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A high order finite difference method with Richardson extrapolation for 3D convection diffusion equation

Yuezhen Ma, Yongbin Ge *

Institute of Applied Mathematics and Mechanics, Ningxia University, Yinchuan, Ningxia 750021, China

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ABSTRACT

In this paper, we extend the Sun and Zhang's [24] work on high order finite difference method, which is based on the Richardson extrapolation technique and an operator interpolation scheme for the one and two dimensional steady convection diffusion equations to the three dimensional case. Firstly, we employ a fourth order compact difference scheme to get the fourth order accurate solution on the fine and the coarse grids. Then, we use the Richardson extrapolation technique by combining the two approximate solutions to get a sixth order accurate solution on coarse grid. Finally, we apply an operator interpolation scheme to achieve the sixth order accurate solution on the fine grid. During this process, we use alternating direction implicit (ADI) method to solve the resulting linear systems. Numerical experiments are conducted to verify the accuracy and effectiveness of the present method.

1. Introduction

A great deal of effort has been devoted in recent years to the development of numerical approximation of convection diffusion problems. It is well known that the traditional numerical schemes have low accuracy and thus need fine discretization to obtain desired accuracy. This will present many computational challenges due to the prohibitive computer memory and CPU time requirements, especially for solving 3D problems. One approach to meet these challenges is to use higher order finite difference approximations or Richardson extrapolation [1,2]. Suppose existing a problem with Dirichlet boundary conditions and the second order central difference approximations are used, then for all internal grid points, the truncation error has the form $\alpha h^2 + \beta h^4 + \gamma h^6 + \cdots$, where h is mesh size and $\alpha,\ \beta,\ \gamma, \ldots$ are constants. Doing the computation with two or three different mesh sizes and carrying out one or two extrapolations to eliminate the error terms of second order or of second and fourth order we derive a solution with fourth or sixth order accuracy.

In the past two decades, high order compact difference methods have generated renewed interest and a variety of specialized techniques have been developed [3–26]. For 2D convection diffusion equations, Gupta et al. [3] employed Taylor series expansions to the differential equation and derived a fourth order polynomial nine-point compact difference scheme. Similar fourth order polynomial compact difference methods have been developed and applied to the 2D convection diffusion equations and the incompressible Navier–Stokes equations by several authors [5,10,11,13–15]. Dennis and Hudson [10] derived the same scheme as in [3] using another approach. As an alternative approach to high order polynomial compact difference scheme, high order compact exponential difference schemes for the 1D and 2D convection diffusion equations are developed by several authors [4,6,9]. Zhang et al. [7] proposed a fourth order compact finite difference scheme with different mesh sizes in different coordinate directions for the 2D convection diffusion equation and a multilevel local mesh

* Corresponding author.
E-mail address: gyb@nxu.edu.cn (Y. Ge).

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refinement strategy was used to deal with the local singularity problem. Kalita et al. [8] developed a high order compact finite difference scheme on non-uniform grids for the 2D convection diffusion equation involving no transformation from the physical space to the computational space. The high order compact difference techniques have also been generalized to 3D [18–22]. These discretization schemes have been shown to have better numerical stability and provide higher accurate approximations than standard lower order finite difference schemes. For the sixth order compact schemes, Chu and Fan [23] proposed a three point combined compact difference (CCD) scheme for solving 2D convection diffusion equation. The scheme can achieve sixth order accuracy for the inner grid points and fifth order accuracy for the boundary grid points. Recently, Sun and Zhang [24] proposed a new high order finite difference discretization strategy for solving 1D and 2D convection diffusion equations. They firstly used a fourth order compact difference scheme to obtain a fine grid solution and a coarse grid solution. Then, they used the Richardson extrapolation technique and an operator interpolation scheme to improve the accuracy order of computed solutions from four to six. They applied the new strategy to solve general 1D and 2D convection diffusion problems and compared with sixth order CCD scheme [23]. Numerical results show that the method is more efficacious than the CCD scheme [23] or the classical fourth order compact scheme [19].

As far as we know, the higher order compact difference schemes on a single scale grid are more complicated to develop in higher dimensions. So, using the multiscale grid methods and extrapolation techniques to achieve the higher order accuracy is a good choice. In this paper, we are aiming at extending the finite difference discretization strategy by using muliscale method and operator based interpolation with an extrapolation technique proposed in [24] for solving 1D and 2D convection diffusion equations to 3D case. We restrict our attention to use a fourth order compact difference scheme for solving 3D convection diffusion equation and improve the accuracy order of the computed solutions from four to six by using the Richardson extrapolation technique and an operator interpolation scheme. In the process of present computational strategy, the alternating direction implicit (ADI) iteration is also used, as in [24] for 2D case, to solve the resulting sparse linear systems. Numerical experiments show that the present sixth order discretization method is more efficient than the classical fourth order compact scheme.

The rest of the paper is organized as follows. Section 2 is a brief review about the fourth order compact difference schemes for 3D convection diffusion equation. Then, we outline a sixth order compact difference discretization strategy by using Richardson extrapolation and an ADI type iteration technique in Section 3. In order to demonstrate the accuracy and effectiveness of the present method, we conduct some numerical experiments in Section 4. Finally, concluding remarks are included in Section 5.

2. Fourth order compact difference scheme

We consider 3D convection diffusion equation in form of

$$u_{xx} + u_{yy} + u_{zz} + p(x,y,z)u_x + q(x,y,z)u_y + r(x,y,z)u_z = f(x,y,z) \tag{1}$$

For a specified forcing function f in a continuous domain Ω in 3D space with suitable boundary conditions prescribed on $\partial\Omega$. Here the coefficients $p,\ q,\ r$, the forcing function f, as well as the unknown function u, are assumed to be continuously differentiable and have the required partial derivatives on Ω, where Ω is a union of rectangular solids.

