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High-order blended compact difference schemes for the 3D elliptic partial differential equation with mixed derivatives and variable coefficients

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Abstract

Blended compact difference (BCD) schemes with fourth- and sixth-order accuracy are proposed for approximating the three-dimensional (3D) variable coefficients elliptic partial differential equation (PDE) with mixed derivatives. With truncation error analyses, the proposed BCD schemes can reach their theoretical accuracy, respectively, for the interior gird points and require 19 points compact stencil. They fully blend the implicit compact difference (CD) scheme and the explicit CD scheme together to make the derivation method and programming easier. The BCD schemes are also decoupled, which means the unknown function and its derivatives are separately resolved by different finite difference equations. Moreover, the sixth-order schemes are developed to solve the first-order derivatives, the second-order derivatives and the second-order mixed derivatives on boundaries. Several test problems are applied to show that the present BCD schemes are more accurate than those in the literature.

Keywords: 3D elliptic equation; Mixed derivative; Variable coefficients; BCD scheme; High-order accuracy

1 Introduction

In the paper, we study the steady 3D elliptic PDE

$$au_{xx} + bu_{yy} + cu_{zz} + pu_x + qu_y + ru_z + d_1u_{xy} + d_2u_{yz} + d_3u_{zx} + su = f(x, y, z), \tag{1}$$

where a, b, c, p, q, r, d_1, d_2, d_3, s and f are sufficiently smooth functions and have the required partial derivatives on Ω. The computational domain Ω is a union of rectangular solid. $\partial\Omega$ is the boundary of Ω.

The elliptic PDE like (1) is of primary importance in various fields of engineering and science [1, 2]. The numerical solution to the elliptic PDE has important interest in numerical analysis. In the past few decades, a lot of numerical methods, which include meshless methods [3], spline collocation methods [4], finite element methods [5], fast domain de-

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composition methods [6], Sinc-Galerkin methods [7] and finite difference methods [2, 8–44], have been proposed by many authors. Among the methods above, the finite difference method has been widely used in scientific research and engineering practice because of its simple structure, it being easy to understand and needing only a small amount of calculation.

The traditional difference schemes generally have low accuracy and calculation instability. And the non-compact high-order finite difference schemes are computational not efficient for a conventional type problem. However, high-order CD schemes have the advantages of having small discrete stencil, high-order accuracy, smaller element sensitivity and good numerical stability, which make it attractive in the fields of partial differential equations and computational fluid dynamics.

According to the difference of discrete objects, the compact difference scheme is divided into an explicit CD scheme and an implicit CD scheme. The former mainly discretize the differential equation (or model equation). The latter only discretizes derivatives of the unknown function involved in the model equation (or differential equation). Various special techniques have been developed rapidly based on implicit compact difference schemes [8–18]. In 1975, Adam [8], Kreiss [9] and Hirsh [10] proposed fourth-order CD schemes for different types of partial differential equations based on the Hermite formula, respectively. In Ref. [10], Hirsh solved the Burgers equation, the boundary layer problem and the driven cavity problem. In 1992, Lele [11] independently proposed a new type of CD method with quasi-spectral resolution and obtained a variety of symmetric compact difference schemes. Ma and Fu [12] proposed the upwind CD scheme with arbitrary-order accuracy in order to suppress the non-physical high frequency oscillation of the numerical solution near the shock wave. Deng and Zhang [13] developed the nonlinear CD scheme and overcame the non-physical oscillation of the symmetric compact difference scheme, which directly improved the quality of the stability simulation. Chu and Fan [14] derived a sixth-order combined CD scheme which is known as (CCD) scheme. In 1998, Mahesh [15] also proposed a CCD scheme of first-order and second-order derivatives with quasi-spectral resolution. Subsequently, the combined compact difference scheme is applied to resolve the wave propagation problem and the solution of the Navier-Stokes equation by Sengupta et al. [16, 17]. On the basis of Ref. [14], Lee et al. [18] constructed a new CCD scheme (CCD2) to solve two-dimensional (2D) elliptic problems with mixed derivative. Meanwhile, many explicit CD schemes have been also developed. Using Taylor series expansion and the method of undetermined coefficients, Gupta et al. [19] developed a fourth-order polynomial CD scheme for the 2D convection-diffusion equation with variable coefficients. Dennis and Hudson [20] developed a fourth-order CD scheme for solving the 2D convection-diffusion equation by using Numerov approximation and applied it to solve the Navier-Stokes equations. Spotz and Carey [21], Li et al. [22] and Gupta [23] proposed a nine-point fourth-order CD method for the Navier-Stokes equations in the form of incompressible vorticity-stream function, respectively. Ananthakrishnaiah et al. [24] also developed a fourth-order CD scheme for the 3D elliptic equations by using a Taylor series expansion and the method of undetermined coefficients. Chen et al. [25] developed a perturbation fourth-order exponential compact difference scheme for convection-diffusion equations with constant and variable coefficients. Tian and Dai [26] and Radhakrishna-Pillai [27] proposed fourth-order exponential CD schemes for the 1D and 2D steady convection-diffusion equations, respectively. Mohanty [28] constructed a

fourth-order CD scheme for the 3D nonlinear elliptic PDE. Gupta and Kouatchou [29] derived a 19-point fourth-order and a 27-point sixth-order CD schemes for the 3D Poisson equation by using the symbol software named Mathematica. Ge and Zhang [30] developed a 19-point fourth-order CD scheme for resolving the 3D linear elliptic equations by using Maple software. For the 3D steady convection-diffusion equation, Tian and Cui [31] and Zhang [32] proposed an explicit fourth-order CD scheme, respectively; Ma and Ge [33] developed a sixth-order CD scheme by using extrapolation technology; Mohamed et al. [34] proposed a fourth-order exponential CD scheme. Recently, Ma and Ge [35] developed a new class of BCD schemes to solve the 2D elliptic PDE with mixed derivatives by combining the advantages of the explicit CD and implicit CD. The BCD schemes cannot only achieve higher-order accuracy, but they also reduce the complexity of algebraic equations, so that they can be solved iteratively by the decoupling method.

As far as we know, there are few reports about the BCD schemes for the 3D elliptic equations with mixed derivatives, especially those with sixth-order accuracy. The main aim of the present paper is to extend our research work for 2D elliptic equations [35] to the 3D cases with variable coefficients and mixed derivatives to derive fourth- and sixth-order BCD schemes. The outline of this paper is organized as follows. Section 2 presents the two kinds of BCD schemes for the 3D elliptic PDE. In Sect. 3, we give truncation error analyses of the BCD schemes, respectively. Next, in Sect. 4, we compare our schemes with other schemes in the literature when numerical tests are conducted. Finally, some concluding remarks are given in Sect. 5.

2 The blended compact difference (BCD) schemes

In this section, the development of BCD formulations for Eq. (1) is briefly discussed. For convenience, the derivatives are symbolized as $u, u_x, u_y, u_z, u_{xx}, u_{yy}, u_{zz}, \partial_x \partial_y u, \partial_y \partial_z u, \partial_z \partial_x u,$ $\partial_x^2 \partial_y u, \partial_x^2 \partial_z u, \partial_y^2 \partial_x u, \partial_y^2 \partial_z u, \partial_z^2 \partial_x u, \partial_z^2 \partial_y u, \partial_x \partial_y \partial_z u, \partial_x^5 u, \partial_x^6 u, \partial_x^7 u, \partial_x^8 u, \partial_y^5 u, \partial_y^6 u, \partial_y^7 u, \partial_y^8 u,$ $\partial_z^5 u, \partial_z^6 u, \partial_z^7 u, \partial_z^8 u,$ respectively. The general Dirichlet boundary condition is considered. Here we use the notations

$$\frac{\partial^i}{\partial \zeta^i} \equiv \partial_\zeta^i \quad \text{and} \quad \frac{\partial^{i+j}}{\partial \zeta^i \partial \lambda^j} \equiv \partial_\zeta^i \partial_\lambda^j.$$

2.1 Inner grid points

Assume the problem domain to be cubical and construct on it a uniform Cartesian mesh of steps h_x, h_y and h_z in the x, y and z directions, respectively. For convenience, we use a local coordinate system [30]. The approximate values of functions $u, u_x, u_y, u_z, u_{xx}, u_{yy}, u_{zz},$ $\partial_x \partial_y u, \partial_y \partial_z u, \partial_z \partial_x u$ at an internal mesh point (x_i, y_j, z_k) are denoted by $u_0, u_{x0} u_{y0}, u_{z0}, u_{xx0},$ $u_{yy0}, u_{zz0}, \partial_x \partial_y u_0, \partial_y \partial_z u_0, \partial_z \partial_x u_0$. The approximate values of its immediate 18 neighboring points are denoted by $u_l, u_{xl}, u_{yl}, u_{zl}, u_{xxl}, u_{yyl}, u_{zzl}, \partial_x \partial_y u_l, \partial_y \partial_z u_l, \partial_z \partial_x u_l, l = 1, 2, \ldots, 18,$ as in Fig. 1. We use the Taylor series expansions at point (x_i, y_j, z_k) for u_x, u_y, u_z.

We obtain

$$u_x = \delta_x u - \frac{h_x^2}{6} \partial_x^3 u - \frac{h_x^4}{120} \partial_x^5 u + O(h_x^6), \tag{2}$$

$$u_y = \delta_y u - \frac{h_y^2}{6} \partial_y^3 u - \frac{h_y^4}{120} \partial_y^5 u + O(h_y^6), \tag{3}$$

$$u_z = \delta_z u - \frac{h_z^2}{6} \partial_z^3 u - \frac{h_z^4}{120} \partial_z^5 u + O(h_z^6), \tag{4}$$

Figure 1 The 19-point stencil of 3D
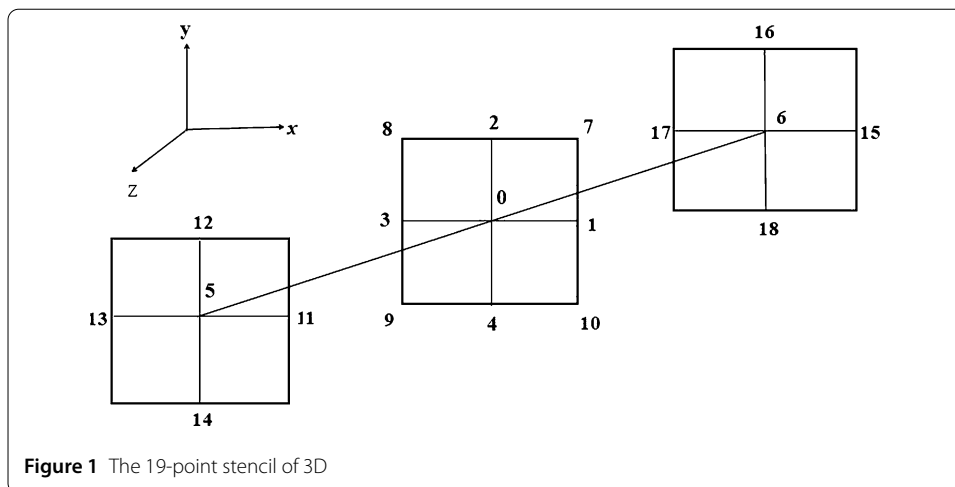
here δ_x, δ_y and δ_z are central difference operators for u_x, u_y, u_z. Substituting Eqs. (2)–(4) into Eq. (1), we obtain

$$
au_{xx} + bu_{yy} + cu_{zz} + p\left(\delta_x u - \frac{h_x^2}{6}\partial_x^3 u - \frac{h_x^4}{120}\partial_x^5 u\right) + q\left(\delta_y u - \frac{h_y^2}{6}\partial_y^3 u - \frac{h_y^4}{120}\partial_y^5 u\right)
$$
$$
+ r\left(\delta_z u - \frac{h_z^2}{6}\partial_z^3 u - \frac{h_z^4}{120}\partial_z^5 u\right) + d_1\partial_x\partial_y u + d_2\partial_y\partial_z u + d_3\partial_z\partial_x u + su
$$
$$
+ O\left(h_x^6 + h_y^6 + h_z^6\right) = f. \tag{5}
$$

Differentiating Eq. (1) with respect to x, y and z, we get

$$
\partial_x^3 u = \frac{1}{a}\big(f_x - b\partial_y^2\partial_x u - b_x u_{yy} - c\partial_z^2\partial_x u - c_x u_{zz} - pu_{xx} - p_x u_x - q\partial_y\partial_x u - q_x u_y - r_x u_z
$$
$$
- r\partial_z\partial_x u - d_1\partial_x^2\partial_y u - d_{1x}\partial_x\partial_y u - d_{2x}\partial_y\partial_z u - d_2\partial_x\partial_y\partial_z u
$$
$$
- d_{3x}\partial_z\partial_x u - d_3\partial_x^2\partial_z u - s_x u - su_x\big)
$$
$$
- \frac{a_x}{a^2}(f - bu_{yy} - cu_{zz} - pu_x - qu_y - ru_z - d_1\partial_x\partial_y u - d_2\partial_y\partial_z u - d_3\partial_z\partial_x u - su), \quad (6)
$$
$$
\partial_y^3 u = \frac{1}{b}\big(f_y - a\partial_x^2\partial_y u - a_y u_{xx} - c\partial_z^2\partial_y u - c_y u_{zz} - p\partial_x\partial_y u - p_y u_x - qu_{yy} - q_y u_y - r_y u_z
$$
$$
- r\partial_z\partial_y u - d_1\partial_y^2\partial_x u - d_{1y}\partial_x\partial_y u - d_{2y}\partial_z\partial_y u - d_2\partial_y^2\partial_z u - d_{3y}\partial_z\partial_x u
$$
$$
- d_3\partial_x\partial_y\partial_z u - s_y u - su_y\big)
$$
$$
- \frac{b_y}{b^2}(f - au_{xx} - cu_{zz} - pu_x - qu_y - ru_z - d_1\partial_x\partial_y u - d_2\partial_y\partial_z u - d_3\partial_z\partial_x u - su), \quad (7)
$$
$$
\partial_z^3 u = \frac{1}{c}\big(f_z - a\partial_x^2\partial_z u - a_z u_{xx} - b\partial_y^2\partial_z u - b_z u_{yy} - p\partial_x\partial_z u - p_z u_x - q\partial_y\partial_z u - q_z u_y - r_z u_z
$$
$$
- ru_{zz} - d_1\partial_x\partial_y\partial_z u - d_{1z}\partial_x\partial_y u - d_{2z}\partial_y\partial_z u - d_2\partial_z^2\partial_y u - d_{3z}\partial_x\partial_z u
$$
$$
- d_3\partial_z^2\partial_x u - s_z u - su_z\big)
$$
$$
- \frac{c_z}{c^2}(f - bu_{yy} - cu_{zz} - pu_x - qu_y - ru_z - d_1\partial_x\partial_y u - d_2\partial_y\partial_z u - d_3\partial_z\partial_x u - su), \quad (8)
$$

substituting Eqs. (6)–(8) into Eq. (5), we get

$$
\begin{aligned}
& A_1 u_{xx} + A_2 u_{yy} + A_3 u_{zz} + A_4 u_x + A_5 u_y + A_6 u_z + A_7 \partial_x \partial_y u + A_8 \partial_y \partial_z u \\
& \quad + A_9 \partial_z \partial_x u + A_{10} \partial_x \partial_y \partial_z u \\
& \quad + A_{11} \partial_x^2 \partial_y u + A_{12} \partial_y^2 \partial_x u + A_{13} \partial_z^2 \partial_x u + A_{14} \partial_x^2 \partial_z u + A_{15} \partial_y^2 \partial_z u \\
& \quad + A_{16} \partial_z^2 \partial_y u + A_{17} u + p \delta_x u + q \delta_y u \\
& \quad + r \delta_z u - \frac{h_x^4 p}{120} \partial_x^5 u - \frac{h_y^4 q}{120} \partial_y^5 u - \frac{h_z^4 r}{120} \partial_z^5 u + O\big(h_x^6 + h_y^6 + h_z^6\big) = F,
\end{aligned}
\tag{9}
$$

