1}{2^3}$	3.2546E-08	11.6	$\frac{1}{2^4}$	1.2392E+01	4.0	$\frac{1}{2^9}$	1.0391E-06	4.0
$\frac{1}{2^4}$	9.7771E-12	11.7	$\frac{1}{2^5}$	5.6600E-01	4.5	$\frac{1}{2^{10}}$	6.4844E-08	4.0
			$\frac{1}{2^6}$	4.8071E-03	6.9	$\frac{1}{2^{11}}$	4.0514E-09	4.0

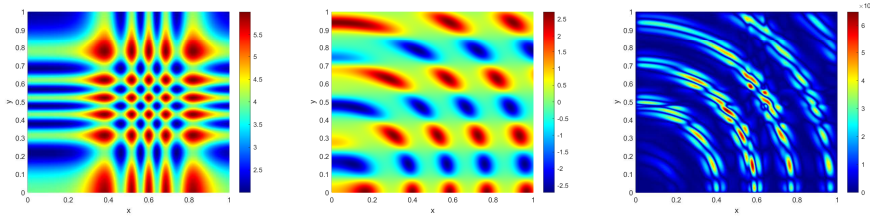


Fig. 1: Theorem 5.2: The coefficient a (left), the exact solution u (middle), and the error $|u_h - u|$ (right) on $[0, 1]^2$ with $h = 2^{-10}$, where u_h is obtained by using the compact, symmetric, and 4th-order 2D FDM.

and f, g are obtained by plugging a, u into (1.1). The numerical results are presented in Table 2 and Figure 2. Due to the size of the linear system produced from discretizing this 3D problem, we compare the speed, accuracy, and convergence rates of solutions obtained from the built-in `cgm` (the conjugate gradient method, which is an iterative solver) and the built-in `mldivide` functions in MATLAB (a direct solver). For the former, we specify error tolerances according to the grid size, while at the same time ensuring that the errors and convergence rates remain unaffected. From the computational speed's perspective, we observe that, on average, the conjugate gradient method is at least 2.5 times faster than `mldivide` for all $h > 2^{-5}$. Meanwhile, when $h = 2^{-6}$, the conjugate gradient method is around 40 times faster than `mldivide`. The efficiency of conjugate gradient method again verifies that the underlying linear system of our FDM is symmetric and positive definite.

Overall, the numerical convergence rates observed from all of our numerical experiments coincide with the theoretically derived consistency orders.

6. Derivations of compact, symmetric, and high-order FDMs in general dimensions. In this section, we adopt the approach of [4, 8] to present a general framework for the proposed finite difference schemes. We present the structure of all possible stencil coefficients and prove that the maximum consistency order is generally 4 for compact symmetric finite difference schemes in higher dimensions.

6.1. Expansion of the solution. This subsection contains key relations used in the upcoming lemmas, propositions, and ultimately our main result, Theorem 4.1.

Table 2: Numerical results for Theorem 5.3. The built-in `cgm` and `mldivide` MATLAB functions are used to solve the linear system $A_h u_h = b_h$ obtained from discretizing (1.1) using a compact, symmetric, and 4th-order 3D FDM. Below, we define $R := \frac{\|A_h u_h - b_h\|_2}{\|b_h\|_2}$. Furthermore, we denote I as the number of iterations of the conjugate gradient method, and T_{CG}, T_D as the computational times (in seconds) for `cgm` and `mldivide` respectively to solve the linear system.

h	Compact, symmetric, and 4th-order 3D FDM									
	<code>cgm</code>						<code>mldivide</code>			T_{CG}/T_D
	$\ u_h - u\ _\infty$	order	tolerance	R	I	T_{CG}	$\ u_h - u\ _\infty$	order	T_D	
$\frac{2}{2^2}$	1.89E+0		10^{-2}	8.1E-3	4	2.6E-3	1.89E+0		9.4E-3	3.7
$\frac{2}{2^3}$	1.30E-1	3.9	10^{-2}	9.4E-3	4	2.0E-3	1.31E-1	3.8	7.8E-3	3.9
$\frac{2}{2^4}$	6.69E-3	4.3	10^{-4}	7.5E-5	27	1.6E-2	6.77E-3	4.3	5.2E-2	3.4
$\frac{2}{2^5}$	3.90E-4	4.1	10^{-6}	9.0E-7	83	3.8E-1	3.90E-4	4.1	9.5E-1	2.5
$\frac{2}{2^6}$	2.43E-5	4.0	10^{-8}	9.2E-9	208	8.3E+0	2.43E-5	4.0	4.3E+1	5.2
$\frac{2}{2^7}$	1.51E-6	4.0	10^{-10}	9.9E-11	518	1.6E+2	1.51E-6	4.0	6.6E+3	40.6

We first rewrite the PDE in (1.1) as

$$(6.1) \quad \partial^{2\vec{e}_1} u = \nabla \tilde{a} \cdot \nabla u - \sum_{j=2}^d \partial^{2\vec{e}_j} u + \tilde{f} \quad \text{with} \quad \tilde{a} := -\ln a \quad \text{and} \quad \tilde{f} := -\frac{f}{a}.$$