We assume that the equation is discretized on a uniform 3D grid in each direction and $h_x,\ h_y$ and h_z are the mesh sizes of $x,\ y$ and z-direction, respectively. We use a local coordinate system as referred in [19], and the grid points are labeled as in

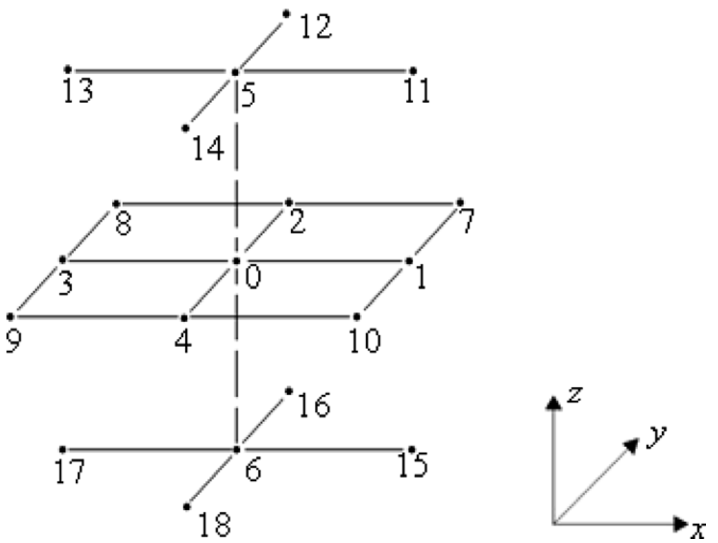

Fig. 1. Computational stencil of the 3D grid points.

Fig. 1. The approximate value of a function $u(x, y, z)$ at an internal mesh point (i, j, k) is denoted by u_0. The approximate values of its immediate 18 neighboring points are denoted by $u_l, l = 1, 2, \ldots 18$, as in Fig. 1.

For the 3D general linear elliptic equations with variable coefficients, Ananthakrishnaiah et al. [18] proposed a procedure of developing fourth order compact finite difference schemes. But the formulas given in [18] are implicit and abstract, so much time and effort have to be spent in deriving explicit schemes for their individual equations. Zhang [19] derived an explicit fourth order scheme for Eq. (1) from the general implicit formulas of [18] by employing the computer algebra package Mathematica. Tian and Cui [20] derived a fourth order compact finite difference scheme of Eq. (1) with unequal mesh sizes on each coordinate direction using the techniques developed by Li et al. [14], who employed the techniques to get the fourth order compact discretization scheme for the vorticity equation in the 2D incompressible Navier–Stokes equations, which is expressed in streamfunction-vorticity form. The fourth order compact finite difference scheme derived in [20] for 3D convection diffusion equation (1) can be written as

$$\sum_{l=0}^{18} A_l u_l = f_0 + \frac{1}{12}(h_x^2 p f_x + h_y^2 q f_y + h_z^2 r f_z + h_x^2 f_{xx} + h_y^2 f_{yy} + h_z^2 f_{zz})_0 \tag{2}$$

where the coefficients are given by

$$A_0 = -\frac{1}{6}\left[8\left(\frac{1}{h_x^2}+\frac{1}{h_y^2}+\frac{1}{h_z^2}\right) + (p^2+q^2+r^2) + 2(p_x+q_y+r_z)\right]_0$$

$$A_1 = \frac{1}{6}\left[\left(\frac{4}{h_x}-\frac{1}{h_y}-\frac{1}{h_z}\right) + \frac{3p}{h_x} - p\left(\frac{h_x^2+h_y^2}{2h_x h_y^2}+\frac{h_x^2+h_z^2}{2h_x h_z^2}\right) + \frac{1}{2}(p^2+2p_x) + \frac{1}{24h_x}\left(h_x^2 p_{xx} + h_y^2 p_{yy} + h_z^2 p_{zz} + h_x^2 p p_x + h_y^2 q p_y + h_z^2 r p_z\right)\right]_0$$

$$A_2 = \frac{1}{6}\left[\left(\frac{4}{h_y}-\frac{1}{h_x}-\frac{1}{h_z}\right) + \frac{3q}{h_y} - q\left(\frac{h_x^2+h_y^2}{2h_y h_x^2}+\frac{h_x^2+h_z^2}{2h_y h_z^2}\right) + \frac{1}{2}(q^2+2q_y) + \frac{1}{24h_y}\left(h_x^2 q_{xx} + h_y^2 q_{yy} + h_z^2 q_{zz} + h_x^2 p q_x + h_y^2 q q_y + h_z^2 r q_z\right)\right]_0$$

$$A_3 = \frac{1}{6}\left[\left(\frac{4}{h_x}-\frac{1}{h_y}-\frac{1}{h_z}\right) - \frac{3p}{h_x} + p\left(\frac{h_x^2+h_y^2}{2h_x h_y^2}+\frac{h_x^2+h_z^2}{2h_x h_z^2}\right) + \frac{1}{2}(p^2+2p_x) - \frac{1}{24h_x}\left(h_x^2 p_{xx} + h_y^2 p_{yy} + h_z^2 p_{zz} + h_x^2 p p_x + h_y^2 q p_y + h_z^2 r p_z\right)\right]_0$$

$$A_4 = \frac{1}{6}\left[\left(\frac{4}{h_y}-\frac{1}{h_x}-\frac{1}{h_z}\right) - \frac{3q}{h_y} + q\left(\frac{h_x^2+h_y^2}{2h_y h_x^2}+\frac{h_x^2+h_z^2}{2h_y h_z^2}\right) + \frac{1}{2}(q^2+2q_y) - \frac{1}{24h_y}\left(h_x^2 q_{xx} + h_y^2 q_{yy} + h_z^2 q_{zz} + h_x^2 p q_x + h_y^2 q q_y + h_z^2 r q_z\right)\right]_0$$

$$A_5 = \frac{1}{6}\left[\left(\frac{4}{h_z}-\frac{1}{h_x}-\frac{1}{h_y}\right) + \frac{3r}{h_z} - r\left(\frac{h_x^2+h_z^2}{2h_z h_x^2}+\frac{h_y^2+h_z^2}{2h_z h_y^2}\right) + \frac{1}{2}(r^2+2r_z) + \frac{1}{24h_z}\left(h_x^2 r_{xx} + h_y^2 r_{yy} + h_z^2 r_{zz} + h_x^2 p r_x + h_y^2 q r_y + h_z^2 r r_z\right)\right]_0$$