where

$$
A_1 = a + \frac{h_x^2 p^2}{6a} - \frac{ab_y h_y^2 q}{6b^2} - \frac{ac_z h_z^2 r}{6c^2} + \frac{a_y h_y^2 q}{6b} + \frac{a_z h_z^2 r}{6c},
\tag{10}
$$

$$
A_2 = b + \frac{h_y^2 q^2}{6b} - \frac{a_x b h_x^2 p}{6a^2} - \frac{c_z b h_z^2 r}{6c^2} + \frac{b_x h_x^2 p}{6a} + \frac{b_z h_z^2 r}{6c},
\tag{11}
$$

$$
A_3 = c + \frac{h_z^2 r^2}{6c} - \frac{a_x c h_x^2 p}{6a^2} - \frac{b_y c h_y^2 q}{6b^2} + \frac{c_x h_x^2 p}{6a} + \frac{c_y h_y^2 q}{6b},
\tag{12}
$$

$$
A_4 = \frac{h_x^2 p}{6a}(p_x + s) + \frac{h_y^2 q p_y}{6b} + \frac{h_z^2 r p_z}{6c} - \frac{a_x h_x^2 p^2}{6a^2} - \frac{b_y p h_y^2 q}{6b^2} - \frac{c_z p h_z^2 r}{6c^2},
\tag{13}
$$

$$
A_5 = \frac{h_y^2 q}{6b}(q_y + s) + \frac{h_x^2 p q_x}{6a} + \frac{h_z^2 r q_z}{6c} - \frac{a_x h_x^2 p q}{6a^2} - \frac{b_y h_y^2 q^2}{6b^2} - \frac{c_z q h_z^2 r}{6c^2},
\tag{14}
$$

$$
A_6 = \frac{h_z^2 r}{6c}(r_z + s) + \frac{h_x^2 p r_x}{6a} + \frac{h_y^2 q r_y}{6b} - \frac{a_x r h_x^2 p}{6a^2} - \frac{b_y r h_y^2 q}{6b^2} - \frac{c_z h_z^2 r^2}{6c^2},
\tag{15}
$$

$$
\begin{aligned}
A_7 &= \frac{h_x^2 p q}{6a} + \frac{h_y^2 q p}{6b} + d_1 + \frac{h_x^2 p d_{1x}}{6a} + \frac{h_y^2 q d_{1y}}{6b} + \frac{h_z^2 r d_{1z}}{6c} - \frac{h_x^2 p a_x d_1}{6a^2} \\
& \quad - \frac{h_y^2 q b_y d_1}{6b^2} - \frac{h_z^2 r c_z d_1}{6c^2},
\end{aligned}
\tag{16}
$$

$$
\begin{aligned}
A_8 &= \frac{h_y^2 q r}{6b} + \frac{h_z^2 r q}{6c} + d_2 + \frac{h_x^2 p d_{2x}}{6a} + \frac{h_y^2 q d_{2y}}{6b} + \frac{h_z^2 r d_{2z}}{6c} - \frac{h_x^2 p a_x d_2}{6a^2} \\
& \quad - \frac{h_y^2 q b_y d_2}{6b^2} - \frac{h_z^2 r c_z d_2}{6c^2},
\end{aligned}
\tag{17}
$$

$$
\begin{aligned}
A_9 &= \frac{h_x^2 p r}{6a} + \frac{h_z^2 r p}{6c} + d_3 + \frac{h_x^2 p d_{3x}}{6a} + \frac{h_y^2 q d_{3y}}{6b} + \frac{h_z^2 r d_{3z}}{6c} - \frac{h_x^2 p a_x d_3}{6a^2} \\
& \quad - \frac{h_y^2 q b_y d_3}{6b^2} - \frac{h_z^2 r c_z d_3}{6c^2},
\end{aligned}
\tag{18}
$$

$$
A_{10} = \frac{h_x^2 p d_2}{6a} + \frac{h_y^2 q d_3}{6b} + \frac{h_z^2 r d_1}{6c},
\tag{19}
$$

$$
A_{11} = \frac{h_x^2 p d_1}{6a} + \frac{h_y^2 q a}{6b},
\tag{20}
$$

$$
A_{12} = \frac{h_x^2 p b}{6a} + \frac{h_y^2 q d_1}{6b},
\tag{21}
$$

$$
A_{13} = \frac{h_x^2 p c}{6a} + \frac{h_z^2 r d_3}{6c},
\tag{22}
$$

$$A_{14} = \frac{h_z^2 ra}{6c} + \frac{h_x^2 pd_3}{6a}, \tag{23}$$

$$A_{15} = \frac{h_z^2 rb}{6c} + \frac{h_y^2 qd_2}{6b}, \tag{24}$$

$$A_{16} = \frac{h_y^2 qc}{6b} + \frac{h_z^2 rd_2}{6c}, \tag{25}$$

$$A_{17} = \left(1 - \frac{a_x h_x^2 p}{6a^2} - \frac{b_y h_y^2 q}{6b^2} - \frac{c_z h_z^2 r}{6c^2}\right)s + \frac{s_x h_x^2 p}{6a} + \frac{s_y h_y^2 q}{6b} + \frac{s_z h_z^2 r}{6c}, \tag{26}$$

$$F = \left(1 - \frac{a_x p h_x^2}{6a^2} - \frac{b_y q h_y^2}{6b^2} - \frac{c_z r h_z^2}{6c^2}\right)f + \frac{p h_x^2}{6a}f_x + \frac{q h_y^2}{6b}f_y + \frac{r h_z^2}{6c}f_z. \tag{27}$$

In order to get a fourth-order formulation for Eq. (9), all the derivatives $\{u_{xx}, u_{yy}, u_{zz}, \partial_x\partial_y u, \partial_y\partial_z u, \partial_z\partial_x u, \partial_x^2\partial_y u, \partial_x^2\partial_z u, \partial_y^2\partial_x u, \partial_y^2\partial_z u, \partial_z^2\partial_x u, \partial_z^2\partial_y u, \partial_x\partial_y\partial_z u\}$ are approximated as follows:

$$u_{xx} = 2\delta_x^2 u - \delta_x u_x + O(h_x^4), \tag{28}$$

$$u_{yy} = 2\delta_y^2 u - \delta_y u_y + O(h_y^4), \tag{29}$$

$$u_{zz} = 2\delta_z^2 u - \delta_z u_z + O(h_z^4), \tag{30}$$

$$\partial_x\partial_y u = \delta_x u_y + \delta_y u_x - \delta_x\delta_y u + O(h_x^4 + h_y^4 + h_x^2 h_y^2), \tag{31}$$

$$\partial_y\partial_z u = \delta_y u_z + \delta_z u_y - \delta_y\delta_z u + O(h_y^4 + h_z^4 + h_y^2 h_z^2), \tag{32}$$

$$\partial_z\partial_x u = \delta_z u_x + \delta_x u_z - \delta_z\delta_x u + O(h_z^4 + h_x^4 + h_z^2 h_x^2), \tag{33}$$

$$\partial_x^2\partial_y u = \delta_x^2 u_y + O(h_x^2), \tag{34}$$

$$\partial_x^2\partial_z u = \delta_x^2 u_z + O(h_x^2), \tag{35}$$

$$\partial_y^2\partial_x u = \delta_y^2 u_x + O(h_y^2), \tag{36}$$

$$\partial_y^2\partial_z u = \delta_y^2 u_z + O(h_y^2), \tag{37}$$

$$\partial_z^2\partial_x u = \delta_z^2 u_x + O(h_z^2), \tag{38}$$

$$\partial_z^2\partial_y u = \delta_z^2 u_y + O(h_z^2), \tag{39}$$

$$\partial_x\partial_y\partial_z u = \frac{1}{3}(\delta_y\delta_z u_x + \delta_x\delta_z u_y + \delta_x\delta_y u_z) + O(h_x^2 + h_y^2 + h_z^2). \tag{40}$$

Here Eqs. (28)–(30) have been studied in Refs. [43, 44]. Substituting Eqs. (28)–(40) into Eq. (9), we have

$$\begin{aligned}
&\left(2A_1\delta_x^2 + 2A_2\delta_y^2 + 2A_3\delta_z^2 + p\delta_x + q\delta_y + r\delta_z - A_7\delta_x\delta_y - A_8\delta_y\delta_z - A_9\delta_z\delta_x\right)u \\
&\quad + \left(A_4 - A_1\delta_x + A_7\delta_y + A_9\delta_z + \frac{A_{10}}{3}\delta_y\delta_z + A_{12}\delta_y^2 + A_{13}\delta_z^2\right)u_x \\
&\quad + \left(A_5 - A_2\delta_y + A_7\delta_x + A_8\delta_z + \frac{A_{10}}{3}\delta_x\delta_z + A_{11}\delta_x^2 + A_{16}\delta_z^2\right)u_y \\
&\quad + \left(A_6 - A_3\delta_z + A_8\delta_y + A_9\delta_x + \frac{A_{10}}{3}\delta_x\delta_y + A_{14}\delta_x^2 + A_{15}\delta_y^2\right)u_z \\
&= \left(1 - \frac{a_x p h_x^2}{6a^2} - \frac{b_y q h_y^2}{6b^2} - \frac{c_z r h_z^2}{6c^2} + \frac{p h_x^2}{6a}\delta_x + \frac{q h_y^2}{6b}\delta_y + \frac{r h_z^2}{6c}\delta_z\right)f.
\end{aligned} \tag{41}$$

Substituting δ_x, δ_y, δ_z, δ_x^2, δ_y^2, δ_z^2, $\delta_x\delta_y$, $\delta_y\delta_z$, $\delta_z\delta_x$ given in Appendix A at grid point 0 into Eq. (41). Then eliminating the sixth-order truncation error terms, we obtain the required fourth-order BCD scheme with 19 grid points

$$-4\left(\frac{A_1}{h_x^2} + \frac{A_2}{h_y^2} + \frac{A_3}{h_z^2}\right)u_0 + \left(\frac{2A_1}{h_x^2} + \frac{p_0}{2h_x}\right)u_1 + \left(\frac{2A_2}{h_y^2} + \frac{q_0}{2h_y}\right)u_2$$

$$+ \left(\frac{2A_1}{h_x^2} - \frac{p_0}{2h_x}\right)u_3 + \left(\frac{2A_2}{h_y^2} - \frac{q_0}{2h_y}\right)u_4$$

$$+ \left(\frac{2A_3}{h_z^2} + \frac{r_0}{2h_z}\right)u_5 + \left(\frac{2A_3}{h_z^2} - \frac{r_0}{2h_z}\right)u_6 - \frac{A_7}{4h_xh_y}u_7 + \frac{A_7}{4h_xh_y}u_8 - \frac{A_7}{4h_xh_y}u_9$$

$$+ \frac{A_7}{4h_xh_y}u_{10} - \frac{A_9}{4h_xh_z}u_{11}$$

$$- \frac{A_8}{4h_yh_z}u_{12} + \frac{A_9}{4h_xh_z}u_{13} + \frac{A_8}{4h_yh_z}u_{14} + \frac{A_9}{4h_xh_z}u_{15} + \frac{A_8}{4h_yh_z}u_{16}$$

$$- \frac{A_9}{4h_xh_z}u_{17} - \frac{A_8}{4h_yh_z}u_{18}$$

$$+ \left(A_4 - \frac{2A_{12}}{h_y^2} - \frac{2A_{13}}{h_z^2}\right)u_{x0} - \frac{A_1}{2h_x}u_{x1} + \left(\frac{A_7}{2h_y} + \frac{A_{12}}{h_y^2}\right)u_{x2} + \frac{A_1}{2h_x}u_{x3}$$

$$+ \left(-\frac{A_7}{2h_y} + \frac{A_{12}}{h_y^2}\right)u_{x4}$$

$$+ \left(\frac{A_9}{2h_z} + \frac{A_{13}}{h_z^2}\right)u_{x5} + \left(-\frac{A_9}{2h_z} + \frac{A_{13}}{h_z^2}\right)u_{x6} + \frac{A_{10}}{12h_yh_z}u_{x12} - \frac{A_{10}}{12h_yh_z}u_{x14}$$

$$- \frac{A_{10}}{12h_yh_z}u_{x16} + \frac{A_{10}}{12h_yh_z}u_{x18}$$

$$+ \left(A_5 - \frac{2A_{11}}{h_x^2} - \frac{2A_{16}}{h_z^2}\right)u_{y0} + \left(\frac{A_7}{2h_x} + \frac{A_{11}}{h_x^2}\right)u_{y1} - \frac{A_2}{2h_y}u_{y2}$$

$$+ \left(-\frac{A_7}{2h_x} + \frac{A_{11}}{h_x^2}\right)u_{y3} + \frac{A_2}{2h_y}u_{y4}$$

$$+ \left(\frac{A_8}{2h_z} + \frac{A_{16}}{h_z^2}\right)u_{y5} + \left(-\frac{A_8}{2h_z} + \frac{A_{16}}{h_z^2}\right)u_{y6} + \frac{A_{10}}{12h_xh_z}u_{y11} - \frac{A_{10}}{12h_xh_z}u_{y13}$$

$$- \frac{A_{10}}{12h_xh_z}u_{y15} + \frac{A_{10}}{12h_xh_z}u_{y17}$$

$$+ \left(A_6 - \frac{2A_{14}}{h_x^2} - \frac{2A_{15}}{h_y^2}\right)u_{z0} + \left(\frac{A_9}{2h_x} + \frac{A_{14}}{h_x^2}\right)u_{z1} + \left(\frac{A_8}{2h_y} + \frac{A_{15}}{h_y^2}\right)u_{z2}$$

$$+ \left(-\frac{A_9}{2h_x} + \frac{A_{14}}{h_x^2}\right)u_{z3} - \frac{A_3}{2h_z}u_{z5}$$

$$+ \left(-\frac{A_8}{2h_y} + \frac{A_{15}}{h_y^2}\right)u_{z4} + \frac{A_3}{2h_z}u_{z6} + \frac{A_{10}}{12h_xh_y}u_{z7} - \frac{A_{10}}{12h_xh_y}u_{z8}$$

$$+ \frac{A_{10}}{12h_xh_y}u_{z9} - \frac{A_{10}}{12h_xh_y}u_{z10}$$

$$= \left(1 - \frac{a_{x0}p_0h_x^2}{6a^2} - \frac{b_{y0}q_0h_y^2}{6b^2} - \frac{c_{z0}r_0h_z^2}{6c^2}\right)f_0 + \frac{p_0h_x^2}{6a}f_{x0} + \frac{q_0h_y^2}{6b}f_{y0} + \frac{r_0h_z^2}{6c}f_{z0}. \qquad (42)$$