Taking partial derivatives of both sides of (6.1), applying the Leibniz rule with $\mathbf{k} \geq 2\vec{e}_1$ to the first term, and rearranging the indices, we get

$$(6.2) \quad \begin{aligned} \partial^{\mathbf{k}} u &= \sum_{\vec{0} \leq \ell \leq \mathbf{k} - 2\vec{e}_1} \binom{\mathbf{k} - 2\vec{e}_1}{\ell} \sum_{j=1}^d \partial^{\mathbf{k} - \ell - 2\vec{e}_1 + \vec{e}_j} \tilde{a} \partial^{\ell + \vec{e}_j} u - \sum_{j=2}^d \partial^{\mathbf{k} - 2\vec{e}_1 + 2\vec{e}_j} u + \partial^{\mathbf{k} - 2\vec{e}_1} \tilde{f} \\ &= \sum_{\substack{\vec{0} \leq \ell \leq \mathbf{k} \\ \ell_1 < k_1}} \tilde{a}_\ell^{\mathbf{k}} \partial^\ell u + \partial^{\mathbf{k} - 2\vec{e}_1} \tilde{f}, \end{aligned}$$

where

$$(6.3) \quad \tilde{a}_\ell^{\mathbf{k}} = \begin{cases} -\sum_{j=2}^d \delta(|\mathbf{k} - \ell - 2\vec{e}_1 + 2\vec{e}_j|), & \text{if } |\ell| = |\mathbf{k}|, \\ \sum_{j=1}^d (1 - \delta(\ell_j)) \binom{\mathbf{k} - 2\vec{e}_1}{\ell - \vec{e}_j} \partial^{\mathbf{k} - \ell - 2\vec{e}_1 + 2\vec{e}_j} \tilde{a}, & \text{if } |\ell| < |\mathbf{k}|. \end{cases}$$

Now, if we use (6.2) repeatedly, we can represent $\partial^{\mathbf{k}} u$ in terms of $\partial^\ell u$ for $\ell \in \Pi_{|\mathbf{k}|}$, where Π_M is defined in (4.2). More concisely, we have

$$(6.4) \quad \partial^{\mathbf{k}} u = \sum_{\ell \in \Pi_{|\mathbf{k}|}} \tilde{A}_\ell^{\mathbf{k}} \partial^\ell u + \tilde{F}_{\mathbf{k}},$$

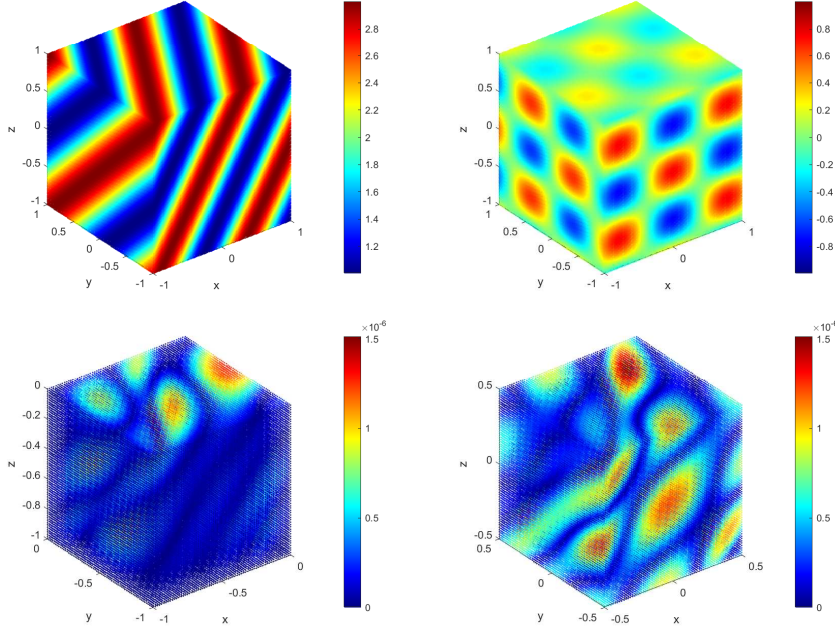


Fig. 2: Theorem 5.3: The coefficient a on $[-1, 1]^3$ (top left), the exact solution u on $[-1, 1]^3$ (top right), the error $|u_h - u|$ on the subdomain $[-1, 0]^3$ (bottom left), and the error $|u_h - u|$ on the subdomain $[-1/2, 1/2]^3$ (bottom right) with $h = 2/2^7$, where u_h is obtained by using the compact, symmetric, and 4th-order 3D FDM.

where the coefficients $\tilde{A}_\ell^{\mathbf{k}}$ and $\tilde{F}_\ell^{\mathbf{k}}$ are uniquely determined through the following recursive formulas:

$$(6.5) \quad \tilde{A}_\ell^{\mathbf{k}} := \begin{cases} \delta(|\mathbf{k} - \ell|), & \text{if } k_1 \leq 1, \\ \sum_{\substack{|\ell| \leq |j| \leq |\mathbf{k}| \\ j_1 < k_1}} \tilde{a}_j^{\mathbf{k}} \tilde{A}_\ell^j, & \text{if } k_1 \geq 2, \end{cases} \quad \tilde{F}_\ell^{\mathbf{k}} := \begin{cases} 0, & \text{if } k_1 \leq 1, \\ \sum_{\substack{|\ell| \leq |\mathbf{k}| \\ \ell_1 < k_1}} \tilde{a}_\ell^{\mathbf{k}} \tilde{F}_\ell + \partial^{\mathbf{k} - 2\bar{e}_1} \tilde{f}, & \text{if } k_1 \geq 2. \end{cases}$$