$$A_6 = \frac{1}{6}\left[\left(\frac{4}{h_z}-\frac{1}{h_x}-\frac{1}{h_y}\right) - \frac{3r}{h_z} + r\left(\frac{h_x^2+h_z^2}{2h_z h_x^2}+\frac{h_y^2+h_z^2}{2h_z h_y^2}\right) + \frac{1}{2}(r^2+2r_z) - \frac{1}{24h_z}\left(h_x^2 r_{xx} + h_y^2 r_{yy} + h_z^2 r_{zz} + h_x^2 p r_x + h_y^2 q r_y + h_z^2 r r_z\right)\right]_0$$

$$A_7 = \frac{1}{12}\left[\left(\frac{1}{h_x^2}+\frac{1}{h_y^2}\right) + \frac{1}{2h_x h_y}\left(\frac{h_x^2+h_y^2}{2}pq + h_x^2 q_x + h_y^2 p_y\right) + \frac{h_x^2+h_y^2}{2h_x h_y}\left(\frac{p}{h_y}+\frac{q}{h_x}\right)\right]_0$$

$$A_8 = \frac{1}{12}[\left(\frac{1}{h_x^2}+\frac{1}{h_y^2}\right) - \frac{1}{2h_x h_y}\left(\frac{h_x^2+h_y^2}{2}pq + h_x^2 q_x + h_y^2 p_y\right) - \frac{h_x^2+h_y^2}{2h_x h_y}\left(\frac{p}{h_y}-\frac{q}{h_x}\right)]_0$$

$$A_9 = \frac{1}{12}\left[\left(\frac{1}{h_x^2}+\frac{1}{h_y^2}\right) + \frac{1}{2h_x h_y}\left(\frac{h_x^2+h_y^2}{2}pq + h_x^2 q_x + h_y^2 p_y\right) - \frac{h_x^2+h_y^2}{2h_x h_y}\left(\frac{p}{h_y}+\frac{q}{h_x}\right)\right]_0$$

$$A_{10} = \frac{1}{12}\left[\left(\frac{1}{h_x^2}+\frac{1}{h_y^2}\right) - \frac{1}{2h_x h_y}\left(\frac{h_x^2+h_y^2}{2}pq + h_x^2 q_x + h_y^2 p_y\right) + \frac{h_x^2+h_y^2}{2h_x h_y}\left(\frac{p}{h_y}-\frac{q}{h_x}\right)\right]_0$$

$$A_{11} = \frac{1}{12}\left[\left(\frac{1}{h_x^2}+\frac{1}{h_z^2}\right) + \frac{1}{2h_x h_z}\left(\frac{h_x^2+h_z^2}{2}pr + h_x^2 r_x + h_z^2 p_z\right) + \frac{h_x^2+h_z^2}{2h_x h_z}\left(\frac{p}{h_z}+\frac{r}{h_x}\right)\right]_0$$

$$A_{12} = \frac{1}{12}\left[\left(\frac{1}{h_y^2}+\frac{1}{h_z^2}\right) + \frac{1}{2h_y h_z}\left(\frac{h_y^2+h_z^2}{2}qr + h_y^2 r_y + h_z^2 q_z\right) + \frac{h_y^2+h_z^2}{2h_y h_z}\left(\frac{q}{h_z}+\frac{r}{h_y}\right)\right]_0$$

$$A_{13} = \frac{1}{12}\left[\left(\frac{1}{h_x^2}+\frac{1}{h_z^2}\right) - \frac{1}{2h_x h_z}\left(\frac{h_x^2+h_z^2}{2}pr + h_x^2 r_x + h_z^2 p_z\right) - \frac{h_x^2+h_z^2}{2h_x h_z}\left(\frac{p}{h_z}-\frac{r}{h_x}\right)\right]_0$$

$$A_{14} = \frac{1}{12}\left[\left(\frac{1}{h_y^2}+\frac{1}{h_z^2}\right) - \frac{1}{2h_y h_z}\left(\frac{h_y^2+h_z^2}{2}qr + h_y^2 r_y + h_z^2 q_z\right) - \frac{h_y^2+h_z^2}{2h_y h_z}\left(\frac{q}{h_z}-\frac{r}{h_y}\right)\right]_0$$

$$A_{15} = \frac{1}{12}\left[\left(\frac{1}{h_x^2}+\frac{1}{h_z^2}\right) - \frac{1}{2h_x h_z}\left(\frac{h_x^2+h_z^2}{2}pr + h_x^2 r_x + h_z^2 p_z\right) + \frac{h_x^2+h_z^2}{2h_x h_z}\left(\frac{p}{h_z}-\frac{r}{h_x}\right)\right]_0$$

$$A_{16}=\frac{1}{12}\left[\left(\frac{1}{h_y^2}+\frac{1}{h_z^2}\right)-\frac{1}{2h_yh_z}\left(\frac{h_y^2+h_z^2}{2}qr+h_y^2r_y+h_z^2q_z\right)+\frac{h_y^2+h_z^2}{2h_yh_z}\left(\frac{q}{h_z}-\frac{r}{h_y}\right)\right]_0$$
$$A_{17}=\frac{1}{12}\left[\left(\frac{1}{h_x^2}+\frac{1}{h_z^2}\right)+\frac{1}{2h_xh_z}\left(\frac{h_x^2+h_z^2}{2}pr+h_x^2r_x+h_z^2p_z\right)-\frac{h_x^2+h_z^2}{2h_xh_z}\left(\frac{p}{h_z}+\frac{r}{h_x}\right)\right]_0$$
$$A_{18}=\frac{1}{12}\left[\left(\frac{1}{h_y^2}+\frac{1}{h_z^2}\right)+\frac{1}{2h_yh_z}\left(\frac{h_y^2+h_z^2}{2}qr+h_y^2r_y+h_z^2q_z\right)-\frac{h_y^2+h_z^2}{2h_yh_z}\left(\frac{q}{h_z}+\frac{r}{h_y}\right)\right]_0$$