Notice that there are four unknowns $\{u, u_x, u_y, u_z\}$ to be determined for fourth-order scheme. In order to match the system, in the inner field, u_x, u_y and u_z are computed, respectively, by

$$\frac{1}{6}u_{x1} + \frac{4}{6}u_{x0} + \frac{1}{6}u_{x3} = \frac{u_1 - u_3}{2h_x}, \tag{43}$$

$$\frac{1}{6}u_{y2} + \frac{4}{6}u_{y0} + \frac{1}{6}u_{y4} = \frac{u_2 - u_4}{2h_y}, \tag{44}$$

and

$$\frac{1}{6}u_{z5} + \frac{4}{6}u_{z0} + \frac{1}{6}u_{z6} = \frac{u_5 - u_6}{2h_z}, \tag{45}$$

to get a sixth-order compact formulation for Eq. (9), consider the following approximations for all the derivatives:

$$u_{xx} = 2\delta_x^2 u - \delta_x u_x + \frac{h_x^4}{360}\partial_x^6 u + O(h_x^6), \tag{46}$$

$$u_{yy} = 2\delta_y^2 u - \delta_y u_y + \frac{h_y^4}{360}\partial_y^6 u + O(h_y^6), \tag{47}$$

$$u_{zz} = 2\delta_z^2 u - \delta_z u_z + \frac{h_z^4}{360}\partial_z^6 u + O(h_z^6), \tag{48}$$

$$\partial_x^2 \partial_y u = \delta_x^2 u_y + \delta_x^2 \delta_y u - \delta_x \delta_y u_x + O(h_x^4 + h_y^4 + h_x^2 h_y^2), \tag{49}$$

$$\partial_x^2 \partial_z u = \delta_x^2 u_z + \delta_x^2 \delta_z u - \delta_x \delta_z u_x + O(h_x^4 + h_z^4 + h_x^2 h_z^2), \tag{50}$$

$$\partial_y^2 \partial_x u = \delta_y^2 u_x + \delta_y^2 \delta_x u - \delta_y \delta_x u_y + O(h_y^4 + h_x^4 + h_y^2 h_x^2), \tag{51}$$

$$\partial_y^2 \partial_z u = \delta_y^2 u_z + \delta_y^2 \delta_z u - \delta_y \delta_z u_y + O(h_y^4 + h_z^4 + h_y^2 h_z^2), \tag{52}$$

$$\partial_z^2 \partial_x u = \delta_z^2 u_x + \delta_z^2 \delta_x u - \delta_z \delta_x u_z + O(h_z^4 + h_x^4 + h_z^2 h_x^2), \tag{53}$$

$$\partial_z^2 \partial_y u = \delta_z^2 u_y + \delta_z^2 \delta_y u - \delta_z \delta_y u_z + O(h_z^4 + h_y^4 + h_z^2 h_y^2), \tag{54}$$

$$\partial_x \partial_y \partial_z u = \frac{1}{3}(2\delta_x \partial_y \partial_z u + 2\delta_y \partial_x \partial_z u + 2\delta_z \partial_x \partial_y u - \delta_x \delta_y u_z$$
$$- \delta_y \delta_z u_x - \delta_z \delta_x u_y) + O(h_x^4 + h_y^4 + h_z^4 + h_x^2 h_y^2 + h_y^2 h_z^2 + h_z^2 h_x^2), \tag{55}$$

$$\partial_x^5 u = \frac{360}{7h_x^4}\left(u_x - \delta_x u + \frac{h_x^2}{6}\delta_x u_{xx}\right) + O(h_x^2), \tag{56}$$

$$\partial_x^6 u = \frac{240}{h_x^4}\left(u_{xx} - \delta_x^2 u + \frac{h_x^2}{12}\delta_x^2 u_{xx}\right) + O(h_x^2), \tag{57}$$

$$\partial_y^5 u = \frac{360}{7h_y^4}\left(u_y - \delta_y u + \frac{h_y^2}{6}\delta_y u_{yy}\right) + O(h_y^2), \tag{58}$$

$$\partial_y^6 u = \frac{240}{h_y^4}\left(u_{yy} - \delta_y^2 u + \frac{h_y^2}{12}\delta_y^2 u_{yy}\right) + O(h_y^2), \tag{59}$$

$$\partial_z^5 u = \frac{360}{7h_z^4}\left(u_z - \delta_z u + \frac{h_z^2}{6}\delta_z u_{zz}\right) + O(h_z^2), \tag{60}$$

$$\partial_z^6 u = \frac{240}{h_z^4}\left(u_{zz} - \delta_z^2 u + \frac{h_z^2}{12}\delta_z^2 u_{zz}\right) + O(h_z^2). \tag{61}$$

Substituting Eqs. (46)–(61) into Eq. (9) and rearranging it, we have

$$
\begin{aligned}
&\left[\frac{4}{3}\left(A_1\delta_x^2 + A_2\delta_y^2 + A_3\delta_z^2\right) + \frac{10}{7}(p\delta_x + q\delta_y + r\delta_z) + A_{11}\delta_x^2\delta_y + A_{12}\delta_y^2\delta_x \right. \\
&\quad \left. + A_{13}\delta_z^2\delta_x A_{14}\delta_x^2\delta_z + A_{15}\delta_y^2\delta_z + A_{16}\delta_z^2\delta_y \right]u + \left(A_7 + \frac{2A_{10}}{3}\delta_z \right)\partial_x\partial_y u \\
&\quad + \left(A_4 - \frac{3}{7}p - A_1\delta_x - A_{11}\delta_x\delta_y + A_{12}\delta_y^2 + A_{13}\delta_z^2 - A_{14}\delta_x\delta_z - \frac{A_{10}}{3}\delta_y\delta_z \right)u_x \\
&\quad + \left(A_5 - \frac{3}{7}q - A_2\delta_y + A_{11}\delta_x^2 - A_{12}\delta_y\delta_x - A_{15}\delta_y\delta_z + A_{16}\delta_z^2 - \frac{A_{10}}{3}\delta_z\delta_x \right)u_y \\
&\quad + \left(A_6 - \frac{3}{7}r - A_3\delta_z - A_{13}\delta_z\delta_x + A_{14}\delta_x^2 + A_{15}\delta_y^2 - A_{16}\delta_z\delta_y - \frac{A_{10}}{3}\delta_x\delta_y \right)u_z \\
&\quad + \left(\frac{2A_1}{3} + \frac{A_1 h_x^2}{18}\delta_x^2 - \frac{p h_x^2}{14}\delta_x \right)u_{xx} + \left(\frac{2A_2}{3} + \frac{A_2 h_y^2}{18}\delta_y^2 - \frac{q h_y^2}{14}\delta_y \right)u_{yy} \\
&\quad + \left(\frac{2A_3}{3} + \frac{A_3 h_z^2}{18}\delta_z^2 - \frac{r h_z^2}{14}\delta_z \right)u_{zz} + \left(A_8 + \frac{2A_{10}}{3}\delta_x \right)\partial_y\partial_z u + \left(A_9 + \frac{2A_{10}}{3}\delta_y \right)\partial_z\partial_x u \\
&= \left(1 - \frac{a_x p h_x^2}{6a^2} - \frac{b_y q h_y^2}{6b^2} - \frac{c_z r h_z^2}{6c^2} + \frac{p h_x^2}{6a}\delta_x + \frac{q h_y^2}{6b}\delta_y + \frac{r h_z^2}{6c}\delta_z \right)f \\
&\quad + O\left(h_x^6 + h_y^6 + h_z^6 + h_x^4 h_y^2 + h_x^2 h_y^4 + h_x^4 h_z^2 + h_z^2 h_x^4 + h_y^4 h_z^2 + h_y^2 h_z^4\right).
\end{aligned} \tag{62}
$$

Substituting δ_x, δ_y, δ_z, δ_x^2, δ_y^2, δ_z^2, $\delta_x\delta_y$, $\delta_y\delta_z$, $\delta_z\delta_x$ (see Appendix A) at grid point 0 into (62), and neglecting the truncation error terms, the 19-point sixth-order BCD scheme can be derived as follows:

$$
\begin{aligned}
&-\frac{8}{3}\left(\frac{A_1}{h_x^2} + \frac{A_2}{h_y^2} + \frac{A_3}{h_z^2} \right)u_0 + \left(\frac{4A_1}{3h_x^2} + \frac{5p_0}{7h_x} - \frac{A_{13}}{h_z^2 h_x} - \frac{A_{12}}{h_y^2 h_x} \right)u_1 \\
&\quad + \left(\frac{4A_2}{3h_y^2} + \frac{5q_0}{7h_y} - \frac{A_{11}}{h_x^2 h_y} - \frac{A_{16}}{h_z^2 h_y} \right)u_2 \\
&\quad + \left(\frac{4A_1}{3h_x^2} - \frac{5p_0}{7h_x} + \frac{A_{13}}{h_x h_z^2} + \frac{A_{12}}{h_x h_y^2} \right)u_3 + \left(\frac{4A_2}{3h_y^2} - \frac{5q_0}{7h_y} + \frac{A_{11}}{h_x^2 h_y} + \frac{A_{16}}{h_z^2 h_y} \right)u_4 \\
&\quad + \left(\frac{4A_3}{3h_z^2} + \frac{5r_0}{7h_z} - \frac{A_{14}}{h_x^2 h_z} - \frac{A_{15}}{h_y^2 h_z} \right)u_5 \\
&\quad + \left(\frac{4A_3}{3h_z^2} - \frac{5r_0}{7h_z} + \frac{A_{14}}{h_x^2 h_z} + \frac{A_{15}}{h_y^2 h_z} \right)u_6 + \left(\frac{A_{11}}{2h_x^2 h_y} + \frac{A_{12}}{2h_y^2 h_x} \right)u_7 \\
&\quad + \left(\frac{A_{11}}{2h_x^2 h_y} - \frac{A_{12}}{2h_y^2 h_x} \right)u_8 - \left(\frac{A_{11}}{2h_x^2 h_y} + \frac{A_{12}}{2h_y^2 h_x} \right)u_9 \\
&\quad + \left(-\frac{A_{11}}{2h_x^2 h_y} + \frac{A_{12}}{2h_y^2 h_x} \right)u_{10} + \left(\frac{A_{13}}{2h_z^2 h_x} + \frac{A_{14}}{2h_x^2 h_z} \right)u_{11} \\
&\quad + \left(\frac{A_{15}}{2h_y^2 h_z} + \frac{A_{16}}{2h_z^2 h_y} \right)u_{12} + \left(-\frac{A_{13}}{2h_z^2 h_x} + \frac{A_{14}}{2h_x^2 h_z} \right)u_{13} \\
&\quad + \left(\frac{A_{15}}{2h_y^2 h_z} - \frac{A_{16}}{2h_z^2 h_y} \right)u_{14} + \left(\frac{A_{13}}{2h_z^2 h_x} - \frac{A_{14}}{2h_x^2 h_z} \right)u_{15}
\end{aligned}
$$

$$+ \left(-\frac{A_{15}}{2h_y^2 h_z} + \frac{A_{16}}{2h_z^2 h_y} \right) u_{16} - \left(\frac{A_{13}}{2h_z^2 h_x} + \frac{A_{14}}{2h_x^2 h_z} \right) u_{17}$$

$$- \left(\frac{A_{15}}{2h_y^2 h_z} + \frac{A_{16}}{2h_z^2 h_y} \right) u_{18} + \left(A_4 - \frac{3p_0}{7} - \frac{2A_{12}}{h_y^2} + \frac{2A_{13}}{h_z^2} \right) u_{x0} - \frac{A_1}{2h_x} u_{x1}$$

$$+ \frac{A_{12}}{h_y^2} u_{x2} + \frac{A_1}{2h_x} u_{x3} + \frac{A_{12}}{h_y^2} u_{x4}$$

$$+ \frac{A_{13}}{h_z^2} u_{x5} + \frac{A_{13}}{h_z^2} u_{x6} - \frac{A_{11}}{4h_x h_y} u_{x7} + \frac{A_{11}}{4h_x h_y} u_{x8} - \frac{A_{11}}{4h_x h_y} u_{x9} + \frac{A_{11}}{4h_x h_y} u_{x10}$$

$$- \frac{A_{14}}{4h_x h_z} u_{x11} - \frac{A_{10}}{12h_z h_y} u_{x12}$$

$$+ \frac{A_{14}}{4h_x h_z} u_{x13} + \frac{A_{10}}{12h_z h_y} u_{x14} + \frac{A_{14}}{4h_x h_z} u_{x15} + \frac{A_{10}}{12h_z h_y} u_{x16} - \frac{A_{14}}{4h_x h_z} u_{x17}$$

$$- \frac{A_{10}}{12h_z h_y} u_{x18} + \frac{A_{11}}{h_x^2} u_{y1}$$

$$+ \left(A_5 - \frac{3q_0}{7} - \frac{2A_{11}}{h_x^2} - \frac{2A_{16}}{h_z^2} \right) u_{y0} - \frac{A_2}{2h_y} u_{y2} + \frac{A_{11}}{h_x^2} u_{y3} + \frac{A_2}{2h_y} u_{y4}$$

$$+ \frac{A_{16}}{h_z^2} u_{y5} + \frac{A_{16}}{h_z^2} u_{y6} - \frac{A_{10}}{12h_x h_y} u_{y7}$$

$$+ \frac{A_{10}}{12h_x h_y} u_{y8} - \frac{A_{10}}{12h_x h_y} u_{y9} + \frac{A_{10}}{12h_x h_y} u_{y10} - \frac{A_{13}}{4h_x h_z} u_{y11} - \frac{A_{16}}{4h_y h_z} u_{y12}$$

$$+ \frac{A_{13}}{4h_x h_z} u_{y13} + \frac{A_{16}}{4h_y h_z} u_{y14}$$

$$+ \frac{A_{13}}{4h_x h_z} u_{y15} + \frac{A_{16}}{4h_y h_z} u_{y16} - \frac{A_{13}}{4h_x h_z} u_{y17} - \frac{A_{16}}{4h_y h_z} u_{y18}$$

$$+ \left(A_6 - \frac{3r_0}{7} - \frac{2A_{14}}{h_x^2} + \frac{2A_{15}}{h_y^2} \right) u_{z0} + \frac{A_{14}}{h_x^2} u_{z1}$$

$$+ \frac{A_{15}}{h_y^2} u_{z2} + \frac{A_{14}}{h_x^2} u_{z3} + \frac{A_{15}}{h_y^2} u_{z4} - \frac{A_3}{2h_z} u_{z5} + \frac{A_3}{2h_z} u_{z6} - \frac{A_{10}}{12h_x h_y} u_{z7}$$

$$+ \frac{A_{10}}{12h_x h_y} u_{z8} - \frac{A_{10}}{12h_x h_y} u_{z9}$$

$$+ \frac{A_{10}}{12h_x h_y} u_{z10} - \frac{A_{13}}{4h_x h_z} u_{z11} - \frac{A_{16}}{4h_y h_z} u_{z12} + \frac{A_{13}}{4h_x h_z} u_{z13} + \frac{A_{16}}{4h_y h_z} u_{z14}$$

$$+ \frac{A_{13}}{4h_x h_z} u_{z15} + \frac{A_{16}}{4h_y h_z} u_{z16}$$

$$- \frac{A_{13}}{4h_x h_z} u_{z17} - \frac{A_{16}}{4h_y h_z} u_{z18} + \frac{5A_1}{9} u_{xx0} + \left(\frac{A_1}{18} - \frac{h_x p_0}{28} \right) u_{xx1}$$

$$+ \left(\frac{A_1}{18} + \frac{h_x p_0}{28} \right) u_{xx3} + \left(\frac{A_2}{18} - \frac{h_y q}{28} \right) u_{yy2}$$

$$+ \frac{5A_2}{9} u_{yy0} + \left(\frac{A_2}{18} + \frac{h_y q_0}{28} \right) u_{yy4} + \frac{5A_3}{9} u_{zz0} + \left(\frac{A_3}{18} - \frac{h_z r_0}{28} \right) u_{zz5}$$

$$+ \left(\frac{A_3}{18} + \frac{h_z r_0}{28} \right) u_{zz6} + A_7 \partial_x \partial_y u_0$$

$$+ \frac{A_{10}}{3h_z} \partial_x \partial_y u_5 - \frac{A_{10}}{3h_z} \partial_x \partial_y u_6 + A_8 \partial_y \partial_z u_0 + \frac{A_{10}}{3h_x} \partial_y \partial_z u_1 - \frac{A_{10}}{3h_x} \partial_y \partial_z u_3$$

$$+ A_9 \partial_x \partial_z u_0 + \frac{A_{10}}{3h_y} \partial_x \partial_z u_2$$

$$- \frac{A_{10}}{3h_y} \partial_x \partial_z u_4$$

$$= \left(1 - \frac{a_{x0} p_0 h_x^2}{6a^2} - \frac{b_{y0} q_0 h_y^2}{6b^2} - \frac{c_{z0} r_0 h_z^2}{6c^2} \right) f_0 + \frac{p_0 h_x^2}{6a} f_{x0} + \frac{q_0 h_y^2}{6b} f_{y0} + \frac{r_0 h_z^2}{6c} f_{z0}. \tag{63}$$