For $M \in \mathbb{N}_0$, a base point $\mathbf{b}^* \in \bar{\Omega}$ and $p = (p_1, \dots, p_d) \in \mathbb{Z}^d$, we have the Taylor expansion

$$u(\mathbf{b}^* + ph) = \sum_{0 \leq |\mathbf{k}| \leq M+1} \left(\prod_{j=1}^d \frac{p_j^{k_j}}{k_j!} \right) h^{|\mathbf{k}|} \partial^{\mathbf{k}} u(\mathbf{b}^*) + \mathcal{O}_u(h^{M+2}).$$

Now we incorporate (6.4) into the Taylor expansion of u to obtain (4.1), where $A_\ell^{\mathbf{k}}(p)$ and $F(p)$ are explicitly defined below:

$$(6.6) \quad A_\ell^{\mathbf{k}}(p) := \sum_{|\mathbf{k}|=k} \left(\prod_{j=1}^d \frac{p_j^{k_j}}{k_j!} \right) \tilde{A}_\ell^{\mathbf{k}} \quad \text{for } \ell \in \Pi_{M+1} \quad \text{and} \quad k = 0, \dots, M+1,$$

and

$$(6.7) \quad F(p) := \sum_{|\mathbf{k}| \leq M+1} \left(\prod_{j=1}^d \frac{p_j^{k_j}}{k_j!} \right) \tilde{F}_{\mathbf{k}} h^{|\mathbf{k}|}.$$

We also consider the converse to guarantee that our FDMs are exhaustive. It will be used in the proof of Lemma 6.1. For any real numbers $(u_{\ell})_{\ell \in \Pi_{M+1}}$, we construct a function v with

$$v(\mathbf{b}^* + ph) = \sum_{0 \leq |\mathbf{k}| \leq M+1} \left(\prod_{j=1}^d \frac{p_j^{k_j}}{k_j!} \right) h^{|\mathbf{k}|} v_{\mathbf{k}}, \quad v_{\mathbf{k}} = \begin{cases} u_{\mathbf{k}}, & \text{if } \mathbf{k} \in \Pi_{M+1}, \\ \sum_{\ell \in \Pi_{|\mathbf{k}|}} \tilde{A}_{\ell}^{\mathbf{k}} v_{\ell} + \tilde{F}_{\mathbf{k}}, & \text{if } \mathbf{k} \notin \Pi_{M+1}, \end{cases}$$

(compare with (6.4)), then $\partial^{\ell} v(\mathbf{b}^*) = u_{\ell}$ for $\ell \in \Pi_{M+1}$ and $\partial^{\ell} \nabla \cdot (a \nabla v) = \partial^{\ell} f$ at $\mathbf{b}^*$ for $|\ell| \leq M-1$.

In preparation for Section 6.2 (particularly for the proof of Lemma 6.1), we mention some special values for the quantities defined above. When $k_1 \geq 2$, we have $\tilde{a}_0^{\mathbf{k}} = 0$ by (6.3). Now we can deduce recursively from (6.5) that $\tilde{A}_0^{\mathbf{k}} = \delta(|\mathbf{k}|)$ for all $\mathbf{k} \in \mathbb{N}_0^d$. It follows from (6.6) that $A_0^k(p) = \delta(k)$ for $k \in \mathbb{N}_0$. Besides, we can calculate from (6.5) and (6.7) that

$$(6.8) \quad F(p) = \frac{1}{2} p_1^2 h^2 \tilde{f}(\mathbf{c}^*) + \mathcal{O}_{\tilde{a}, \tilde{f}}(h^3) = -\frac{1}{2a(\mathbf{c}^*)} p_1^2 h^2 f(\mathbf{c}^*) + \mathcal{O}_{\tilde{a}, \tilde{f}}(h^3),$$

where p_1 is the first entry of $p \in \mathbb{Z}^d$ and we recall that $\tilde{f} = -f/a$ as stated in (6.1). The coefficient $\tilde{A}_{\ell}^{\mathbf{k}}$ is of particular interest when $|\mathbf{k}| = |\ell|$ and $\ell \in \Pi_{|\mathbf{k}|}$. In this case, (6.3) and (6.5) imply

$$\tilde{A}_{\ell}^{\mathbf{k}} = \begin{cases} \delta(|\mathbf{k} - \ell|), & \text{if } k_1 \leq 1, \\ -\sum_{j=2}^d \tilde{A}_{\ell}^{\mathbf{k} - 2\vec{e}_1 + 2\vec{e}_j}, & \text{if } k_1 \geq 2. \end{cases}$$

Combined with (6.6), we can see that $A_{\ell}^k(p)$ is a constant independent of the functions a , f , and g in the PDE (1.1). In the particular case of $d = 2$, we can deduce that

$$(6.9) \quad \tilde{A}_{\ell}^{\mathbf{k}} = 0 \quad \text{if } \frac{1}{2}(\mathbf{k} - \ell) \notin \mathbb{N}_0^d \quad \text{and} \quad \tilde{A}_{\ell}^{\mathbf{k}} = (-1)^{(k_1 - l_1)/2} \quad \text{if } \frac{1}{2}(\mathbf{k} - \ell) \in \mathbb{N}_0^d.$$

This yields the following closed form of $A_{\ell}^k(p)$ when $d = 2$:

$$(6.10) \quad A_{(0,k)}^k(p) = \sum_{\substack{j \leq k \\ j \text{ is even}}} \frac{p_1^j p_2^{k-j}}{j!(k-j)!} (-1)^{j/2} = \frac{1}{k!} \operatorname{Re}(\mathbf{i}p_1 + p_2)^k.$$

Similarly, $A_{(1,k-1)}^k(p) = \frac{1}{k!} \operatorname{Im}(\mathbf{i}p_1 + p_2)^k$ for $k \in \mathbb{N}$.