and the first and second derivatives of $p,\ q,\ r$ and f are discretized by the standard second order central difference approximation. This scheme is denoted as FDS in [20]. If letting $h_x=h_y=h_z$ and substituting the standard second order central difference approximation for the first and second derivatives of $p,\ q,\ r$ and f, the scheme (2) is equivalent to the fourth order compact (FOC) scheme derived by Zhang [19] with equal mesh size. However, this substitution is not necessary for the scheme since the first and second derivatives can be calculated in advance in the program. Recently, Ge and Zhang [22] presented a 19 point fourth order compact difference scheme for solving a general 3D linear elliptic partial differential equation by using the Maple software package.

The fourth order compact finite difference scheme (2) results in a system of linear equations of the form $Ax=b$, where A is the coefficient matrix, x is the solution vector, and b is the right-hand side vector, which includes the forcing term and boundary condition information. Each row of A corresponding to an interior node away from the boundary contains 19 nonzero entries. Those rows corresponding to the nodes next to the boundary contain fewer nonzero entries. In general, A has 19 nonzero diagonals and is usually nonsymmetric and indefinite for large cell Reynolds number Re_Δ, where Re_Δ is defined as

$$Re_\Delta=\max(\sup_{(x,y,z)\in\Omega}|p(x,y,z)|h_x,\ \sup_{(x,y,z)\in\Omega}|q(x,y,z)|h_y,\ \sup_{(x,y,z)\in\Omega}|r(x,y,z)|h_z)/2. \tag{3}$$

For $Re_\Delta\leqslant 1$, we say that Eq. (1) is diffusion dominated, otherwise it is convection dominated. For 2D convection diffusion problems with the second order central difference scheme, classical iterative methods for solving the resulting linear system do not converge when the Re_Δ is greater than a certain constant [25]. In contrast, for the fourth order compact difference scheme, classical iterative methods can still converge for large Re_Δ problems [19,25]. A rigorous convergence proof for the 2D analogous problem with constant coefficients is given in [26] and its generalization to the 3D problem is straightforward.

3. Richardson extrapolation algorithm

The finite difference discretization algorithm in [24] can be implemented by three steps: (i) computing the fourth order accurate solution on the fine and the coarse grids, (ii) applying the Richardson extrapolation technique to obtain a sixth order solution on the coarse grid, which is directly interpolated on many points of the fine grid and (iii) using an operator based interpolation scheme with the fourth order compact different scheme to obtain the sixth order solution on other points of the fine grid.

In this section, based on the idea used to compute a sixth order solution for 1D and 2D convection diffusion equations in [24], we will still use the ADI method, which is similar to a line relaxation method, to compute a sixth order approximate solution for the 3D convection diffusion equation (1).

The ADI method, first introduced by Peaceman and Rachford, is a finite difference method for solving the heat equation or the diffusion equation or to the iterative solution of the linear systems associated with usual difference approximation to the Laplace equation [27]. From then on, it is used frequently to the numerical solution of parabolic, hyperbolic and elliptic partial differential equations [28–31,24]. It can be viewed as an iterative method to solve a higher dimensional problem by solving a series of lower dimensional problems repeatedly. For the 3D case, the ADI iteration process from n to $(n+1)$ can be separated into three parts, the x-axis sweeping, the y-axis sweeping and the z-axis sweeping. The sixth order compact method in the 3D case is based on the fourth order compact difference scheme (2). The computational space contains three components Ω_h^4, Ω_{2h}^4 and Ω_h^6, where Ω_h^4 means the fourth order solution space with accuracy order $O(h_x^4+h_y^4+h_z^4)$, Ω_{2h}^4 denotes the fourth order solution space with accuracy order $O((2h_x)^4+(2h_y)^4+(2h_z)^4)$, Ω_h^6 is the sixth order solution space with accuracy order $O((2h_x)^6+(2h_y)^6+(2h_z)^6)$.

As in [24], we rewrite the fourth order compact difference scheme (2) in previous section as the following form:

$$\begin{aligned}&A^h_{i,j,k}(0)u_{i,j,k}+A^h_{i,j,k}(1)u_{i+1,j,k}+A^h_{i,j,k}(2)u_{i,j+1,k}+A^h_{i,j,k}(3)u_{i-1,j,k}+A^h_{i,j,k}(4)u_{i,j+1,k}+A^h_{i,j,k}(5)u_{i,j,k+1}+A^h_{i,j,k}(6)u_{i,j,k-1}\\&+A^h_{i,j,k}(7)u_{i+1,j+1,k}+A^h_{i,j,k}(8)u_{i-1,j+1,k}+A^h_{i,j,k}(9)u_{i-1,j-1,k}++A^h_{i,j,k}(10)u_{i+1,j-1,k}+A^h_{i,j,k}(11)u_{i+1,j,k+1}\\&+A^h_{i,j,k}(12)u_{i,j+1,k+1}+A^h_{i,j,k}(13)u_{i-1,j,k+1}+A^h_{i,j,k}(14)u_{i,j-1,k+1}+A^h_{i,j,k}(15)u_{i+1,j,k-1}+A^h_{i,j,k}(16)u_{i,j+1,k-1}\\&+A^h_{i,j,k}(17)u_{i-1,j,k-1}+A^h_{i,j,k}(18)u_{i,j-1,k-1}=F^h_{i,j,k}\end{aligned} \tag{4}$$

The Richardson extrapolation formula which is used in this study is

$$\tilde{u}^{2h}_{i,j,k}=\frac{16u^h_{2i,2j,2k}-u^{2h}_{i,j,k}}{15}. \tag{5}$$

Here the notation $A^h_{i,j,k}(0)$ is a simplified version of $A^{h_x,h_y,h_z}_{i,j,k}(0)$, and the notation $u^h_{i,j,k}$ is a simplified version of $u^{h_x,h_y,h_z}_{i,j,k}$. In fact, the mesh sizes in the three coordinate directions do not have to be equal.