Notice that all the derivatives are separately computed and are demanded to achieve sixth-order accuracy. In the study, we directly use the sixth-order schemes of u_x, u_y, u_z, u_{xx}, u_{yy} and u_{zz} in Ref. [14] as well as the sixth-order CCD2 schemes of $\partial_x \partial_y u$, $\partial_y \partial_z u$ and $\partial_z \partial_x u$ in Ref. [18]. The sixth-order schemes of u_x, u_y, u_z, u_{xx}, u_{yy} and u_{zz} in x-, y- and z-directions are as follows:

$$\frac{7}{16} (u_x)_{i+1,j,k} + (u_x)_{i,j,k} + \frac{7}{16} (u_x)_{i-1,j,k}$$

$$= \frac{15}{16h_x} (u_{i+1,j,k} - u_{i-1,j,k}) + \frac{h_x}{16} \left[(u_{xx})_{i+1,j,k} - (u_{xx})_{i-1,j,k} \right] + O(h_x^6), \tag{64}$$

$$-\frac{1}{8} (u_{xx})_{i+1,j,k} + (u_{xx})_{i,j,k} - \frac{1}{8} (u_{xx})_{i-1,j,k}$$

$$= \frac{3}{h_x^2} (u_{i+1,j,k} - 2u_{i,j,k} + u_{i-1,j,k}) - \frac{9}{8h_x} \left[(u_x)_{i+1,j,k} - (u_x)_{i-1,j,k} \right] + O(h_x^6), \tag{65}$$

$$\frac{7}{16} (u_y)_{i,j+1,k} + (u_y)_{i,j,k} + \frac{7}{16} (u_y)_{i,j-1,k}$$

$$= \frac{15}{16h_y} (u_{i,j+1,k} - u_{i,j-1,k}) + \frac{h_y}{16} \left[(u_{yy})_{i,j+1,k} - (u_{yy})_{i,j-1,k} \right] + O(h_y^6), \tag{66}$$

$$-\frac{1}{8} (u_{yy})_{i,j+1,k} + (u_{yy})_{i,j,k} - \frac{1}{8} (u_{yy})_{i,j-1,k}$$

$$= \frac{3}{h_y^2} (u_{i,j+1,k} - 2u_{i,j,k} + u_{i,j-1,k}) - \frac{9}{8h_y} \left[(u_y)_{i,j+1,k} - (u_y)_{i,j-1,k} \right] + O(h_y^6), \tag{67}$$

$$\frac{7}{16} (u_z)_{i,j,k+1} + (u_z)_{i,j,k} + \frac{7}{16} (u_z)_{i,j,k-1}$$

$$= \frac{15}{16h_z} (u_{i,j,k+1} - u_{i,j,k-1}) + \frac{h_z}{16} \left[(u_{zz})_{i,j,k+1} - (u_{zz})_{i,j,k-1} \right] + O(h_z^6), \tag{68}$$

$$-\frac{1}{8} (u_{zz})_{i,j,k+1} + (u_{zz})_{i,j,k} - \frac{1}{8} (u_{zz})_{i,j,k-1}$$

$$= \frac{3}{h_z^2} (u_{i,j,k+1} - 2u_{i,j,k} + u_{i,j,k-1}) - \frac{9}{8h_z} \left[(u_z)_{i,j,k+1} - (u_z)_{i,j,k-1} \right] + O(h_z^6). \tag{69}$$

The mixed derivatives $\{\partial_x \partial_y u, \partial_y \partial_z u, \partial_z \partial_x u\}$ are computed with the nine-point sixth-order schemes in Ref. [18], which are expressed as follows:

$$\partial_x \partial_y u_0 + \frac{1}{16} (\partial_x \partial_y u_1 + \partial_x \partial_y u_2 + \partial_x \partial_y u_3 + \partial_x \partial_y u_4)$$

$$- \frac{1}{32} (\partial_x \partial_y u_5 + \partial_x \partial_y u_6 + \partial_x \partial_y u_7 + \partial_x \partial_y u_8) + \frac{9}{16h_y} (u_{x2} - u_{x4})$$

$$= -\frac{9}{32h_x h_y}(u_5 - u_6 + u_7 - u_8) + \frac{9}{16h_x}(u_{y1} - u_{y3}) + O(h_x^6 + h_y^6), \tag{70}$$

$$\partial_y \partial_z u_0 + \frac{1}{16}(\partial_y \partial_z u_2 + \partial_y \partial_z u_5 + \partial_y \partial_z u_4 + \partial_y \partial_z u_6)$$
$$- \frac{1}{32}(\partial_y \partial_z u_{12} + \partial_y \partial_z u_{14} + \partial_y \partial_z u_{16} + \partial_y \partial_z u_{18}) + \frac{9}{16h_z}(u_{y5} - u_{y6})$$
$$= -\frac{9}{32h_y h_z}(u_{12} - u_{14} + u_{18} - u_{16}) + \frac{9}{16h_y}(u_{z2} - u_{z4}) + O(h_y^6 + h_z^6), \tag{71}$$

$$\partial_z \partial_x u_0 + \frac{1}{16}(\partial_z \partial_x u_1 + \partial_z \partial_x u_3 + \partial_z \partial_x u_5 + \partial_z \partial_x u_6)$$
$$- \frac{1}{32}(\partial_z \partial_x u_{11} + \partial_z \partial_x u_{13} + \partial_z \partial_x u_{15} + \partial_z \partial_x u_{17}) + \frac{9}{16h_z}(u_{x5} - u_{x6})$$
$$= -\frac{9}{32h_x h_z}(u_{11} - u_{13} - u_{15} + u_{17}) + \frac{9}{16h_z}(u_{z1} - u_{z3}) + O(h_x^6 + h_z^6). \tag{72}$$

In the explicit fourth-order CD scheme [32], the third- and fourth-order derivatives of the truncation errors are represented by the original differential equation. But in the BCD schemes, the fifth- and sixth-order derivatives are represented by an unknown function, its first- and second-order derivatives, while the third-order derivatives are represented by means of the method in Ref. [32].

2.2 Boundary formulas for derivatives

It is of great significance to construct higher-order boundaries schemes for the BCD schemes at inner points. If the boundaries schemes are not well constructed, the accuracy and stability of the numerical solution will be affected. For the fourth-order BCD scheme, we adopt the consistent fourth-order boundary schemes [37], which have good stability and accuracy (see Appendix B).

For the sixth-order BCD scheme, because the first-order, second-order and second-order mixed derivatives are unknown at the boundaries, so we need to construct sixth-order boundaries schemes for them. Firstly, we consider the left boundary. In order to obtain the sixth-order scheme of the left boundary ($i = 0$ and $i = N_x$ in x-direction) of u_x, we assume that the unknown function and its first-order derivative u_x have the following relationship:

$$(u_x)_{0,j,k} + \alpha(u_x)_{1,j,k} = \frac{1}{h_x}\sum_{i=0}^{6} b_i u_{i,j,k} \quad (j = 0, 1, \dots, N_y; k = 0, 1, \dots, N_z). \tag{73}$$

The left boundary format discrete template is shown in Fig. 2.

Figure 2 Grid point discretization for the left boundary
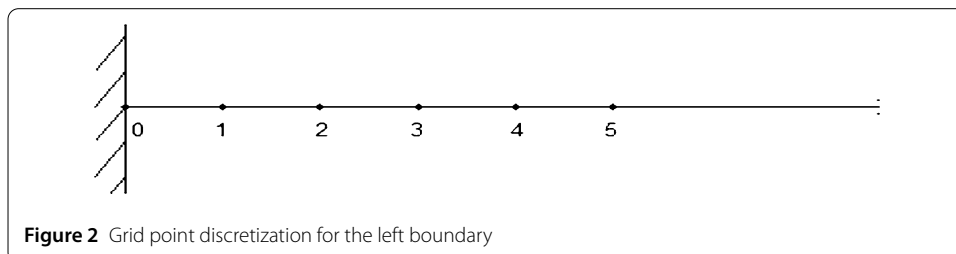
Next, the unknown function u and its first-order derivative u_x in Eq. (73) are expanded by a Taylor series at point $i = 0$. By matching the coefficients of the unknown function and its derivatives, we can obtain the following constrained linear equations:

$$
\begin{cases}
b_0 + b_1 + b_2 + b_3 + b_4 + b_5 = 0, \\
\frac{1}{2!}(b_1 + 2^2 b_2 + 3^2 b_3 + 4^2 b_4 + 5^2 b_5) = \alpha, \\
\frac{1}{3!}(b_1 + 2^3 b_2 + 3^3 b_3 + 4^3 b_4 + 5^3 b_5) = \frac{\alpha}{2}, \\
\frac{1}{4!}(b_1 + 2^4 b_2 + 3^4 b_3 + 4^4 b_4 + 5^4 b_5) = \frac{\alpha}{6}, \\
\frac{1}{5!}(b_1 + 2^5 b_2 + 3^5 b_3 + 4^5 b_4 + 5^5 b_5) = \frac{\alpha}{24}, \\
\frac{1}{6!}(b_1 + 2^6 b_2 + 3^6 b_3 + 4^6 b_4 + 5^6 b_5) = \frac{\alpha}{120}, \\
\frac{1}{7!}(b_1 + 2^7 b_2 + 3^7 b_3 + 4^7 b_4 + 5^7 b_5) = \frac{\alpha}{720}.
\end{cases}
\tag{74}
$$

With the help the Matlab software, we obtain the sixth-order scheme of the left boundary:

$$
(u_x)_{0,j,k} - \frac{1}{5}(u_x)_{1,j,k}
$$

$$
= \frac{1}{h_x}\left(-\frac{149}{60}u_{0,j,k} + \frac{1723}{300}u_{1,j,k} - 7u_{2,j,k} + \frac{19}{3}u_{3,j,k} - \frac{43}{12}u_{4,j,k}\right.
$$

$$
\left. + \frac{23}{20}u_{5,j,k} - \frac{4}{25}u_{6,j,k}\right) \quad (j = 0,1,\dots,N_y; k = 0,1,\dots,N_z),
\tag{75}
$$

similarly, the remaining sixth-order schemes of the boundaries (right, down, up, rear and front) for $\{u_x, u_y, u_z\}$ are given as follows:

$$
(u_x)_{N_x,j,k} - \frac{1}{5}(u_x)_{N_x-1,j,k}
$$

$$
= \frac{1}{h_x}\left(\frac{29}{12}u_{N_x,j,k} - \frac{1877}{300}u_{N_x-1,j,k} + 8u_{N_x-2,j,k} + \frac{5}{3}u_{N_x-3,j,k} - 7u_{N_x-4,j,k}\right.
$$

$$
\left. + \frac{47}{12}u_{N_x-5,j,k} - \frac{5}{4}u_{N_x-5,j,k}\right) \quad (j = 0,1,\dots,N_y; k = 0,1,\dots,N_z),
\tag{76}
$$

$$
(u_y)_{i,0,k} + \frac{1}{5}(u_y)_{i,1,k}
$$

$$
= \frac{1}{h_y}\left(-\frac{149}{60}u_{i,0,k} + \frac{1723}{300}u_{i,1,k} - 7u_{i,2,k} + \frac{19}{3}u_{i,3,k} - \frac{43}{12}u_{i,4,k} + \frac{23}{20}u_{i,5,k} - \frac{4}{25}u_{i,6,k}\right)
$$

$$
(i = 0,1,\dots,N_x; k = 0,1,\dots,N_z),
\tag{77}
$$

$$
(u_y)_{i,N_y,k} - \frac{1}{5}(u_y)_{i,N_y-1,k}
$$

$$
= \frac{1}{h_y}\left(\frac{29}{12}u_{i,N_y,k} - \frac{1877}{300}u_{i,N_y-1,k} + 8u_{i,N_y-2,k} + \frac{5}{3}u_{i,N_y-3,k} - 7u_{i,N_y-4,k}\right.
$$

$$
\left. + \frac{47}{12}u_{i,N_y-5,k} - \frac{5}{4}u_{i,N_y-6,k}\right) \quad (i = 0,1,\dots,N_x; k = 0,1,\dots,N_z),
\tag{78}
$$

$$
(u_z)_{i,j,0} + \frac{1}{5}(u_z)_{i,j,1}
$$

$$
= \frac{1}{h_z}\left(-\frac{149}{60}u_{i,j,0} + \frac{1723}{300}u_{i,j,1} - 7u_{i,j,2} + \frac{19}{3}u_{i,j,3} - \frac{43}{12}u_{i,j,4} + \frac{23}{20}u_{i,j,5}\right.
$$

$$-\frac{4}{25}u_{i,j,6}\Big) \quad (i = 0, 1, \ldots, N_x; j = 0, 1, \ldots, N_y), \tag{79}$$

$$(u_z)_{i,j,N_z} - \frac{1}{5}(u_z)_{i,j,N_z-1}$$

$$= \frac{1}{h_z}\left(\frac{29}{12}u_{i,j,N_z} - \frac{1877}{300}u_{i,j,N_z-1} + 8u_{i,j,N_z-2} + \frac{5}{3}u_{i,j,N_z-3} - 7u_{i,j,N_z-4}\right.$$

$$\left. + \frac{47}{12}u_{i,j,N_z-5} - \frac{5}{4}u_{i,j,N_z-6}\right) \quad (i = 0, 1, \ldots, N_x; j = 0, 1, \ldots, N_y). \tag{80}$$