6.2. Structure of the stencil coefficients. Let $\mathbf{c}^* \in \Omega_h$ and $\mathcal{S} = \{-1, 0, 1\}^d$. We expand the solution u at each point $\mathbf{c}^* + ph$ according to (4.1) with the base point $\mathbf{b}^* = \mathbf{c}^*$. In view of this, we aim to construct a finite difference scheme in the form of (2.1) that satisfies (2.3) with $f_h = \sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) F(p)$. The conditions on C_p are given by the following lemma.

LEMMA 6.1. *Let $M \geq -1$ be an integer. Consider the finite difference scheme $\mathcal{L}_h u_h = f_h$ for (1.1) on Ω_h satisfying the assumptions of Theorem 4.1. Then, the following statements are equivalent:*

(a) *The discretization operator $\mathcal{L}_h$ satisfies the following relation*

$$(6.11) \quad \mathcal{L}_h u(\mathbf{c}^*) = \sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) F(p) + \mathcal{O}_{\bar{a},u}(h^{M+2}), \quad \forall \mathbf{c}^* \in \Omega_h,$$

where $F(p)$ is defined in (6.7).

(b) *For all $\mathbf{c}^* \in \Omega_h$, we have*

$$(6.12) \quad \sum_{p \in \mathcal{S}} A_{\ell}^{|\ell|}(p) c_{p,j} = - \sum_{k=0}^{j-1} \sum_{p \in \mathcal{S}} A_{\ell}^{|\ell|+j-k}(p) c_{p,k}, \quad \forall j = 0, \dots, M+1, \quad \ell \in \Pi_{M+1-j},$$

where $A_{\ell}^k(p)$ is defined in (6.6). In particular, $\sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) = 0$.

(c) *If $\sum_{p \in \mathcal{S}} p_1^2 c_{p,0} \neq 0$, where p_1 is the first entry of $p \in \mathcal{S}$, holds, then there exists a grid function f_h such that the scheme $\mathcal{L}_h u_h = f_h$ is M th-order consistent.*

In addition, if M_ is the largest integer such that (6.12) has a solution, then any finite difference scheme $\mathcal{L}_h u_h = f_h$ has at most M_* th-order of consistency.*

Proof. The equivalence of (6.11) and (6.12) is treated in [8, Lemma 3.1] with a slight modification of the summation indices. Since we need to refer to the proof when we prove the equivalence of (b) and (c), we still present it for the sake of clarity. Additionally, we observe that expanding $u(\mathbf{c}^* + ph)$ at the base point $\mathbf{b}^* = \mathbf{c}^*$ via (4.1) yields

$$(6.13) \quad \mathcal{L}_h u(\mathbf{c}^*) = \sum_{\ell \in \Pi_{M+1}} P_{\ell}(h) \partial^{\ell} u(\mathbf{c}^*) + \sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) F(p) + \mathcal{O}_{\bar{a},u}(h^{M+2}),$$

where

$$P_{\ell}(h) := \sum_{k=|\ell|}^{M+1} \sum_{p \in \mathcal{S}} A_{\ell}^k(p) C_p(\mathbf{c}^*) h^k, \quad \ell \in \Pi_{M+1}.$$

(a) $\Leftrightarrow$ (b): Treating all $\partial^{\ell} u$, $\ell \in \Pi_{M+1}$ as independent variables, we deduce from (6.13) that $P_{\ell}(h) = \mathcal{O}_{\bar{a},u}(h^{M+2})$, $\forall \ell \in \Pi_{M+1}$. Now plugging $C_p(\mathbf{c}^*) = \sum_{j=0}^{M+1} c_{p,j} h^j + \mathcal{O}_{\bar{a}}(h^{M+2})$ into $P_{\ell}(h)$, we have

$$\begin{aligned} \mathcal{O}_{\bar{a},u}(h^{M+2}) &= \sum_{k=|\ell|}^{M+1} \sum_{j=0}^{M+1} \sum_{p \in \mathcal{S}} A_{\ell}^k(p) c_{p,j} h^{j+k} + \mathcal{O}_{\bar{a},u}(h^{M+2}) \\ &= \sum_{j=|\ell|}^{M+1} \sum_{k=0}^{j-|\ell|} \sum_{p \in \mathcal{S}} A_{\ell}^{j-k}(p) c_{p,k} h^j + \mathcal{O}_{\bar{a},u}(h^{M+2}). \end{aligned}$$