Assuming that $N_x,\ N_y$ and N_z are both even numbers, one ADI iteration (from the nth to the $(n+1)$) of the sixth order algorithm based on the Richardson extrapolation technique is outlined as follows.

3.1. The x-axis sweeping

- Solve a tridiagonal linear system of the order (N_x-1) by (N_x-1) for each x-direction on the fine grid Ω^4_h, i.e.,

$$\begin{aligned}A^h_{i,j,k}(0)u^{h,*}_{i,j,k}+A^h_{i,j,k}(1)u^{h,*}_{i+1,j,k}+A^h_{i,j,k}(3)u^{h,*}_{i-1,j,k}=F^h_{i,j,k}-\Big(&A^h_{i,j,k}(2)u^{h,n}_{i,j+1,k}+A^h_{i,j,k}(4)u^{h,n}_{i,j-1,k}+A^h_{i,j,k}(5)u^{h,n}_{i,j,k+1}+A^h_{i,j,k}(6)u^{h,n}_{i,j,k-1}\\&+A^h_{i,j,k}(7)u^{h,n}_{i+1,j+1,k}+A^h_{i,j,k}(8)u^{h,n}_{i-1,j+1,k}+A^h_{i,j,k}(9)u^{h,n}_{i-1,j-1,k}+A^h_{i,j,k}(10)u^{h,n}_{i+1,j-1,k}\\&+A^h_{i,j,k}(11)u^{h,n}_{i+1,j,k+1}+A^h_{i,j,k}(12)u^{h,n}_{i,j+1,k+1}+A^h_{i,j,k}(13)u^{h,n}_{i-1,j,k+1}+A^h_{i,j,k}(14)u^{h,n}_{i,j-1,k+1}\\&+A^h_{i,j,k}(15)u^{h,n}_{i+1,j,k-1}+A^h_{i,j,k}(16)u^{h,n}_{i,j+1,k-1}+A^h_{i,j,k}(17)u^{h,n}_{i-1,j,k-1}+A^h_{i,j,k}(18)u^{h,n}_{i,j-1,k-1}\Big),\end{aligned}$$

  for the fine grid x-direction lines $j=1,2,\dots(N_y-1),\ k=1,2,\dots(N_z-1)$.

- Solve a tridiagonal linear system of the order $(N_x/2-1)$ by $(N_x/2-1)$ for each x-direction on the coarse grid Ω^4_{2h}, i.e.,

$$\begin{aligned}A^{2h}_{i,j,k}(0)u^{2h,*}_{i,j,k}+A^{2h}_{i,j,k}(1)u^{2h,*}_{i+1,j,k}+A^{2h}_{i,j,k}(3)u^{2h,*}_{i-1,j,k}=F^{2h}_{i,j,k}-(&A^{2h}_{i,j,k}(2)u^{2h,n}_{i,j+1,k}+A^{2h}_{i,j,k}(4)u^{2h,n}_{i,j-1,k}+A^{2h}_{i,j,k}(5)u^{2h,n}_{i,j,k+1}+A^{2h}_{i,j,k}(6)u^{2h,n}_{i,j,k-1}\\&+A^{2h}_{i,j,k}(7)u^{2h,n}_{i+1,j+1,k}+A^{2h}_{i,j,k}(8)u^{2h,n}_{i-1,j+1,k}+A^{2h}_{i,j,k}(9)u^{2h,n}_{i-1,j-1,k}+A^{2h}_{i,j,k}(10)u^{2h,n}_{i+1,j-1,k}\\&+A^{2h}_{i,j,k}(11)u^{2h,n}_{i+1,j,k+1}+A^{2h}_{i,j,k}(12)u^{2h,n}_{i,j+1,k+1}+A^{2h}_{i,j,k}(13)u^{2h,n}_{i-1,j,k+1}\\&+A^{2h}_{i,j,k}(14)u^{2h,n}_{i,j-1,k+1}+A^{2h}_{i,j,k}(15)u^{2h,n}_{i+1,j,k-1}+A^{2h}_{i,j,k}(16)u^{2h,n}_{i,j+1,k-1}\\&+A^{2h}_{i,j,k}(17)u^{2h,n}_{i-1,j,k-1}+A^{2h}_{i,j,k}(18)u^{2h,n}_{i,j-1,k-1}),\end{aligned}$$

  for the coarse grid x-direction lines $j=1,2,\dots(N_y/2-1),\ k=1,2,\dots(N_z/2-1)$.

- From $u^{h,*}_{2i,2j,2k}\in\Omega^4_h$ and $u^{2h,*}_{i,j,k}\in\Omega^4_{2h}$, we compute $\tilde{u}^{h,*}_{2i,2j,2k}\in\Omega^6_h$ by (4).
- From $\tilde{u}^{h,n}_{i,2j,2k-1}\in\Omega^6_h$, $\tilde{u}^{h,n}_{i,2j-1,k}\in\Omega^6_h$ and $\tilde{u}^{h,*}_{2i,2j,2k}\in\Omega^6_h$ with (3), we obtain $\tilde{u}^{h,*}_{2i-1,2j,2k}\in\Omega^6_h$.
- From $\tilde{u}^{h,*}_{i,2j,2k}\in\Omega^6_h$ and $\tilde{u}^{h,n}_{i,j,2k-1}\in\Omega^6_h$ with (3), we obtain $\tilde{u}^{h,*}_{i,2j-1,2k}\in\Omega^6_h$.
- From $\tilde{u}^{h,*}_{i,j,2k}\in\Omega^6_h$ with (3), by solving a tridiagonal linear system of the order (N_x-1) by (N_x-1) for each x-direction on the fine grid, we obtain $\tilde{u}^{h,*}_{i,j,2k-1}\in\Omega^6_h$.