With a similar method, we can get the boundary schemes for $\{u_{xx}, u_{yy}, u_{zz}\}$ on boundaries. All sixth-order boundaries schemes (left, right, down, up, rear and front) for $\{u_{xx}, u_{yy}, u_{zz}\}$ are given as follows:

$$(u_{xx})_{0,j,k} - 6(u_{xx})_{1,j,k}$$

$$= \frac{1}{h_x^2}\left(-\frac{403}{18}u_{0,j,k} + 33u_{1,j,k} - \frac{21}{2}u_{2,j,k} - \frac{4}{9}u_{3,j,k}\right) - \frac{26}{3h_x}(u_x)_{0,j,k}$$

$$+ \frac{1}{h_x}\left[-6(u_x)_{1,j,k} + 3(u_x)_{2,j,k}\right] \quad (j = 0, 1, \ldots, N_y; k = 0, 1, \ldots, N_z), \tag{81}$$

$$(u_{xx})_{N_x,j,k} - 6(u_{xx})_{N_x-1,j,k}$$

$$= \frac{1}{h_x^2}\left(-\frac{403}{18}u_{N_x,j,k} + 33u_{N_x-1,j,k} - \frac{21}{2}u_{N_x-2,j,k} - \frac{4}{9}u_{N_x-3,j,k}\right) + \frac{26}{3h_x}(u_x)_{N_x,j,k}$$

$$+ \frac{1}{h_x}\left[6(u_x)_{N_x-1,j,k} - 3(u_x)_{N_x-2,j,k}\right] \quad (j = 0, 1, \ldots, N_y; k = 0, 1, \ldots, N_z), \tag{82}$$

$$(u_{yy})_{i,0,k} - 6(u_{yy})_{i,1,k}$$

$$= \frac{1}{h_y^2}\left(-\frac{403}{18}u_{i,0,k} + 33u_{i,1,k} - \frac{21}{2}u_{i,2,k} - \frac{4}{9}u_{i,3,k}\right) - \frac{26}{3h_y}(u_y)_{i,0,k}$$

$$+ \frac{1}{h_y}\left[-6(u_y)_{i,1,k} + 3(u_y)_{i,2,k}\right] \quad (i = 0, 1, \ldots, N_x; k = 0, 1, \ldots, N_z), \tag{83}$$

$$(u_{yy})_{i,N_y,k} - 6(u_{yy})_{i,N_y-1,k}$$

$$= \frac{1}{h_y^2}\left(-\frac{403}{18}u_{i,N_y,k} + 33u_{i,N_y-1,k} - \frac{21}{2}u_{i,N_y-2,k} - \frac{4}{9}u_{i,N_y-3,k}\right) + \frac{26}{3h_y}(u_y)_{i,N_y,k}$$

$$+ \frac{1}{h_y}\left[6(u_y)_{i,N_y-1,k} - 3(u_y)_{i,N_y-2,k}\right] \quad (i = 0, 1, \ldots, N_x; k = 0, 1, \ldots, N_z), \tag{84}$$

$$(u_{zz})_{i,j,0} - 6(u_{zz})_{i,j,1}$$

$$= \frac{1}{h_z^2}\left(-\frac{403}{18}u_{i,j,0} + 33u_{i,j,1} - \frac{21}{2}u_{i,j,2} - \frac{4}{9}u_{i,j,3}\right) - \frac{26}{3h_z}(u_z)_{i,j,0}$$

$$+ \frac{1}{h_z}\left[-6(u_z)_{i,j,1} + 3(u_z)_{i,j,2}\right] \quad (i = 0, 1, \ldots, N_x; j = 0, 1, \ldots, N_y), \tag{85}$$

$$(u_{zz})_{i,j,N_z} - 6(u_{zz})_{i,j,N_z-1}$$

$$= \frac{1}{h_z^2}\left(-\frac{403}{18}u_{i,j,N_z} + 33u_{i,j,N_z-1} - \frac{21}{2}u_{i,j,N_z-2} - \frac{4}{9}u_{i,j,N_z-3}\right) + \frac{26}{3h_z}(u_z)_{i,j,N_z}$$

$$+ \frac{1}{h_z}\left[6(u_z)_{i,j,N_z-1} - 3(u_z)_{i,j,N_z-2}\right] \quad (i = 0, 1, \ldots, N_x; j = 0, 1, \ldots, N_y). \tag{86}$$

Finally, all sixth-order boundaries schemes for $\{\partial_x\partial_y u, \partial_y\partial_z u, \partial_z\partial_x u\}$ are derived, similar to deriving the boundaries schemes of $\{u_x, u_y, u_z\}$ (see Appendix C). Taking $\partial_x\partial_y u$ as an example, the $\partial_x\partial_y u$ can be regarded as $(u_x)_y$ or $(u_y)_x$. All sixth-order boundaries schemes (left, right, down, up) for $\partial_x\partial_y u$ are given as follows:

$$
\partial_x\partial_y u_{0,j,k} + \frac{1}{5}\partial_x\partial_y u_{1,j,k}
$$

$$
= \left[-\frac{149}{60}(u_y)_{0,j,k} + \frac{1723}{300}(u_y)_{1,j,k} - 7(u_y)_{2,j,k} + \frac{19}{3}(u_y)_{3,j,k} - \frac{43}{12}(u_y)_{4,j,k} \right.
$$

$$
\left. + \frac{23}{20}(u_y)_{5,j,k} - \frac{4}{25}(u_y)_{6,j,k} \right] \Big/ h_x \quad (j = 0, 1, \dots, N_y; k = 0, 1, \dots, N_z), \tag{87}
$$

$$
\partial_x\partial_y u_{N_x,j,k} - \frac{1}{5}\partial_x\partial_y u_{N_x-1,j,k}
$$

$$
= \left[\frac{29}{12}(u_y)_{N_x,j,k} - \frac{1877}{300}(u_y)_{N_x-1,j,k} + 8(u_y)_{N_x-2,j,k} - 7(u_y)_{N_x-3,j,k} + \frac{47}{12}(u_y)_{N_x-4,j,k} \right.
$$

$$
\left. - \frac{5}{4}(u_y)_{N_x-5,j,k} + \frac{13}{75}(u_y)_{N_x-6,j,k} \right] \Big/ h_x \quad (j = 0, 1, \dots, N_y; k = 0, 1, \dots, N_z), \tag{88}
$$

$$
\partial_x\partial_y u_{i,0,k} + \frac{1}{5}\partial_x\partial_y u_{i,1,k}
$$

$$
= \left[-\frac{149}{60}(u_x)_{i,0,k} + \frac{1723}{300}(u_x)_{i,1,k} - 7(u_x)_{i,2,k} + \frac{19}{3}(u_x)_{i,3,k} - \frac{43}{12}(u_x)_{i,4,k} \right.
$$

$$
\left. + \frac{23}{20}(u_x)_{i,5,k} - \frac{4}{25}(u_x)_{i,6,k} \right] \Big/ h_y \quad (i = 0, 1, \dots, N_x; k = 0, 1, \dots, N_z), \tag{89}
$$

$$
\partial_x\partial_y u_{i,N_y,k} - \frac{1}{5}\partial_x\partial_y u_{i,N_y-1,k}
$$

$$
= \left[\frac{29}{12}(u_x)_{i,N_y,k} - \frac{1877}{300}(u_x)_{i,N_y-1,k} + 8(u_x)_{i,N_y-2,k} - 7(u_x)_{i,N_y-3,k} + \frac{47}{12}(u_x)_{i,N_y-4,k} \right.
$$

$$
\left. - \frac{5}{4}(u_x)_{i,N_y-5,k} + \frac{13}{75}(u_x)_{i,N_y-6,k} \right] \Big/ h_y \quad (i = 0, 1, \dots, N_x; k = 0, 1, \dots, N_z). \tag{90}
$$

With a similar method, we are able to obtain the boundaries schemes for $\{\partial_y\partial_z u, \partial_z\partial_x u\}$. All sixth-order boundaries schemes (rear, front, down, up,) are given for $\partial_y\partial_z u$ as follows:

$$
\partial_y\partial_z u_{i,j,0} + \frac{1}{5}\partial_y\partial_z u_{i,j,1}
$$

$$
= \left[-\frac{149}{60}(u_y)_{i,j,0} + \frac{1723}{300}(u_y)_{i,j,1} - 7(u_y)_{i,j,2} + \frac{19}{3}(u_y)_{i,j,3} - \frac{43}{12}(u_y)_{i,j,4} \right.
$$

$$
\left. + \frac{23}{20}(u_y)_{i,j,5} - \frac{4}{25}(u_y)_{i,j,6} \right] \Big/ h_z \quad (i = 0, 1, \dots, N_x; j = 0, 1, \dots, N_y), \tag{91}
$$

$$
\partial_y\partial_z u_{i,j,N_z} - \frac{1}{5}\partial_y\partial_z u_{i,j,N_z-1}
$$

$$
= \left[\frac{29}{12}(u_y)_{i,j,N_z} - \frac{1877}{300}(u_y)_{i,j,N_z-1} + 8(u_y)_{i,j,N_z-2} - 7(u_y)_{i,j,N_z-3} + \frac{47}{12}(u_y)_{i,j,N_z-4} \right.
$$

$$
\left. - \frac{5}{4}(u_y)_{i,j,N_z-5} + \frac{13}{75}(u_y)_{i,jN_z-6} \right] \Big/ h_z \quad (i = 0, 1, \dots, N_x; j = 0, 1, \dots, N_y), \tag{92}
$$

$$\partial_y \partial_z u_{i,0,k} + \frac{1}{5} \partial_y \partial_z u_{i,1,k}$$

$$= \left[-\frac{149}{60}(u_z)_{i,0,k} + \frac{1723}{300}(u_z)_{i,1,k} - 7(u_z)_{i,2,k} + \frac{19}{3}(u_z)_{i,3,k} - \frac{43}{12}(u_z)_{i,4,k} + \frac{23}{20}(u_z)_{i,5,k} \right.$$

$$\left. - \frac{4}{25}(u_z)_{i,6,k} \right] \Big/ h_y \quad (i = 0, 1, \ldots, N_x; k = 0, 1, \ldots, N_z), \tag{93}$$

$$\partial_y \partial_z u_{i,N_y,k} - \frac{1}{5} \partial_y \partial_z u_{i,N_y-1,k}$$

$$= \left[\frac{29}{12}(u_z)_{i,N_y,k} - \frac{1877}{300}(u_z)_{i,N_y-1,k} + 8(u_z)_{i,N_y-2,k} - 7(u_z)_{i,N_y-3,k} + \frac{47}{12}(u_z)_{i,N_y-4,k} \right.$$

$$\left. - \frac{5}{4}(u_z)_{i,N_y-5,k} + \frac{13}{75}(u_z)_{i,N_y-6,k} \right] \Big/ h_y \quad (i = 0, 1, \ldots, N_x; k = 0, 1, \ldots, N_z). \tag{94}$$

All sixth-order boundaries schemes are given for $\partial_x \partial_z u$ as follows:

$$\partial_z \partial_x u_{0,j,k} + \frac{1}{5} \partial_z \partial_x u_{1,j,k}$$

$$= \left[-\frac{149}{60}(u_z)_{0,j,k} + \frac{1723}{300}(u_z)_{1,j,k} - 7(u_z)_{2,j,k} + \frac{19}{3}(u_z)_{3,j,k} - \frac{43}{12}(u_z)_{4,j,k} \right.$$

$$\left. + \frac{23}{20}(u_z)_{5,j,k} - \frac{4}{25}(u_z)_{6,j,k} \right] \Big/ h_x \quad (j = 0, 1, \ldots, N_y; k = 0, 1, \ldots, N_z), \tag{95}$$

$$\partial_z \partial_x u_{N_x,j,k} - \frac{1}{5} \partial_z \partial_x u_{N_x-1,j,k}$$

$$= \left[\frac{29}{12}(u_z)_{N_x,j,k} - \frac{1877}{300}(u_z)_{N_x-1,j,k} + 8(u_z)_{N_x-2,j,k} - 7(u_z)_{N_x-3,j,k} + \frac{47}{12}(u_z)_{N_x-4,j,k} \right.$$

$$\left. - \frac{5}{4}(u_z)_{N_x-5,j,k} + \frac{13}{75}(u_z)_{N_x-6,j,k} \right] \Big/ h_x \quad (j = 0, 1, \ldots, N_y; k = 0, 1, \ldots, N_z), \tag{96}$$

$$\partial_z \partial_x u_{i,j,0} + \frac{1}{5} \partial_z \partial_x u_{i,j,1}$$

$$= \left[-\frac{149}{60}(u_x)_{i,j,0} + \frac{1723}{300}(u_x)_{i,j,1} - 7(u_x)_{i,j,2} + \frac{19}{3}(u_x)_{i,j,3} - \frac{43}{12}(u_x)_{i,j,4} \right.$$

$$\left. + \frac{23}{20}(u_x)_{i,j,5} - \frac{4}{25}(u_x)_{i,j,6} \right] \Big/ h_z \quad (i = 0, 1, \ldots, N_x; k = 0, 1, \ldots, N_z), \tag{97}$$

$$\partial_z \partial_x u_{i,j,N_z} - \frac{1}{5} \partial_z \partial_x u_{i,j,N_z-1}$$

$$= \left[\frac{29}{12}(u_x)_{i,j,N_z} - \frac{1877}{300}(u_x)_{i,j,N_z-1} + 8(u_x)_{i,j,N_z-2} - 7(u_x)_{i,j,N_z-3} + \frac{47}{12}(u_x)_{i,j,N_z-4} \right.$$

$$\left. - \frac{5}{4}(u_x)_{i,j,N_z-5} + \frac{13}{75}(u_x)_{i,j,N_z-6} \right] \Big/ h_z \quad (i = 0, 1, \ldots, N_x; j = 0, 1, \ldots, N_y). \tag{98}$$

In the section, we obtain all sixth-order boundaries schemes which require more than 3 grid points. Although they are not compact in the traditional sense, the major compact structure is from the interior difference equations.

2.3 Computing process

Next, we will give computing process of the sixth-order BCD scheme. Computation of the fourth-order BCD is close to it, so we will not talk about it more.

Step 1: Giving any initial guess values for $\{u^0, u_x^0, u_y^0, u_z^0, u_{xx}^0, u_{yy}^0, u_{zz}^0, \partial_x\partial_y u^0,$ $\partial_y\partial_z u^0, \partial_z\partial_x u^0\}$.

Step 2: Computing $u_x^{(m)}$, $u_y^{(m)}$, $u_z^{(m)}$ by interior difference equations (64), (66), (68) and boundaries difference equations (75)–(80), respectively.

Step 3: Computing $u_{xx}^{(m)}$, $u_{yy}^{(m)}$, $u_{zz}^{(m)}$ by interior difference equations (65), (67), (69) and boundaries difference equations (81)–(86), respectively.

Step 4: Computing $\partial_x\partial_y u^m$, $\partial_y\partial_z u^m$, $\partial_z\partial_x u^m$ by interior difference equations (70)–(72) and boundaries difference equations (87)–(98), respectively.

Step 5: Computing $u^{(m)}$ by the present sixth-order BCD scheme (63) to compute the transport variable u.

If the condition $\|F - Lu^{(m)}\| < \varepsilon$ is satisfied, then stop. Otherwise, let $m = m + 1$ and repeat steps 2–5.

Here m – the iteration number; L – the linear difference operator of the scheme (63); $\|\cdot\| - L_\infty$ norm; ε – the convergence tolerance.