Since h is independent, the above identity implies $\sum_{k=0}^{j-|\ell|} \sum_{p \in \mathcal{S}} A_{\ell}^{j-k} c_{p,k} = 0$ for $\ell \in \Pi_{M+1}$ and $|\ell| \leq j \leq M+1$, which is equivalent to (6.12) by replacing $j - |\ell|$ with the new index j . Besides, setting $\ell = \vec{0}$ in (6.12), we get

$$\sum_{p \in \mathcal{S}} A_{\vec{0}}^0(p) c_{p,j} = - \sum_{k=0}^{j-1} \sum_{p \in \mathcal{S}} A_{\vec{0}}^{j-k}(p) c_{p,k}, \quad \forall j = 0, \dots, M+1.$$

Since $A_0^k(p) = \delta(k)$, we have $\sum_{p \in \mathcal{S}} c_{p,j} = 0$ for $0 \leq j \leq M+1$. Hence, $\sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) = 0$. This proves the equivalence between (a) and (b).

(a) $\Rightarrow$ (c): Suppose that $\sum_{p \in \mathcal{S}} p_1^2 c_{p,0} \neq 0$ and set $f_h := \sum_{p \in \mathcal{S}} C_p F(p)$. Then, (6.8) implies that $f_h = \mathcal{O}_{\tilde{a}, \tilde{f}}(h^2)$ with a nonzero leading term. This confirms the M th-order consistency of the scheme according to Definition 2.1, and proves item (c).

(c) $\Rightarrow$ (b): We want to show that if (6.12) fails for some $\mathbf{c}^* \in \Omega_h$, then we cannot find a grid function f_h , which makes the finite difference scheme M th-order consistent. In this case, $P_\ell(h)$ is not simultaneously zero for $\ell \in \Pi_{M+1}$ by the argument used in proving (a) $\Leftrightarrow$ (b). From the discussion in Section 6.1, for any given values $(u_\ell)_{\ell \in \Pi_{M+1}}$, there exists a smooth function v such that $\partial^\ell v(\mathbf{c}^*) = u_\ell$ for $\ell \in \Pi_{M+1}$ and $\partial^\ell \nabla \cdot (a \nabla v)(\mathbf{c}^*) = \partial^\ell f(\mathbf{c}^*)$ for $|\ell| \leq M-1$. From (6.5) and (6.7), we can see that $F(p) \in \text{span}\{\partial^\ell f(\mathbf{c}^*) : |\ell| \leq M-1\}$, which implies that $\sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) F(p)$ remains constant for such a function v . On the other hand, $\sum_{\ell \in \Pi_{M+1}} P_\ell(h) \partial^\ell v(\mathbf{c}^*)$ can be equal to any number as $(u_\ell)_{\ell \in \Pi_{M+1}}$ varies. Thus, neglecting the $\mathcal{O}_{\tilde{a}, u}(h^{M+2})$ term, the right-hand side of (6.13) must be dependent of u in addition to a and f . This proves that we cannot find f_h that forms an M th-order consistent scheme. Thus, (c) implies (b).

For the last statement, consider (6.13) with $M = M_* + 1$ for an arbitrary discretization operator $\mathcal{L}_h$. Since item (b), or equivalently item (a), is impossible for $M = M_* + 1$, there exists $\ell \in \Pi_{M_*+2}$ such that $P_\ell(h) \neq 0$. Now by repeating the argument of (c) $\Rightarrow$ (b), we can show that there is no $(M_* + 1)$ th-order consistent finite difference scheme $\mathcal{L}_h u_h = f_h$. The proof is complete. $\square$

Equation (6.12) provides an efficient way to find the stencil coefficients. We view (6.12) as a cascade of linear systems $\mathbb{A}_j \vec{c}_j = \vec{b}_j$ with unknowns $c_{p,j}$ for $j = 0, \dots, M+1$, where $\mathbb{A}_j$ is an $\#\Pi_{M+1-j} \times \#\mathcal{S}$ matrix and $\vec{b}_j, \vec{c}_j \in \mathbb{R}^{\#\mathcal{S}}$. Note that $\mathbb{A}_j$ is a constant matrix according to the end of Section 6.1 and it consists of merely the first $\#\Pi_{M+1-j}$ rows of $\mathbb{A}_0$. Moreover, when $d = 2$, the matrix $\mathbb{A}_j$ in this article and [8] only differ by a reordering of the columns.

Following the result of Lemma 6.1, the next proposition shows that the set of all possible stencil coefficients has a cascade structure. A more explicit explanation of this proposition is provided after the proof.

PROPOSITION 6.2. *For any integer $M \geq -1$ and $\mathbf{c}^* \in \Omega_h$, denote $\mathcal{N}_M$ to be the solution space of (6.12) viewed as a single linear system for $\{c_{p,j} : 0 \leq j \leq M+1, p \in \mathcal{S}\}$. Moreover, writing $\vec{c}_j = (c_{p,j})_{p \in \mathcal{S}}$, we define a shifting operator $T : \mathbb{R}^{(M+1)\#\mathcal{S}} \rightarrow \mathbb{R}^{(M+2)\#\mathcal{S}}$, $(\vec{c}_0, \dots, \vec{c}_M) \mapsto (\vec{0}, \vec{c}_0, \dots, \vec{c}_M)$, where $\vec{0} \in \mathbb{R}^{\#\mathcal{S}}$. Then $\mathcal{N}_M$ is a linear space with a decomposition*

$$(6.14) \quad \mathcal{N}_M = T\mathcal{N}_{M-1} + \mathcal{N}_M^* = \sum_{m=-1}^M T^{M-m} \mathcal{N}_m^*,$$

where $\mathcal{N}_m^*$ is a linear space and $\dim \mathcal{N}_M^*$ is equal to the dimension of the solution space of (6.12) with $j = 0$.