3.2. The y-axis sweeping

- Solve a tridiagonal linear system of the order (N_y-1) by (N_y-1) for each y-direction on the fine grid Ω^4_h, i.e.,

$$\begin{aligned}A^h_{i,j,k}(0)u^{h,**}_{i,j,k}+A^h_{i,j,k}(2)u^{h,**}_{i,j+1,k}+A^h_{i,j,k}(4)u^{h,**}_{i,j-1,k}=F^h_{i,j,k}-(&A^h_{i,j,k}(1)u^{h,*}_{i+1,j,k}+A^h_{i,j,k}(3)u^{h,*}_{i-1,j,k}+A^h_{i,j,k}(5)u^{h,*}_{i,j,k+1}+A^h_{i,j,k}(6)u^{h,*}_{i,j,k-1}\\&+A^h_{i,j,k}(7)u^{h,*}_{i+1,j+1,k}+A^h_{i,j,k}(8)u^{h,*}_{i-1,j+1,k}+A^h_{i,j,k}(9)u^{h,*}_{i-1,j-1,k}+A^h_{i,j,k}(10)u^{h,*}_{i+1,j-1,k}\\&+A^h_{i,j,k}(11)u^{h,*}_{i+1,j,k+1}+A^h_{i,j,k}(12)u^{h,*}_{i,j+1,k+1}+A^h_{i,j,k}(13)u^{h,*}_{i-1,j,k+1}\\&+A^h_{i,j,k}(14)u^{h,*}_{i,j-1,k+1}+A^h_{i,j,k}(15)u^{h,*}_{i+1,j,k-1}+A^h_{i,j,k}(16)u^{h,*}_{i,j+1,k-1}\\&+A^h_{i,j,k}(17)u^{h,*}_{i-1,j,k-1}+A^h_{i,j,k}(18)u^{h,*}_{i,j-1,k-1}),\end{aligned}$$

  for the fine grid y-direction lines $i=1,2,\dots(N_x-1),\ k=1,2,\dots(N_z-1)$.

- Solve a tridiagonal linear system of the order $(N_y/2-1)$ by $(N_y/2-1)$ for each y-direction on the coarse grid Ω^4_{2h}, i.e.,

$$\begin{aligned}A^{2h}_{i,j,k}(0)u^{2h,**}_{i,j,k}+A^{2h}_{i,j,k}(2)u^{2h,**}_{i,j+1,k}+A^{2h}_{i,j,k}(4)u^{2h,**}_{i,j-1,k}=F^{2h}_{i,j,k}-(&A^{2h}_{i,j,k}(1)u^{2h,*}_{i+1,j,k}+A^{2h}_{i,j,k}(3)u^{2h,*}_{i-1,j,k}+A^{2h}_{i,j,k}(5)u^{2h,*}_{i,j,k+1}+A^{2h}_{i,j,k}(6)u^{2h,*}_{i,j,k-1}\\&+A^{2h}_{i,j,k}(7)u^{2h,*}_{i+1,j+1,k}+A^{2h}_{i,j,k}(8)u^{2h,*}_{i-1,j+1,k}+A^{2h}_{i,j,k}(9)u^{2h,*}_{i-1,j-1,k}+A^{2h}_{i,j,k}(10)u^{2h,*}_{i+1,j-1,k}\\&+A^{2h}_{i,j,k}(11)u^{2h,*}_{i+1,j,k+1}+A^{2h}_{i,j,k}(12)u^{2h,*}_{i,j+1,k+1}+A^{2h}_{i,j,k}(13)u^{2h,*}_{i-1,j,k+1}\\&+A^{2h}_{i,j,k}(14)u^{2h,*}_{i,j-1,k+1}+A^{2h}_{i,j,k}(15)u^{2h,*}_{i+1,j,k-1}+A^{2h}_{i,j,k}(16)u^{2h,*}_{i,j+1,k-1}\\&+A^{2h}_{i,j,k}(17)u^{2h,*}_{i-1,j,k-1}+A^{2h}_{i,j,k}(18)u^{2h,*}_{i,j-1,k-1}),\end{aligned}$$

  for the coarse grid y-direction lines $i=1,2,\dots(N_x/2-1),\ k=1,2,\dots(N_z/2-1)$.

- From $u^{h,**}_{2i,2j,2k} \in \Omega^4_h$ and $u^{2h,**}_{i,j,k} \in \Omega^4_{2h}$, we compute $\tilde{u}^{h,**}_{2i,2j,2k} \in \Omega^6_h$ by (4).
- From $\tilde{u}^{h,*}_{2i,j,2k-1} \in \Omega^6_h, \tilde{u}^{h,*}_{2i-1,j,k} \in \Omega^6_h$ and $\tilde{u}^{h,**}_{2i,2j,2k} \in \Omega^6_h$ with (3), we obtain $\tilde{u}^{h,**}_{2i,2j-1,2k} \in \Omega^6_h$.
- From $\tilde{u}^{h,**}_{2i,j,2k} \in \Omega^6_h$ and $\tilde{u}^{h,*}_{i,j,2k-1} \in \Omega^6_h$ with (3), we obtain $\tilde{u}^{h,**}_{2i-1,j,2k} \in \Omega^6_h$.
- From $\tilde{u}^{h,**}_{i,j,2k} \in \Omega^6_h$ with (3), by solving a tridiagonal linear system of the order $(N_y - 1)$ by $(N_y - 1)$ for each y-direction on the fine grid, we obtain $\tilde{u}^{h,**}_{i,j,2k-1} \in \Omega^6_h$.