3 Truncation error analysis

For simplicity, it is supposed that h_x, h_y and h_z is equal to h. Truncation error analysis is given as follows. Using the Taylor series expansions at point (x_i, y_j, z_k)

$$u_x = \delta_x u - \frac{h^2}{6}\partial_x^3 u - \frac{h^4}{120}\partial_x^5 u - \frac{h^6}{5040}\partial_x^7 u + O(h^8), \tag{99}$$

$$u_y = \delta_y u - \frac{h^2}{6}\partial_y^3 u - \frac{h^4}{120}\partial_y^5 u - \frac{h^6}{5040}\partial_y^7 u + O(h^8), \tag{100}$$

$$u_z = \delta_z u - \frac{h^2}{6}\partial_z^3 u - \frac{h^4}{120}\partial_z^5 u - \frac{h^6}{5040}\partial_z^7 u + O(h^8). \tag{101}$$

Differentiating Eq. (1) with respect to x, y and z, we get

$$\partial_x^3 u = \frac{1}{a}\big(f_x - b\partial_y^2\partial_x u - b_x u_{yy} - c\partial_z^2\partial_x u - c_x u_{zz} - pu_{xx} - p_x u_x - q\partial_y\partial_x u - q_x u_y - r_x u_z$$

$$- ru_{zx} - d_1\partial_x^2\partial_y u - d_{1x}\partial_x\partial_y u - d_{2x}\partial_y\partial_z u - d_2\partial_x\partial_y\partial_z u - d_{3x}\partial_z\partial_x u$$

$$- d_3\partial_x^2\partial_z u - s_x u - su_x\big)$$

$$- \frac{a_x}{a^2}\big(f - bu_{yy} - cu_{zz} - pu_x - qu_y - ru_z - d_1\partial_x\partial_y u - d_2\partial_y\partial_z u$$

$$- d_3\partial_z\partial_x u - su\big), \tag{102}$$

$$\partial_y^3 u = \bigg[\frac{1}{b}\big(f_y - a\partial_x^2\partial_y u - a_y u_{xx} - c\partial_z^2\partial_y u - c_y u_{zz} - p\partial_x\partial_y u - p_y u_x - qu_{yy} - q_y u_y - r_y u_z$$

$$- ru_{zy} - d_1\partial_y^2\partial_x u - d_{1y}\partial_x\partial_y u - d_{2y}\partial_y\partial_z u - d_2\partial_y^2\partial_z u - d_{3y}\partial_z\partial_x u$$

$$- d_3\partial_x\partial_y\partial_z u - s_y u - su_y\big)$$

$$- \frac{b_y}{b^2}\big(f - au_{xx} - cu_{zz} - pu_x - qu_y - ru_z - d_1\partial_x\partial_y u - d_2\partial_y\partial_z u$$

$$- d_3\partial_z\partial_x u - su\bigg], \tag{103}$$

$$\partial_z^3 u = \frac{1}{c}\big(f_z - a\partial_x^2\partial_z u - a_z u_{xx} - b\partial_y^2\partial_z u - b_z u_{yy} - p\partial_x\partial_z u - p_z u_x - q\partial_y\partial_z u - q_z u_y - r_z u_z$$

$$- ru_{zz} - d_1 \partial_x \partial_y \partial_z u - d_{1z} \partial_x \partial_y u - d_{2z} \partial_y \partial_z u - d_2 \partial_z^2 \partial_y u$$

$$- d_{3z} \partial_z \partial_x u - d_3 \partial_z^2 \partial_x u - s_z u - s u_z \big)$$

$$- \frac{c_z}{c^2}(f - b u_{yy} - c u_{zz} - p u_x - q u_y - r u_z - d_1 \partial_x \partial_y u - d_2 \partial_y \partial_z u$$

$$- d_3 \partial_z \partial_x u - s u). \tag{104}$$

Substituting Eqs. (102)–(104) into Eq. (1) and rearranging it:

$$A_1 u_{xx} + A_2 u_{yy} + A_3 u_{zz} + A_4 u_x + A_5 u_y + A_6 u_z + A_7 \partial_x \partial_y u + A_8 \partial_y \partial_z u$$

$$+ A_9 \partial_z \partial_x u + A_{10} \partial_x \partial_y \partial_z u$$

$$+ A_{11} \partial_x^2 \partial_y u + A_{12} \partial_y^2 \partial_x u + A_{13} \partial_z^2 \partial_x u + A_{14} \partial_x^2 \partial_z u + A_{15} \partial_y^2 \partial_z u$$

$$+ A_{16} \partial_z^2 \partial_y u + p \delta_x u + q \delta_y u + A_{17} u$$

$$+ r \delta_z u - \frac{h^4 p}{120} \partial_x^5 u - \frac{h^6 p}{5040} \partial_x^7 u - \frac{h^4 q}{120} \partial_y^5 u \frac{h^6 q}{5040} \partial_y^7 u - \frac{h^4 r}{120} \partial_z^5 u - \frac{h^6 r}{5040} \partial_z^7 u + O\big(h^8\big)$$

$$= F. \tag{105}$$

Here, A_1, A_2, A_3, A_4, A_5, A_6, A_7, A_8, A_9, A_{10}, A_{11}, A_{12}, A_{13}, A_{14}, A_{15}, A_{16}, A_{17} and F are defined in (9). In order to get a sixth-order compact scheme for Eq. (42), consider the following approximations for all the derivatives. These derivatives are approximated as follows:

$$u_{xx} = 2\delta_x^2 u - \delta_x u + \frac{h^4}{360} \partial_x^6 u + \frac{h^6}{10{,}080} \partial_x^8 u + O\big(h^8\big), \tag{106}$$

$$u_{yy} = 2\delta_y^2 u - \delta_y u + \frac{h^4}{360} \partial_y^6 u + \frac{h^6}{10{,}080} \partial_y^8 u + O\big(h^8\big), \tag{107}$$

$$u_{zz} = 2\delta_z^2 u - \delta_z u + \frac{h^4}{360} \partial_z^6 u + \frac{h^6}{10{,}080} \partial_z^8 u + O\big(h^8\big), \tag{108}$$

$$\partial_x \partial_y u = (\delta_x u_y + \delta_y u_x - \delta_x \delta_y u) + \frac{h^4}{36} \partial_x^3 \partial_y^3 u + O\big(h^6\big), \tag{109}$$

$$\partial_y \partial_z u = (\delta_y u_z + \delta_z u_y - \delta_y \delta_z u) + \frac{h^4}{36} \partial_y^3 \partial_z^3 u + O\big(h^6\big), \tag{110}$$

$$\partial_z \partial_x u = (\delta_z u_x + \delta_x u_z - \delta_z \delta_x u) + \frac{h^4}{36} \partial_z^3 \partial_x^3 u + O\big(h^6\big), \tag{111}$$

$$\partial_x \partial_y \partial_z u = \delta_x \partial_y \partial_z u + \delta_y \partial_x \partial_z u - \delta_x \delta_y u_z + \frac{h^4}{36} \partial_x^3 \partial_y^3 \partial_z u + O\big(h^6\big), \tag{112}$$

$$\partial_x^2 \partial_y u = \delta_x^2 u_y + \delta_x^2 \delta_y u - \delta_x \delta_y u_x + \frac{h^4}{36} \partial_x^4 \partial_y^3 u + O\big(h^6\big), \tag{113}$$

$$\partial_y^2 \partial_x u = \delta_y^2 u_x + \delta_y^2 \delta_x u - \delta_x \delta_y u_y + \frac{h^4}{36} \partial_y^4 \partial_x^3 u + O\big(h^6\big), \tag{114}$$

$$\partial_y^2 \partial_z u = \delta_y^2 u_z + \delta_y^2 \delta_z u - \delta_y \delta_z u_y + \frac{h^4}{36} \partial_y^4 \partial_z^3 u + O\big(h^6\big), \tag{115}$$

$$\partial_z^2 \partial_y u = \delta_z^2 u_y + \delta_z^2 \delta_y u - \delta_z \delta_y u_z + \frac{h^4}{36} \partial_z^4 \partial_y^3 u + O\big(h^6\big), \tag{116}$$

$$\partial_x^2 \partial_z u = \delta_x^2 u_z + \delta_x^2 \delta_z u - \delta_x \delta_z u_x + \frac{h^4}{36} \partial_x^4 \partial_z^3 u + O(h^6), \tag{117}$$

$$\partial_z^2 \partial_x u = \delta_z^2 u_x + \delta_z^2 \delta_x u - \delta_x \delta_z u_z + \frac{h^2}{36} \partial_z^4 \partial_x^3 u + O(h^6), \tag{118}$$

$$\partial_x^5 u = \frac{360}{7h^4} \left(u_x - \delta_x u + \frac{h^2}{6} \delta_x u_{xx} \right) - \frac{3h^2}{49} \partial_x^7 u + O(h^4), \tag{119}$$

$$\partial_x^6 u = \frac{240}{h^4} \left(u_{xx} - \delta_x^2 u + \frac{h^2}{12} \delta_x^2 u_{xx} \right) - \frac{11h^2}{252} \partial_x^8 u + O(h^4), \tag{120}$$

$$\partial_y^5 u = \frac{360}{7h^4} \left(u_y - \delta_y u + \frac{h^2}{6} \delta_y u_{yy} \right) - \frac{3h^2}{49} \partial_y^7 u + O(h^4), \tag{121}$$

$$\partial_y^6 u = \frac{240}{h^4} \left(u_{yy} - \delta_y^2 u + \frac{h^2}{12} \delta_y^2 u_{yy} \right) - \frac{11h^2}{252} \partial_y^8 u + O(h^4), \tag{122}$$

$$\partial_z^5 u = \frac{360}{7h^4} \left(u_z - \delta_z u + \frac{h^2}{6} \delta_z u_{zz} \right) - \frac{3h^2}{49} \partial_z^7 u + O(h^4), \tag{123}$$

$$\partial_z^6 u = \frac{240}{h^4} \left(u_{zz} - \delta_z^2 u + \frac{h^2}{12} \delta_z^2 u_{zz} \right) - \frac{11h^2}{252} \partial_z^8 u + O(h^4). \tag{124}$$

Substituting Eqs. (106)–(124) into Eq. (105), we have

$$\begin{aligned}
T &+ \left[\frac{4}{3} \left(A_1 \delta_x^2 + A_2 \delta_y^2 + A_3 \delta_z^2 \right) + \frac{3}{7} (p\delta_x + q\delta_y + r\delta_z) + A_{11} \delta_x^2 \delta_y + A_{12} \delta_y^2 \delta_x \right. \\
&\quad \left. + A_{13} \delta_z^2 \delta_x + A_{14} \delta_x^2 \delta_z + A_{15} \delta_y^2 \delta_z + A_{16} \delta_z^2 \delta_y \right] u \\
&+ \left[A_4 - \frac{3}{7} p - A_1 \delta_x - A_{11} \delta_x \delta_y + A_{12} \delta_y^2 + A_{13} \delta_z^2 - A_{14} \delta_x \delta_z - \frac{10}{3} \delta_y \delta_z \right] u_x \\
&+ \left[A_5 - \frac{3}{7} q - A_2 \delta_y + A_{11} \delta_x^2 - A_{12} \delta_y \delta_x - A_{15} \delta_y \delta_z + A_{16} \delta_z^2 - \frac{10}{3} \delta_z \delta_x \right] u_y \\
&+ \left[A_6 - \frac{3}{7} r - A_3 \delta_z - A_{13} \delta_z \delta_x + A_{14} \delta_x^2 + A_{15} \delta_y^2 - A_{16} \delta_z \delta_y - \frac{10}{3} \delta_x \delta_y \right] u_z \\
&+ \left(\frac{2A_1}{3} + \frac{A_1 h_x^2}{18} \delta_x^2 - \frac{p h_x^2}{14} \delta_x \right) u_{xx} + \left(\frac{2A_2}{3} + \frac{A_2 h_y^2}{18} \delta_y^2 - \frac{q h_y^2}{14} \delta_y \right) u_{yy} \\
&+ \left(A_7 + \frac{2A_{10}}{3} \delta_z \right) \partial_x \partial_y u \\
&+ \left(\frac{2A_3}{3} + \frac{A_3 h_z^2}{18} \delta_z^2 - \frac{r h_z^2}{14} \delta_z \right) u_{zz} + \left(A_8 + \frac{2A_{10}}{3} \delta_x \right) \partial_y \partial_z u + \left(A_9 + \frac{2A_{10}}{3} \delta_y \right) \partial_z \partial_x u \\
&= \left(1 - \frac{a_x p h_x^2}{6a^2} - \frac{b_y q h_y^2}{6b^2} - \frac{c_z r h_z^2}{6c^2} + \frac{p h_x^2}{6a} \delta_x + \frac{q h_y^2}{6b} \delta_y + \frac{r h_z^2}{6c} \delta_z \right) f. \tag{125}
\end{aligned}$$

Here

$$\begin{aligned}
T &= \frac{h^6}{45,360} \left(A_1 \partial_x^8 u + A_2 \partial_y^8 u + A_3 \partial_z^8 u \right) + \frac{h^6}{35,280} \left(p \partial_x^7 u + q \partial_y^7 u + r \partial_z^7 u \right) \\
&\quad + \frac{h^4}{36} \left(A_{11} \partial_x^4 \partial_y^3 u + A_{12} \partial_y^4 \partial_x^3 u + A_{13} \partial_z^4 \partial_x^3 u + A_{14} \partial_x^4 \partial_z^3 u + A_{15} \partial_y^4 \partial_z^3 u + A_{16} \partial_z^4 \partial_y^3 u \right) \\
&\quad + \frac{A_{10} h^4}{108} \left(\partial_x^3 \partial_y^3 \partial_z u + \partial_x^3 \partial_z^3 \partial_y u + \partial_y^3 \partial_z^3 \partial_x u \right). \tag{126}
\end{aligned}$$

Notice that all the derivatives $\{u_x, u_y, u_z, u_{xx}, u_{yy}, u_{zz}, \partial_x\partial_y u, \partial_y\partial_z u, \partial_z\partial_x u\}$ are calculated independently. Detailed derivation of the above discretization can be found in [20]. By substituting the truncation errors of the derivatives, we can get truncation error of the sixth-order BCD scheme as follows:

$$
\begin{aligned}
T_6 = {}& \left(A_4 - \frac{3}{7}p - A_1 - A_{11} + A_{12} + A_{13} - A_{14} - \frac{A_{10}}{3}\right)\frac{h^6}{7!}\partial_x^7 u \\
&+ \left(\frac{4A_3}{3} + \frac{A_3 h^2}{9} - \frac{rh^2}{7}\right)\frac{h^6}{8!}\partial_z^8 u \\
&+ \left(A_5 - \frac{3}{7}q - A_2 + A_{11} - A_{12} - A_{15} + A_{16} - \frac{A_{10}}{3}\right)\frac{h^6}{7!}\partial_y^7 u \\
&+ \left(\frac{4A_2}{3} + \frac{A_2 h^2}{9} - \frac{qh^2}{7}\right)\frac{h^6}{8!}\partial_y^8 u \\
&+ \left(A_6 - \frac{3}{7}r - A_3 - A_{13} + A_{14} + A_{15} - A_{16} - \frac{A_{10}}{3}\right)\frac{h^6}{7!}\partial_z^7 u \\
&+ \left(\frac{4A_1}{3} + \frac{A_1 h^2}{9} - \frac{ph^2}{7}\right)\frac{h^6}{8!}\partial_x^8 u \\
&+ \frac{h^6}{960}\Big[A_7\big(\partial_x^5\partial_y^3 u + \partial_x^3\partial_y^5 u\big) + A_8\big(\partial_y^5\partial_z^3 u + \partial_y^3\partial_z^5 u\big) \\
&+ A_9\big(\partial_z^5\partial_x^3 u + \partial_x^5\partial_z^3 u\big)\Big] + T.
\end{aligned}
\tag{127}
$$

Similarly, we can obtain a truncation error of the fourth-order BCD scheme as follows:

$$
\begin{aligned}
T_4 = {}& \frac{h^4}{360}\big(A_1\partial_x^6 u + A_2\partial_y^6 u + A_3\partial_z^6 u\big) - \frac{h^4}{120}\big(p\partial_x^5 u + q\partial_y^5 u + r\partial_z^5 u\big) \\
&- \frac{h^4}{36}\big(A_7\big(\partial_y^3\partial_x^3 u + A_8\partial_y^3\partial_z^3 u + A_9\partial_z^3\partial_x^3 u\big) \\
&- \frac{h^2 A_{10}}{18}\big(\partial_z^3\partial_y\partial_x u + \partial_z^3\partial_x\partial_y u + \partial_x^3\partial_z\partial_y u + \partial_x^3\partial_y\partial_z u + \partial_y^3\partial_x\partial_z u + \partial_y^3\partial_z\partial_x u\big) \\
&+ \frac{h^2}{12}\big(A_{11}\partial_y\partial_x^4 u + A_{12}\partial_x\partial_y^4 u + A_{13}\partial_x\partial_z^4 u + A_{14}\partial_z\partial_x^4 u + A_{15}\partial_z\partial_y^4 u + A_{16}\partial_y\partial_z^4 u\big) \\
&+ \left(A_4 - A_1 + A_7 + A_9 + \frac{A_{10}}{3} + A_{12} + A_{13}\right)\frac{h^4}{180}\partial_x^5 u \\
&+ \left(A_5 - A_2 + A_7 + A_8 + \frac{A_{10}}{3} + A_{11} + A_{16}\right)\frac{h^4}{180}\partial_y^5 u \\
&+ \left(A_6 - A_3 + A_8 + A_9 + \frac{A_{10}}{3} + A_{14} + A_{15}\right)\frac{h^4}{180}\partial_z^5 u.
\end{aligned}
\tag{128}
$$

4 Numerical experiments

In order to verify the accuracy and reliability of the present BCD schemes, numerical experiments with five test problems which have analytical solutions are carried out in this section. All the test problems, where the right-hand function and the Dirichlet boundary conditions can be given using the analytical solutions, are defined on the unit cube domain $\Omega = (0,1) \times (0,1) \times (0,1)$. The hybrid biconjugate gradient stabilized method (BiCGstab(2)) is selected to resolve the resulting linear systems in the problems. The errors and the con-

vergence order of the method are obtained according to the following definitions:

$$Error = \max_{i,j,k} \left| u_{i,j,k} - u(x_i, y_j, z_k) \right|; \qquad Order = \frac{\log(Error1/Error2)}{\log(h_1/h_2)}.$$

Here $u(x_i, y_j, z_k)$ is the exact solution. $Error1$ and $Error2$ are the maximum absolute errors estimated for two different grid step sizes h_1 and h_2.