Proof. It is clear that $\mathcal{N}_M$ is a linear space from (6.12). We can equivalently write (6.12) as

$$(6.15) \quad \sum_{p \in \mathcal{S}} A_\ell^{|\ell|}(p) c_{p,0} = 0, \quad \forall \ell \in \Pi_{M+1},$$

when $j = 0$ and

(6.16)

$$\sum_{k=1}^j \sum_{p \in \mathcal{S}} A_{\ell}^{|\ell|+j-k}(p) c_{p,j} = - \sum_{p \in \mathcal{S}} A_{\ell}^{|\ell|+j}(p) c_{p,0}, \quad \forall j = 1, \dots, M+1, \ell \in \Pi_{M+1-j}.$$

Viewing (6.16) as a single linear system for $(\vec{c}_1, \dots, \vec{c}_M)$, we know that its solution space $\mathcal{N}(\vec{c}_0)$ can be decomposed into $\mathcal{N}^0 + (\vec{c}_1^*(\vec{c}_0), \dots, \vec{c}_M^*(\vec{c}_0))$, where $\mathcal{N}^0$ is the solution space of the homogeneous equation and $(\vec{c}_1^*(\vec{c}_0), \dots, \vec{c}_M^*(\vec{c}_0))$ is a particular solution that is dependent on $\vec{c}_0$. It follows that

$$\mathcal{N}_M = \{(\vec{c}_0, \dots, \vec{c}_M) : \vec{c}_0 \text{ satisfies (6.15), } (\vec{c}_1, \dots, \vec{c}_M) \in \mathcal{N}(\vec{c}_0)\}.$$

Denote

$$\mathcal{N}_M^* := \{(\vec{c}_0, \vec{c}_1^*(\vec{c}_0), \dots, \vec{c}_M^*(\vec{c}_0)) : \vec{c}_0 \text{ satisfies (6.15)}\},$$

then clearly $\mathcal{N}_M^*$ is a subspace of $\mathcal{N}_M$. Thus, $\mathcal{N}_M = T\mathcal{N}^0 \oplus \mathcal{N}_M^*$. On the other hand, by shifting the index from j to $j+1$, we see that $(\vec{c}_1, \dots, \vec{c}_M) \in \mathcal{N}^0$ if and only if

$$\sum_{k=0}^j \sum_{p \in \mathcal{S}} A_{m,n}^{|\ell|+j-k}(p) c_{p,j+1} = 0, \quad \forall j = 0, \dots, M, \ell \in \Pi_{M-j}.$$

The above equation holds if and only if $(\vec{c}_1, \dots, \vec{c}_M) \in \mathcal{N}_{M-1}$. Therefore, $\mathcal{N}^0 = \mathcal{N}_{M-1}$ and we get $\mathcal{N}_M = T\mathcal{N}_{M-1} \oplus \mathcal{N}_M^*$. The second equality in (6.14) follows directly from the first equality. Lastly, we can see from the above proof that $\dim \mathcal{N}_M^*$ is equal to the dimension of the solution space of (6.15), which is the same as (6.12) with $j = 0$. $\square$

Now we correspond the solution $\{c_{p,j} : 0 \leq j \leq M+1, p \in \mathcal{S}\}$ of (6.12) to the stencil coefficients $\{C_p = \sum_{j=0}^{M+1} c_{p,j} h^j : p \in \mathcal{S}\}$, then the shifting operator T sends C_p into hC_p . Moreover, let $\{(C_p^{[M],k})_{p \in \mathcal{S}} : 1 \leq k \leq K_M := \dim \mathcal{N}_M^*\}$ be a basis of $\mathcal{N}_M^*$. According to Proposition 6.2, any stencil coefficients C_p satisfying (6.11) can be decomposed as

$$(6.17) \quad C_p = \sum_{k=1}^{K_M} \kappa_{M,k} C_p^{[M],k} + hC'_p = \sum_{m=-1}^M \sum_{k=1}^{K_m} \kappa_{m,k} C_p^{[m],k} h^{M-m},$$

where $\kappa_{m,k} \in \mathbb{R}$ for all $k = 1, \dots, K_m$, $m = -1, \dots, M$, and C'_p are some stencil coefficients that satisfy (6.11) with M replaced by $M-1$.

Now we consider the compact stencil, that is, $\mathcal{S} = \{-1, 0, 1\}^d$. Since $\mathbb{A}_j$, $0 \leq j \leq M+1$ are constant matrices, it is easy to perform symbolic calculation and obtain the dimension K_M . The results for 2D and 3D are recorded in (4.5), (4.7), and (4.8). Using these explicit expressions, it is easy to verify whether the stencil coefficients in (6.17) satisfy the condition $\sum_{p \in \mathcal{S}} p_1^2 c_{p,0} \neq 0$ in item (c) of Lemma 6.1, which leads to a compact, symmetric, and M th-order consistent FDM for (1.1).