3.3. The z-axis sweeping

- Solve a tridiagonal linear system of the order $(N_z - 1)$ by $(N_z - 1)$ for each z-direction on the fine grid Ω^4_h, i.e.,

$$\begin{aligned}A^h_{i,j,k}(0)u^{h,n+1}_{i,j,k} + A^h_{i,j,k}(5)u^{h,n+1}_{i,j,k+1} + A^h_{i,j,k}(6)u^{h,n+1}_{i,j,k-1} = F^h_{i,j,k} - (&A^h_{i,j,k}(1)u^{h,**}_{i+1,j,k} + A^h_{i,j,k}(2)u^{h,**}_{i,j+1,k} + A^h_{i,j,k}(3)u^{h,**}_{i-1,j,k} + A^h_{i,j,k}(4)u^{h,**}_{i,j-1,k}\\ &+ A^h_{i,j,k}(7)u^{h,**}_{i+1,j+1,k} + A^h_{i,j,k}(8)u^{h,**}_{i-1,j+1,k} + A^h_{i,j,k}(9)u^{h,**}_{i-1,j-1,k} + A^h_{i,j,k}(10)u^{h,**}_{i+1,j-1,k}\\ &+ A^h_{i,j,k}(11)u^{h,**}_{i+1,j,k+1} + A^h_{i,j,k}(12)u^{h,**}_{i,j+1,k+1} + A^h_{i,j,k}(13)u^{h,**}_{i-1,j,k+1}\\ &+ A^h_{i,j,k}(14)u^{h,**}_{i,j-1,k+1} + A^h_{i,j,k}(15)u^{h,**}_{i+1,j,k-1} + A^h_{i,j,k}(16)u^{h,**}_{i,j+1,k-1}\\ &+ A^h_{i,j,k}(17)u^{h,**}_{i-1,j,k-1} + A^h_{i,j,k}(18)u^{h,**}_{i,j-1,k-1}),\end{aligned}$$

  for the fine grid z-direction lines $i = 1, 2, \ldots (N_x - 1),\ j = 1, 2, \ldots (N_y - 1)$.

- Solve a tridiagonal linear system of the order $(N_z/2 - 1)$ by $(N_z/2 - 1)$ for each z-direction on the coarse grid Ω^4_{2h}, i.e.,

$$\begin{aligned}A^{2h}_{i,j,k}(0)u^{2h,n+1}_{i,j,k} + A^{2h}_{i,j,k}(5)u^{2h,n+1}_{i,j,k+1} + A^{2h}_{i,j,k}(6)u^{2h,n+1}_{i,j,k-1} = F^{2h}_{i,j,k} - (&A^{2h}_{i,j,k}(1)u^{2h,**}_{i+1,j,k} + A^{2h}_{i,j,k}(2)u^{2h,**}_{i,j+1,k} + A^{2h}_{i,j,k}(3)u^{2h,**}_{i-1,j,k} + A^{2h}_{i,j,k}(4)u^{2h,**}_{i,j-1,k}\\ &+ A^{2h}_{i,j,k}(7)u^{2h,**}_{i+1,j+1,k} + A^{2h}_{i,j,k}(8)u^{2h,**}_{i-1,j+1,k} + A^{2h}_{i,j,k}(9)u^{2h,**}_{i-1,j-1,k} + A^{2h}_{i,j,k}(10)u^{2h,**}_{i+1,j-1,k}\\ &+ A^{2h}_{i,j,k}(11)u^{2h,**}_{i+1,j,k+1} + A^{2h}_{i,j,k}(12)u^{2h,**}_{i,j+1,k+1} + A^{2h}_{i,j,k}(13)u^{2h,**}_{i-1,j,k+1}\\ &+ A^{2h}_{i,j,k}(14)u^{2h,**}_{i,j-1,k+1} + A^{2h}_{i,j,k}(15)u^{2h,**}_{i+1,j,k-1} + A^{2h}_{i,j,k}(16)u^{2h,**}_{i,j+1,k-1}\\ &+ A^{2h}_{i,j,k}(17)u^{2h,**}_{i-1,j,k-1} + A^{2h}_{i,j,k}(18)u^{2h,**}_{i,j-1,k-1}),\end{aligned}$$

  for the coarse grid z-direction lines $i = 1, 2, \ldots (N_x/2 - 1),\ j = 1, 2, \ldots (N_y/2 - 1)$.

- From $u^{h,n+1}_{2i,2j,2k} \in \Omega^4_h$ and $u^{2h,n+1}_{i,j,k} \in \Omega^4_{2h}$, we compute $\tilde{u}^{h,n+1}_{2i,2j,2k} \in \Omega^6_h$ by (4).
- From $\tilde{u}^{h,**}_{2i,2j-1,k} \in \Omega^6_h, \tilde{u}^{h,**}_{2i-1,j,k} \in \Omega^6_h$ and $\tilde{u}^{h,n+1}_{2i,2j,2k} \in \Omega^6_h$ with (3), we obtain $\tilde{u}^{h,n+1}_{2i,2j,2k-1} \in \Omega^6_h$.
- From $\tilde{u}^{h,n+1}_{2i,2j,k} \in \Omega^6_h$ and $\tilde{u}^{h,**}_{2i-1,j,k} \in \Omega^6_h$ with (3), we obtain $\tilde{u}^{h,n+1}_{2i,2j-1,k} \in \Omega^6_h$.
- From $\tilde{u}^{h,n+1}_{2i,j,k} \in \Omega^6_h$ with (3), by solving a tridiagonal linear system of the order $(N_z - 1)$ by $(N_z - 1)$ for each z-direction on the fine grid, we obtain $\tilde{u}^{h,n+1}_{2i-1,j,k} \in \Omega^6_h$.

The ADI iterations continue until a certain norm of the correction vector of the approximate solution is reduced to a certain tolerance.

4. Numerical experiments

We use the sixth order Richardson extrapolation discretization strategy discussed in the previous sections to solve two 3D problems, which were studied by Zhang [19]. The domain is defined as the unit cube $(0,1)^3 \subset R^3$.The right hand side function $f(x,y,z)$ and Dirichlet boundary conditions are specified to satisfy the given exact solution $u(x,y,z)$. The programs are run on a P4/2.6G personal computer and we use the Fortrann 77 programming language in double precision. We use the ADI iterations to solve all linear systems resulted from different discretization schemes. The initial approximation for all iterations is taken to be $u(x,y,z) = 0$ and the computations are terminated when the residual in the discrete L_2 norm is reduced by a factor of 10^{-14}. The maximum absolute errors are computed over all the discrete grids. The order of convergence rate of the discretization scheme is computed, as in [18,21], by

$$Order = \ln\left(\frac{error(h1)}{error(h2)}\right) \bigg/ \ln\left(\frac{h1}{h2}\right)$$

where $error(h1)$ and $error(h2)$ are the maximum absolute errors associated with mesh size $h1$ and $h2$. CPU time which excludes any time for input and output operations is derived by making use of inner function TIMEF in the Microsoft Fortran PowerStation Software.