For comparison, the proposed BCD schemes are used to compute the numerical solutions of all problems and the results with those computed by the explicit fourth-order CD scheme [24]. The maximum absolute errors and convergence orders with different values of h are listed in Tables 1–5, respectively. These results show clearly the BCD4 scheme, the explicit fourth-order CD scheme [24] and the BCD6 scheme can reach their fourth- and sixth-order accuracy and the BCD4 scheme gets a slightly better accurate solution than the explicit fourth-order CD scheme. However, the BCD6 scheme produces a much better

Table 1 The maximum error and convergence order for Problem 1

h	Ananthakrishnaiah [24]		BCD4 scheme		BCD6 scheme	
	Error	Order	Error	Order	Error	Order
1/4	7.66(–04)					
1/8	4.93(–05)	3.96	2.15(–05)		2.46(–07)	
1/16	3.14(–06)	3.97	1.32(–06)	4.03	2.81(–09)	6.45
1/32	–	–	8.14(–08)	4.02	2.65(–11)	6.73
1/48	–	–	1.60(–08)	4.01	1.99(–12)	6.39

Table 2 The maximum error and convergence order for Problem 2

h	Ananthakrishnaiah [24]		BCD4 scheme		BCD6 scheme	
	Error	Order	Error	Order	Error	Order
1/4	2.50(–05)					
1/8	1.29(–06)	4.28	6.25(–07)		1.14(–07)	
1/16	8.04(–08)	4.00	2.40(–08)	4.70	1.88(–09)	5.92
1/32	–	–	1.19(–09)	4.33	2.99(–11)	5.97
1/48	–	–	2.10(–10)	4.28	2.60(–12)	6.02

Table 3 The maximum error and convergence order for Problem 3

h	Ananthakrishnaiah [24]		BCD4 scheme		BCD6 scheme	
	Error	Order	Error	Order	Error	Order
1/4	8.88(–05)					
1/8	5.18(–06)	4.10	4.29(–07)		4.35(–08)	
1/16	3.18(–07)	4.03	1.69(–08)	4.67	6.15(–10)	6.14
1/32	–	–	8.63(–10)	4.29	8.68(–12)	6.15
1/48	–	–	1.60(–10)	4.16	6.98(–13)	6.22

Table 4 The maximum error and convergence order for Problem 4

h	Ananthakrishnaiah [24]		BCD4 scheme		BCD6 scheme	
	Error	Order	Error	Order	Error	Order
1/4	2.53(–04)					
1/8	1.64(–05)	3.95	1.17(–05)		2.75(–07)	
1/16	1.04(–06)	3.98	6.12(–07)	4.26	2.95(–09)	6.54
1/32	–	–	3.64(–08)	4.07	2.78(–11)	6.73
1/48	–	–	7.09(–09)	4.03	2.01(–12)	6.48

Table 5 The maximum error and average convergence order for Problem 5

h	Ananthakrishnaiah [24]		BCD4 scheme		BCD6 scheme	
	Error	Order	Error	Order	Error	Order
1/4	4.96(−06)					
1/8	3.06(−07)	4.02	3.77(−07)		1.29(−08)	
1/16	2.06(−08)	3.89	1.21(−08)	4.96	1.73(−10)	6.22
1/32	–	–	5.40(−10)	4.49	1.57(−12)	6.39
1/48	–	–	9.55(−11)	4.27	2.07(−13)	5.00

accurate solution than both the BCD4 scheme and the explicit fourth-order CD scheme [24].

Problem 1 ([24]) We choose the coefficients in Equation (1) as

$$a = 5, \qquad b = 3, \qquad c = 4, \qquad p = 13, \qquad q = 11, \qquad r = 10,$$
$$d_1 = 0, \qquad d_2 = 0, \qquad d_3 = 0, \qquad s = -7.$$

The analytic solution is

$$u(x, y, z) = \exp(x + y + z).$$

Problem 2 ([24]) The coefficients of our second problem is chosen as

$$a = 1 + x^4; \qquad b = 1 + y^4; \qquad c = 1 + z^4; \qquad p = 1 + \cos x; \qquad q = 1 + \cos y;$$
$$r = 1 + \cos z; \qquad d_1 = 0; \qquad d_2 = 0; \qquad d_3 = 0; \qquad s = -1.$$

The analytic solution is

$$u(x, y, z) = \big[\cosh(x) + \cosh(y) + \cosh(z)\big] / \cosh(1).$$

Problem 3 ([24]) The coefficients of our third problem is chosen as

$$a = \exp(2x); \qquad b = \exp(2y); \qquad c = \exp(2z); \qquad p = \exp(x + y + z);$$
$$q = \exp(x + y + z); \qquad r = -\exp(x + y + z); \qquad d_1 = d_2 = d_3 = s = 0.$$

The analytic solution is

$$u(x, y, z) = \cos(x) + \cos(y) + \cos(z).$$

Problem 4 ([24]) The coefficients of our fourth problem is chosen as

$$a = b = c = 10, \qquad p = 13, \qquad q = 11, \qquad r = 10,$$
$$d_1 = 1, \qquad d_2 = 2, \qquad d_3 = 3, \qquad s = -7.$$

The analytic solution is

$$u(x, y, z) = \exp(x + y + z).$$

Problem 5 ([24]) The coefficients of our fifth problem is chosen as

$$a = b = c = 10 + x^4 + y^4 + z^4; \qquad p = 1 + \cos x; \qquad q = 1 + \cos y;$$

$$r = 1 + \cos z; \qquad d_1 = 1 + z; \qquad d_2 = 1 + x; \qquad d_3 = 1 + y; \qquad s = 0.$$

The analytic solution is

$$u(x, y, z) = \bigl(\cosh(x) + \cosh(y) + \cosh(z)\bigr)/\cosh(1).$$

5 Conclusions

In this paper, we have constructed the fourth- and sixth-order BCD schemes for the 3D variable coefficients elliptic PDE with mixed derivatives. Firstly, based on Taylor series expansion and truncation error remainder, combined with the fourth-order Padé schemes of the first-order derivatives, a new fourth-order BCD scheme is constructed. In this new scheme, the unknown function and its first-order derivatives are regarded as the unknown variables in the calculation. Then, on the basis of the fourth-order BCD scheme proposed above, a new sixth-order BCD scheme is proposed by replacing the fifth- and sixth-order derivatives of the truncation errors with the linear combination of the unknown function, the first- and second-order as well as the second-order mixed derivatives. In other words, in the sixth-order BCD scheme, the unknown function, its first- and second-order derivatives as well as the second-order mixed derivatives are regarded as the unknown variables. At the same time, the sixth-order boundaries schemes of the first-order derivatives, the second-order derivatives and the second-order mixed derivatives are proposed. Finally, numerical results indicate that the present BCD schemes exhibit a very good resolution and high accuracy for all test problems.

Appendix A: Details of the finite difference operators

$$\delta_x^2 u_0 = \frac{u_1 - 2u_0 + u_3}{h_x^2}, \qquad \delta_y^2 u_0 = \frac{u_2 - 2u_0 + u_4}{h_y^2}, \qquad \delta_z^2 u_0 = \frac{u_5 - 2u_0 + u_6}{h_z^2},$$

$$\delta_x u_0 = \frac{u_1 - u_3}{2h_x}, \qquad \delta_y u_0 = \frac{u_2 - u_4}{2h_y}, \qquad \delta_z u_0 = \frac{u_5 - u_6}{2h_z},$$

$$\delta_x \delta_y u_0 = \frac{u_7 - u_8 + u_9 - u_{10}}{4h_x h_y},$$

$$\delta_y \delta_z u_0 = \frac{u_{12} - u_{14} - u_{16} + u_{18}}{4h_z h_y},$$

$$\delta_x \delta_z u_0 = \frac{u_{11} - u_{13} - u_{15} + u_{17}}{4h_x h_z},$$

$$\delta_x^2 \delta_y u_0 = \frac{u_7 + u_8 - u_9 - u_{10} - 2u_2 + 2u_4}{2h_x^2 h_y},$$

$$\delta_y^2 \delta_x u_0 = \frac{u_7 - u_8 - u_9 + u_{10} - 2u_1 + 2u_3}{2h_y^2 h_x},$$

$$\delta_y^2 \delta_z u_0 = \frac{u_{12} + u_{14} - u_{16} - u_{18} - 2u_5 + 2u_6}{2h_y^2 h_z},$$

$$\delta_z^2 \delta_y u_0 = \frac{u_{12} - u_{14} + u_{16} - u_{18} - 2u_2 + 2u_4}{2h_z^2 h_y},$$

$$\delta_x^2 \delta_z u_0 = \frac{u_{11} + u_{13} - u_{15} - u_{17} - 2u_5 + 2u_6}{2h_x^2 h_z},$$

$$\delta_z^2 \delta_x u_0 = \frac{u_{11} - u_{13} + u_{15} - u_{17} - 2u_1 + 2u_3}{2h_z^2 h_x}.$$

Appendix B: Fourth-order scheme for boundary conditions of the first-order derivatives [37]

$$(u_x)_{0,j,k} + \frac{14}{15}(u_x)_{1,j,k}$$

$$= \frac{1}{h_x}\left(-\frac{184}{75}u_{0,j,k} + \frac{703}{180}u_{1,j,k} - \frac{89}{30}u_{2,j,k} + \frac{67}{30}u_{3,j,k}\right.$$

$$\left. - \frac{77}{90}u_{4,j,k} + \frac{41}{300}u_{5,j,k}\right) \quad (j = 1, 2, \ldots, N_y; k = 1, 2, \ldots, N_z), \tag{B.1}$$

$$(u_x)_{N_x,j,k} - \frac{14}{15}(u_x)_{N_x-1,j,k}$$

$$= \frac{1}{h_x}\left(\frac{52}{25}u_{N_x,j,k} - \frac{1067}{180}u_{N_x-1,j,k} + \frac{67}{10}u_{N_x-2,j,k} - \frac{41}{10}u_{N_x-3,j,k}\right.$$

$$\left. + \frac{133}{90}u_{N_x-4,j,k} - \frac{69}{300}u_{N_x-5,j,k}\right) \quad (j = 1, 2, \ldots, N_y, k = 1, 2, \ldots, N_z), \tag{B.2}$$

$$(u_y)_{i,0,k} + \frac{14}{15}(u_y)_{i,1,k}$$

$$= \frac{1}{h_y}\left(-\frac{184}{75}u_{i,0,k} + \frac{703}{180}u_{i,1,k} - \frac{89}{30}u_{i,2,k} + \frac{67}{30}u_{i,3,k}\right.$$

$$\left. - \frac{77}{90}u_{i,4,k} + \frac{41}{300}u_{i,5,k}\right) \quad (i = 1, 2, \ldots, N_x; k = 1, 2, \ldots, N_z), \tag{B.3}$$

$$(u_y)_{i,N_y,k} - \frac{14}{15}(u_y)_{i,N_y-1,k}$$

$$= \frac{1}{h_y}\left(\frac{52}{25}u_{i,N_y,k} - \frac{1067}{180}u_{i,N_y-1,k} + \frac{67}{10}u_{i,N_y-2,k} - \frac{41}{10}u_{i,N_y-3,k}\right.$$

$$\left. + \frac{133}{90}u_{i,N_y-4,k} - \frac{69}{300}u_{i,N_y-5,k}\right) \quad (i = 1, 2, \ldots, N_x; k = 1, 2, \ldots, N_z), \tag{B.4}$$

$$(u_z)_{i,j,0} + \frac{14}{15}(u_z)_{i,j,1}$$

$$= \frac{1}{h_z}\left(-\frac{184}{75}u_{i,j,0} + \frac{703}{180}u_{i,j,1} - \frac{89}{30}u_{i,j,2} + \frac{67}{30}u_{i,j,3}\right.$$

$$\left. - \frac{77}{90}u_{i,j,4} + \frac{41}{300}u_{i,j,5}\right) \quad (i = 1, 2, \ldots, N_x; j = 1, 2, \ldots, N_y), \tag{B.5}$$

$$(u_z)_{i,j,N_z} - \frac{14}{15}(u_z)_{i,j,N_z-1}$$

$$= \frac{1}{h_z}\left(\frac{52}{25}u_{i,j,N_z} - \frac{1067}{180}u_{i,j,N_z-1} + \frac{67}{10}u_{i,j,N_z-2} - \frac{41}{10}u_{i,j,N_z-3}\right.$$

$$\left. + \frac{133}{90}u_{i,j,N_z-4} - \frac{69}{300}u_{i,j,N_z-5}\right) \quad (i = 1, 2, \ldots, N_x; j = 1, 2, \ldots, N_y). \tag{B.6}$$
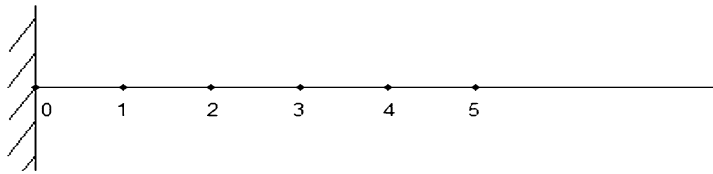
Figure 3 Grid point discretization for left boundary

Appendix C: The sixth-order boundary schemes of the mixed derivatives

The sixth-order approximation of left boundary of mixed derivative may be obtained from a relation of the form

$$
\begin{aligned}
\partial_x \partial_y u_{0,j,k} &+ \alpha \partial_x \partial_y u_{1,j,k} \\
&= \big[(u_y)_x\big]_{0,j,k} + \alpha\big[(u_y)_x\big]_{1,j,k} \\
&= \big[a_0 (u_y)_{0,j,k} + a_1 (u_y)_{1,j,k} \\
&\quad + a_2 (u_y)_{2,j,k} + a_3 (u_y)_{3,j,k} + a_4 (u_y)_{4,j,k} + a_5 (u_y)_{5,j,k} + a_6 (u_y)_{6,j,k} \big] / h_x.
\end{aligned}
\tag{C.1}
$$

Here $j = 0, 1, \ldots, N_y$; $k = 0, 1, \ldots, N_k$ the coefficients $a_0, a_1, a_2, a_3, a_4, a_5, a_6$ (for the subscript see Fig. 3) and α are derived by matching the Taylor series coefficients of various orders. The detailed derivation process is given below.