6.3. Maximum consistency order of d -dimensional compact FDMs for $d \geq 2$. We start this subsection by proving the maximum consistency order of compact nonsymmetric FDMs for (1.1). Recall from the previous subsection that the consistency order of a compact d -dimensional finite difference scheme is closely related to the dimension K_M . It is challenging to directly determine the dimension

K_M for $d > 3$. Hence, to circumvent this issue, we shall employ a key dimensional reduction technique, which enables us to use the dimension K_M in the 2D setting obtained via symbolic computation. This technique is used again in Lemma 6.4.

LEMMA 6.3. *Let $d \geq 2$. Then any compact finite difference scheme $\mathcal{L}_h u_h = f_h$ for (1.1) on Ω_h satisfying the assumptions of Theorem 4.1 is at most 6th-order consistent.*

Proof. We first prove this statement for $d = 2$. As mentioned in the remark just before this subsection, we have $K_M > 0$ if and only if $M \leq 6$, that is, (6.12) has a solution for the compact stencil $\mathcal{S}$ only when $M \leq 6$. According to Lemma 6.1, there is no compact M th-order consistent finite difference schemes for (1.1) with $M \geq 7$.

Now, we prove the statement for $d \geq 3$. We find a set of 2D functions $\tilde{a}$, $\tilde{f}$, $\tilde{u}$ and $\tilde{g}$ that satisfy (1.1) in $\tilde{\Omega} = (0, 1)^2$. Afterwards, we extend these functions to $\Omega = (0, 1)^d$, denoted by a , f , u and g respectively, such that they are constant along each direction x_j , $3 \leq j \leq d$. The extended functions clearly satisfy (1.1) in Ω . Let $\mathcal{L}_h u_h = f_h$ be a d -dimensional compact finite difference scheme for (1.1), where $\mathcal{L}_h u(\mathbf{c}^*) := \sum_{p \in \mathcal{S}} C_p(\mathbf{c}^*) u(\mathbf{c}^* + ph)$ with $\mathbf{c}^* \in \Omega_h$. Then, (2.3) holds in Ω_h . To construct a 2D finite difference scheme $\tilde{\mathcal{L}}_h u_h = \tilde{f}_h$ on $\tilde{\Omega}_h$, for each $\tilde{\mathbf{c}}^* \in \tilde{\Omega}_h$ we find a point $\mathbf{c}^* \in \Omega_h$ such that $\tilde{\mathbf{c}}^*$ consists of its first two components. Now we define

$$\tilde{\mathcal{L}}_h u_h(\tilde{\mathbf{c}}^*) = \sum_{\tilde{p} \in \tilde{\mathcal{S}}} \tilde{C}_{\tilde{p}}(\tilde{\mathbf{c}}^*) u_h(\tilde{\mathbf{c}}^* + \tilde{p}h), \quad \tilde{\mathbf{c}}^* \in \tilde{\Omega}_h,$$

and $\tilde{f}_h(\tilde{\mathbf{c}}^*) = f_h(\mathbf{c}^*)$, where $\tilde{\mathcal{S}} = [-1, 1]^2 \cap \mathbb{Z}^2$ and $\tilde{C}_{\tilde{p}}(\tilde{\mathbf{c}}^*) = \sum_{\{p \in \mathcal{S} : \tilde{p} = (p_1, p_2)\}} C_p(\mathbf{c}^*)$. Due to the way we extend the 2D functions, we have $\tilde{\mathcal{L}}_h \tilde{u}(\tilde{\mathbf{c}}^*) = \mathcal{L}_h u(\mathbf{c}^*)$, and $\tilde{f}_h$ depends only on the 2D functions and their derivatives. It follows that (2.3) also holds for $\tilde{\mathcal{L}}_h u_h = \tilde{f}_h$ in $\tilde{\Omega}_h$. Thus far, we have shown that if there is a compact d -dimensional compact finite difference scheme that is M th-order consistent, then there is a compact 2D M th-order consistent finite difference scheme. This contradicts the first part of the proof and we obtain the stated result of the lemma. $\square$

The following lemma shows that if we additionally require symmetry, than in general the fourth order FDMs in Section 6.3 already reach the maximum consistency order.

LEMMA 6.4. *Let $\frac{|\nabla a|^2}{a^2} - \frac{2\Delta a}{a}$ be non-constant in $\Omega = (0, 1)^d$, $d \geq 2$. Then there is no compact, symmetric, and 5th-order consistent finite difference scheme $\mathcal{L}_h u_h = f_h$ for (1.1) on Ω_h satisfying the assumptions of Theorem 4.1.*

Proof. By the same dimension reduction technique as in Lemma 6.3, we only need to prove the current lemma for $d = 2$. Suppose towards a contradiction that there exists a compact, symmetric, and 5th-order consistent finite difference scheme in Ω_h . On the one hand, all compact 5th-order consistent FDMs must satisfy (6.17) with $M = 5$, where $\kappa_{m,k} = \kappa_{m,k}(\mathbf{c}^*)$ is dependent on the stencil center $\mathbf{c}^*$. On the other hand, the FDM is clearly symmetric on the set $\{\mathbf{c}^* + qh : q \in \{(0, 0), (0, 1), (1, 0), (1, 1)\}\}$ as long as it is a subset of Ω_h . This symmetry condition yields 6 equations $C_{p-q}(\mathbf{c}^* + qh) = C_{q-p}(\mathbf{c}^* + ph)$, $p \neq q \in \{(0, 0), (0, 1), (1, 0), (1, 1)\}$ that the stencil coefficients should satisfy. We substitute (6.17) into these equations. By symbolic calculation, we obtain the following three necessary conditions:

(6.18a)

$$\kappa_{5,1}(\mathbf{c}^*) = \kappa_{5,1}(\mathbf{c}^* + (0, 1)h) = \kappa_{5,1}(\mathbf{c}^* + (1, 0)h) = \kappa_{5,1}(\mathbf{c}^* + (1, 1)h),$$

(6.18b)

$$\kappa_{2,1}(\mathbf{c}^* + (1,1)h) - \kappa_{2,1}(\mathbf{c}^*) = \frac{\kappa_{5,1}(\mathbf{c}^*)}{20}(\partial_x + \partial_y)(2\Delta\tilde{a} - |\nabla\tilde{a}|^2)(\mathbf{c}^* + (1,1)h/2),$$

and

$$\kappa_{2,1}(\mathbf{c}^* + (1,0)h) - \kappa_{2,1}(\mathbf{c}^* + (0,1)h) = \frac{\kappa_{5,1}(\mathbf{c}^*)}{20}(\partial_x - \partial_y)(2\Delta\tilde{a} - |\nabla\tilde{a}|^2)(\mathbf{c}^* + (1,1)h/2).$$

In particular, (6.18a) implies that $\kappa_{5,1}(\mathbf{c}^*)$ is constant over $\mathbf{c}^* \in \Omega_h$, hence we drop $\mathbf{c}^*$ afterwards. Recall the requirement $\sum_{p \in \mathcal{S}} p_1^2 c_{p,0} \neq 0$ in item (c) of Lemma 6.1. From (6.17) and the explicit expression in Section 4.1, we can calculate that $\sum_{p \in \mathcal{S}} p_1^2 c_{p,0} = -12\kappa_{5,1}$. Thus, $\kappa_{5,1} \neq 0$.

Note that $\frac{|\nabla a|^2}{a^2} - \frac{2\Delta a}{a} = 2\Delta\tilde{a} - |\nabla\tilde{a}|^2$ by $\tilde{a} = -\ln a$. Since $2\Delta\tilde{a} - |\nabla\tilde{a}|^2$ is not constant, it cannot be constant along all line segments $y = x + c$ and $y = -x + c$ within Ω . We assume that $2\Delta\tilde{a} - |\nabla\tilde{a}|^2$ is not constant on a line segment of the form $y = x + c$. Then we can choose h arbitrarily close to 0, such that there exists $z_1, z_2 \in \Omega_h$ satisfying $z_2 = z_1 + (1,1)Kh$ for some $K \in \mathbb{N}$ and $2\Delta\tilde{a} - |\nabla\tilde{a}|^2$ takes different values on z_1 and z_2 . It follows from (6.18b) that

$$\begin{aligned} \kappa_{2,1}(z_2) - \kappa_{2,1}(z_1) &= \sum_{k=1}^K \frac{\kappa_{5,1}}{20}(\partial_x + \partial_y)(2\Delta\tilde{a} - |\nabla\tilde{a}|^2)(\mathbf{c}^* + (1,1)(k-1/2)h) \\ &= \frac{\kappa_{5,1}}{10\sqrt{2}h} \left(2\Delta\tilde{a} - |\nabla\tilde{a}|^2\right) \Big|_{z_1}^{z_2} + \mathcal{O}_{\tilde{a}}(1), \end{aligned}$$

where we have treated the first line as a Riemann sum approximation to an integral to obtain the final line. This makes $\kappa_{2,1}$ as well as certain coefficients $c_{p,k}$ unbounded as $h \rightarrow 0$, which contradicts $c_{p,k} = \mathcal{O}_a(1)$. Therefore, such a finite difference scheme does not exist. $\square$

7. Conclusion. In this paper, we presented compact, symmetric, and high-order FDMS for the variable Poisson equation on a d -dimensional hypercube. Under the assumption that a uniform grid is used, we proved that in the one-dimensional case, the consistency order can be as high as we wish; meanwhile, in the general d -dimensional case for $d \geq 2$, the maximum consistency order is 4. For the special case where $d = 2$ and the diffusion coefficient, a , satisfies a certain derivative condition, the maximum consistency order is 6. Generally speaking, if we do not require the finite difference stencil to be symmetric, the highest consistency order that a d -dimensional FDM can achieve on a uniform mesh is 6 for $d \geq 2$. Our calculation and analysis can be extended to the non-uniform grid case. However, we found that a compact symmetric d -dimensional FDM for $d \geq 2$ can achieve at most consistency order 2. For ease of reproducibility, we presented our FDMS explicitly. Our numerical experiments also validated our theoretical findings and demonstrated some benefits of using our proposed symmetric FDMS.

As future work, we shall consider extending our current work to the general elliptic PDE (1.1) with a reaction term, and more general boundary conditions. We expect that some of the techniques used in this paper carry over to that setting. We choose to only consider (1.1) to simplify the presentation and to allow us clearly communicate the main techniques. Additionally, we shall explore the possibility of constructing a compact, symmetric, and high-order FDM for a curved domain.

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