Using the Taylor series expansions at point (x_0, y_j, z_k)

$$
\begin{aligned}
(u_y)_{1,j,k} = (u_y)_{0,j,k} &+ h_x \partial_x \partial_y u_{0,j,k} + \frac{h_x^2}{2!} \partial_x^2 \partial_y u_{0,j,k} + \frac{h_x^3}{3!} \partial_y \partial_x^3 u_{0,j,k} \\
&+ \frac{h_x^4}{4!} \partial_y \partial_x^4 u_{0,j,k} + \frac{h_x^5}{5!} \partial_y \partial_x^5 u_{0,j,k} + \frac{h_x^6}{6!} \partial_y \partial_x^6 u_{0,j,k} + O\big(h_x^7\big),
\end{aligned}
\tag{C.2}
$$

$$
\begin{aligned}
(u_y)_{2,j,k} = (u_y)_{0,j,k} &+ 2 h_x \partial_y \partial_x u_{0,j,k} + \frac{2^2 h_x^2}{2!} \partial_y \partial_x^2 u_{0,j,k} + \frac{2^3 h_x^3}{3!} \partial_y \partial_x^3 u_{0,j,k} \\
&+ \frac{2^4 h_x^4}{4!} \partial_y \partial_x^4 u_{0,j,k} + \frac{2^5 h_x^5}{5!} \partial_y \partial_x^5 u_{0,j,k} + \frac{2^6 h_x^6}{6!} \partial_y \partial_x^6 u_{0,j,k} + O\big(h_x^7\big),
\end{aligned}
\tag{C.3}
$$

$$
\begin{aligned}
(u_y)_{3,j,k} = (u_y)_{0,j,k} &+ 3 h_x \partial_y \partial_x u_{0,j,k} + \frac{3^2 h_x^2}{2!} \partial_y \partial_x^2 u_{0,j,k} + \frac{3^3 h_x^3}{3!} \partial_y \partial_x^3 u_{0,j,k} \\
&+ \frac{3^4 h_x^4}{4!} \partial_y \partial_x^4 u_{0,j,k} + \frac{3^5 h_x^5}{5!} \partial_y \partial_x^5 u_{0,j,k} + \frac{3^6 h_x^6}{6!} \partial_y \partial_x^6 u_{0,j,k} + O\big(h_x^7\big),
\end{aligned}
\tag{C.4}
$$

$$
\begin{aligned}
(u_y)_{4,j,k} = (u_y)_{0,j,k} &+ 4 h_x \partial_y \partial_x u_{0,j,k} + \frac{4^2 h_x^2}{2!} \partial_y \partial_x^2 u_{0,j,k} + \frac{4^3 h_x^3}{3!} \partial_y \partial_x^3 u_{0,j,k} \\
&+ \frac{4^4 h_x^4}{4!} \partial_y \partial_x^4 u_{0,j,k} + \frac{4^5 h_x^5}{5!} \partial_y \partial_x^5 u_{0,j,k} + \frac{4^6 h_x^6}{6!} \partial_y \partial_x^6 u_{0,j,k} + O\big(h_x^7\big),
\end{aligned}
\tag{C.5}
$$

$$
\begin{aligned}
(u_y)_{5,j,k} = (u_y)_{0,j,k} &+ 5 h_x \partial_y \partial_x u_{0,j,k} + \frac{5^2 h_x^2}{2!} \partial_y \partial_x^2 u_{0,j,k} + \frac{5^3 h_x^3}{3!} \partial_y \partial_x^3 u_{0,j,k} \\
&+ \frac{5^4 h_x^4}{4!} \partial_y \partial_x^4 u_{0,j,k} + \frac{5^5 h_x^5}{5!} \partial_y \partial_x^5 u_{0,j,k} + \frac{5^6 h_x^6}{6!} \partial_y \partial_x^6 u_{0,j,k} + O\big(h_x^7\big),
\end{aligned}
\tag{C.6}
$$

$$(u_y)_{6,j,k} = (u_y)_{0,j,k} + 6h_x \partial_y \partial_x u_{0,j,k} + \frac{6^2 h_x^2}{2!}(u_{yxx})\partial_y \partial_x^2 u_{0,j,k} + \frac{6^3 h_x^3}{3!}\partial_y \partial_x^3 u_{0,j,k}$$

$$+ \frac{6^4 h_x^4}{4!}\partial_y \partial_x^4 u_{0,j,k} + \frac{6^5 h_x^5}{5!}\partial_y \partial_x^5 u_{0,j,k} + \frac{6^6 h_x^6}{6!}\partial_y \partial_x^6 u_{0,j,k} + O(h_x^7). \tag{C.7}$$

Substituting Eqs. (C.2)–(C.7) into Eq. (C.1), we are able to obtain linear equations as shown now:

$$a_0 + a_1 + a_2 + a_3 + a_4 + a_5 + a_6 = 0,$$

$$\frac{1}{2!}(a_1 + 2^2 a_2 + 3^2 a_3 + 4^2 a_4 + 5^2 a_5 + 6^2 a_6) = \alpha,$$

$$\frac{1}{3!}(a_1 + 2^3 a_2 + 3^3 a_3 + 4^3 a_4 + 5^3 a_5 + 6^3 a_6) = \frac{\alpha}{2},$$

$$\frac{1}{4!}(a_1 + 2^4 a_2 + 3^4 a_3 + 4^4 a_4 + 5^4 a_5 + 6^4 a_6) = \frac{\alpha}{6}, \tag{C.8}$$

$$\frac{1}{5!}(a_1 + 2^5 a_2 + 3^5 a_3 + 4^5 a_4 + 5^5 a_5 + 6^5 a_6) = \frac{\alpha}{24},$$

$$\frac{1}{6!}(a_1 + 2^6 a_2 + 3^6 a_3 + 4^6 a_4 + 5^6 a_5 + 6^6 a_6) = \frac{\alpha}{120},$$

$$\frac{1}{7!}(a_1 + 2^7 a_2 + 3^7 a_3 + 4^7 a_4 + 5^7 a_5 + 6^7 a_6) = \frac{\alpha}{720}.$$

And resolving it by Matlab Software, we can get the results as follows:

$$\alpha = \frac{1}{5}, \qquad a_0 = -\frac{149}{60}, \qquad a_1 = \frac{1723}{300}, \qquad a_2 = -7,$$

$$a_3 = \frac{19}{3}, \qquad a_4 = -\frac{43}{12}, \qquad a_5 = \frac{23}{20}, \qquad a_6 = -\frac{4}{25}.$$

So, the sixth-order scheme for the left boundary mixed derivative can be written as:

$$\partial_x \partial_y u_{0,j,k} + \frac{1}{5}\partial_x \partial_y u_{1,j,k}$$

$$= \left[-\frac{149}{60}(u_y)_{0,j,k} + \frac{1723}{300}(u_y)_{1,j,k} - 7(u_y)_{2,j,k} + \frac{19}{3}(u_y)_{3,j,k} - \frac{43}{12}(u_y)_{4,j,k} \right.$$

$$\left. + \frac{23}{20}(u_y)_{5,j,k} - \frac{4}{25}(u_y)_{6,j,k} \right] / h_x, \quad j = 0, 1, 2, \ldots, N_y; k = 0, 1, 2, \ldots, N_z. \tag{C.9}$$

With a similar method, we can get the sixth-order boundaries schemes for other second-order derivatives as follows:

$$\partial_x \partial_y u_{N_x,j,k} - \frac{1}{5}\partial_x \partial_y u_{N_x-1,j,k}$$

$$= \left[\frac{29}{12}(u_y)_{N_x,j,k} - \frac{1877}{300}(u_y)_{N_x-1,j,k} + 8(u_y)_{N_x-2,j,k} - 7(u_y)_{N_x-3,j,k} \right.$$

$$+ \frac{47}{12}(u_y)_{N_x-4,j,k} - \frac{5}{4}(u_y)_{N_x-5,j,k}$$

$$\left. + \frac{13}{75}(u_y)_{N_x-6,j,k} \right] / h_x, \quad j = 0, 1, 2, \ldots, N_y; k = 0, 1, 2, \ldots, N_z, \tag{C.10}$$

$$\partial_x \partial_y u_{i,0,k} + \frac{1}{5} \partial_x \partial_y u_{i,1,k}$$

$$= \left(-\frac{149}{60}(u_x)_{i,0,k} + \frac{1723}{300}(u_x)_{i,1,k} - 7(u_x)_{i,2,k} + \frac{19}{3}(u_x)_{i,3,k} - \frac{43}{12}(u_x)_{i,4,k} \right.$$

$$\left. + \frac{3}{20}(u_x)_{i,5,k} - \frac{4}{25}(u_x)_{i,6,k} \right)/h_y, \quad i = 1,2,\ldots,N_x; k = 1,2,\ldots,N_z, \quad\quad (C.11)$$

$$\partial_x \partial_y u_{i,N_y,k} - \frac{1}{5} \partial_x \partial_y u_{i,N_y-1,k}$$

$$= \left[\frac{29}{12}(u_x)_{i,N_y,k} - \frac{1877}{300}(u_x)_{i,N_y-1,k} + 8(u_x)_{i,N_y-2,k} - 7(u_x)_{i,N_y-3,k} \right.$$

$$+ \frac{47}{12}(u_x)_{i,N_y-4,k} - \frac{5}{4}(u_x)_{i,N_y-5,k}$$

$$\left. + \frac{13}{75}(u_x)_{i,N_y-6,k} \right]/h_x, \quad i = 0,1,2,\ldots,N_x; k = 0,1,2,\ldots,N_z, \quad\quad (C.12)$$

$$\partial_y \partial_z u_{i,j,0} + \frac{1}{5} \partial_y \partial_z u_{i,j,1}$$

$$= \left[-\frac{149}{60}(u_y)_{i,j,0} + \frac{1723}{300}(u_y)_{i,j,1} - 7(u_y)_{i,j,2} + \frac{19}{3}(u_y)_{i,j,3} - \frac{43}{12}(u_y)_{i,j,4} \right.$$

$$\left. + \frac{23}{20}(u_y)_{i,j,5} - \frac{4}{25}(u_y)_{i,j,6} \right]/h_z, \quad i = 0,1,\ldots,N_x; j = 0,1,\ldots,N_y, \quad\quad (C.13)$$

$$\partial_y \partial_z u_{i,j,N_z} - \frac{1}{5} \partial_y \partial_z u_{i,j,N_z-1}$$

$$= \left[\frac{29}{12}(u_y)_{i,j,N_z} - \frac{1877}{300}(u_y)_{i,j,N_z-1} + 8(u_y)_{i,j,N_z-2} - 7(u_y)_{i,j,N_z-3} + \frac{47}{12}(u_y)_{i,j,N_z-4} \right.$$

$$\left. - \frac{5}{4}(u_y)_{i,j,N_z-5} + \frac{13}{75}(u_y)_{N_z-6} \right]/h_z, \quad i = 0,1,\ldots,N_x; j = 0,1,\ldots,N_y, \quad\quad (C.14)$$

$$\partial_y \partial_z u_{i,0,k} + \frac{1}{5} \partial_y \partial_z u_{i,1,k}$$

$$= \left[-\frac{149}{60}(u_z)_{i,0,k} + \frac{1723}{300}(u_z)_{i,1,k} - 7(u_z)_{i,2,k} + \frac{19}{3}(u_z)_{i,3,k} - \frac{43}{12}(u_z)_{i,4,k} \right.$$

$$\left. + \frac{23}{20}(u_z)_{i,5,k} - \frac{4}{25}(u_z)_{i,6,k} \right]/h_y, \quad i = 0,1,\ldots,N_x; k = 0,1,\ldots,N_z, \quad\quad (C.15)$$

$$\partial_y \partial_z u_{i,N_y,k} - \frac{1}{5} \partial_y \partial_z u_{i,N_y-1,k}$$

$$= \left[\frac{29}{12}(u_z)_{i,N_y,k} - \frac{1877}{300}(u_z)_{i,N_y-1,k} + 8(u_z)_{i,N_y-2,k} - 7(u_z)_{i,N_y-3,k} + \frac{47}{12}(u_z)_{i,N_y-4,k} \right.$$

$$\left. - \frac{5}{4}(u_z)_{i,N_y-5,k} + \frac{13}{75}(u_z)_{i,N_y-6,k} \right]/h_y, \quad i = 0,1,\ldots,N_x; k = 0,1,\ldots,N_z, \quad\quad (C.16)$$

$$\partial_z \partial_x u_{0,j,k} + \frac{1}{5} \partial_z \partial_x u_{1,j,k}$$

$$= \left[-\frac{149}{60}(u_z)_{0,j,k} + \frac{1723}{300}(u_z)_{1,j,k} - 7(u_z)_{2,j,k} + \frac{19}{3}(u_z)_{3,j,k} - \frac{43}{12}(u_z)_{4,j,k} \right.$$

$$\left. + \frac{23}{20}(u_z)_{5,j,k} - \frac{4}{25}(u_z)_{6,j,k} \right]/h_x, \quad j = 0,1,\ldots,N_y; k = 0,1,\ldots,N_z, \quad\quad (C.17)$$

$$\partial_z \partial_x u_{N_x,j,k} - \frac{1}{5} \partial_z \partial_x u_{N_x-1,j,k}$$

$$= \left[\frac{29}{12} (u_z)_{N_x,j,k} - \frac{1877}{300} (u_z)_{N_x-1,j,k} + 8(u_z)_{N_x-2,j,k} - 7(u_z)_{N_x-3,j,k} + \frac{47}{12} (u_z)_{N_x-4,j,k} \right.$$

$$\left. - \frac{5}{4} (u_z)_{N_x-5,j,k} + \frac{13}{75} (u_z)_{N_x-6,j,k} \right] \Big/ h_x, \quad j = 0, 1, \ldots, N_y; k = 0, 1, \ldots, N_z, \qquad (C.18)$$

$$\partial_z \partial_x u_{i,j,0} + \frac{1}{5} \partial_z \partial_x u_{i,j,1}$$

$$= \left[-\frac{149}{60} (u_x)_{i,j,0} + \frac{1723}{300} (u_x)_{i,j,1} - 7(u_x)_{i,j,2} + \frac{19}{3} (u_x)_{i,j,3} - \frac{43}{12} (u_x)_{i,j,4} \right.$$

$$\left. + \frac{23}{20} (u_x)_{i,j,5} - \frac{4}{25} (u_x)_{i,j,6} \right] \Big/ h_z, \quad i = 0, 1, \ldots, N_x; k = 0, 1, \ldots, N_z, \qquad (C.19)$$

$$\partial_z \partial_x u_{i,j,N_z} - \frac{1}{5} \partial_z \partial_x u_{i,j,N_z-1}$$

$$= \left[\frac{29}{12} (u_x)_{i,j,N_z} - \frac{1877}{300} (u_x)_{i,j,N_z-1} + 8(u_x)_{i,j,N_z-2} - 7(u_x)_{i,j,N_z-3} + \frac{47}{12} (u_x)_{i,j,N_z-4} \right.$$

$$\left. - \frac{5}{4} (u_x)_{i,j,N_z-5} + \frac{13}{75} (u_x)_{i,j,N_z-6} \right] \Big/ h_z, \quad i = 0, 1, \ldots, N_x; j = 0, 1, \ldots, N_y. \qquad (C.20)$$

Availability of data and materials
Not applicable.

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
YG defined the research theme. TM designed numerical method and conducted numerical experiments. TM also interpreted the results and wrote the paper. All authors have seen and approved the final version of the manuscript.

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