We present numerical results for small to moderate Reynolds numbers ($Re \leqslant 10^3$), the same range as tested by several authors [32–34]. For those problems with high Re numbers (convection dominated), the solution changes much more rapidly in some direction or exhibits local behaviors, which demand finer discretization in some direction or in local domain to capture the fine details of the solution. On this aspect, high order compact schemes on uniform grids cannot exploit their superiority. So, some special strategies need to be developed to treat these problems. For example, in [7], a multilevel local mesh refinement strategy is used to deal with 2D convection diffusion singularity problems. And another example, in [21], a grid transformation technique is used to map the 3D convection diffusion equation from a graded mesh to a uniform mesh for problems with boundary Layers. The goal is to put more grid points inside the boundary layers.

4.1. Problem 1

$$p(x,y,z) = Re\sin y\sin z\cos x,$$
$$q(x,y,z) = Re\sin x\sin z\cos y,$$
$$r(x,y,z) = Re\sin x\sin y\cos z,$$

exact solution is

$$u(x,y,z) = \cos(4x + 6y + 8z).$$

4.2. Problem 2

$$p(x,y,z) = Rex(1-2y)(1-z),$$
$$q(x,y,z) = Rey(1-2z)(1-x),$$
$$r(x,y,z) = Rez(1-x)(1-y),$$

exact solution is

$$u(x,y,z) = \sin\pi x\sin\pi y\sin\pi z.$$

Table 1
Comparison of the number of the ADI iterations, the maximum absolution errors and the CPU seconds of the FOC and the REC scheme for solving the Problems 1 with $Re = 1$.

h	Zhang's FOC scheme [19]				Present REC scheme			
	Num	CPU	Error	Order	Num	CPU	Error	Order
1/8	36	0.02	2.58e−3		36	0.03	1.96e−3	
1/16	132	1.22	1.61e−4	4.00	132	2.84	6.88e−5	4.83
1/32	493	48.02	1.01e−5	4.00	494	97.12	1.58e−6	5.45
1/64	1854	1396.68	6.28e−7	4.00	1859	3239.48	2.86e−8	5.79

Table 2
Comparison of the number of the ADI iterations, the maximum absolution errors and the CPU seconds of the FOC and the REC scheme for solving the Problems 1 with $Re = 10$.

h	Zhang's FOC scheme [19]				Present REC scheme			
	Num	CPU	Error	Order	Num	CPU	Error	Order
1/8	36	0.03	4.98e−3		36	0.03	3.51e−3	
1/16	125	1.24	3.11e−4	4.00	125	2.72	1.42e−4	4.62
1/32	456	37.03	1.95e−5	3.99	457	88.94	3.67e−6	5.28
1/64	1684	1162.02	1.22e−6	4.00	1687	2842.32	6.87e−8	5.74

Table 3
Comparison of the number of the ADI iterations, the maximum absolution errors and the CPU seconds of the FOC and the REC scheme for solving the Problems 1 with $Re = 100$.

h	Zhang's FOC scheme [19]				Present REC scheme			
	Num	CPU	Error	Order	Num	CPU	Error	Order
1/8	16	0.02	5.17e−2		15	0.02	4.52e−2	
1/16	44	0.44	4.05e−3	3.68	44	1.03	3.30e−3	3.77
1/32	151	12.68	2.72e−4	3.90	151	30.59	1.19e−4	4.80
1/64	547	380.24	1.72e−5	3.98	548	930.04	2.82e−6	5.39

Tables 1–8 compare the sixth order Richardson extrapolation compact (REC) discretization method with the standard FOC scheme [19]. The maximum absolute errors, the estimated accuracy order, CPU time in seconds and the number of the ADI iterations needed to compute the approximate solution with the REC and the FOC schemes are reported. It is found that, with the same mesh size h, the REC scheme takes the same iterations as the FOC scheme, and the REC scheme is more

Table 4
Comparison of the number of the ADI iterations, the maximum absolution errors and the CPU seconds of the FOC and the REC scheme for solving the Problems 1 with $Re = 1000$.

h	Zhang's FOC scheme [19]				Present REC scheme			
	Num	CPU	Error	Order	Num	CPU	Error	Order
1/8	49	0.03	1.25e−1		49	0.05	1.25e−1	
1/16	91	0.86	2.32e−2	2.44	92	2.00	2.09e−2	2.57
1/32	74	6.14	2.60e−3	3.16	84	16.65	2.06e−3	3.35
1/64	148	104.32	1.93e−4	3.75	148	255.14	1.11e−4	4.22

Table 5
Comparison of the number of the ADI iterations, the maximum absolution errors and the CPU seconds of the FOC and the REC scheme for solving the Problems 2 with $Re = 1$.

h	Zhang's FOC scheme [19]				Present REC scheme			
	Num	CPU	Error	Order	Num	CPU	Error	Order
1/8	40	0.03	2.39e−4		40	0.05	9.86e−5	
1/16	145	1.33	1.48e−5	4.02	145	3.11	2.61e−6	5.24
1/32	544	43.82	9.22e−7	4.00	545	106.72	4.76e−8	5.78
1/64	2059	1411.25	5.76e−8	4.00	2064	3488.20	7.76e−10	5.94

Table 6
Comparison of the number of the ADI iterations, the maximum absolution errors and the CPU seconds of the FOC and the REC scheme for solving the Problems 2 with $Re = 10$.

h	Zhang's FOC scheme [19]				Present REC scheme			
	Num	CPU	Error	Order	Num	CPU	Error	Order
1/8	38	0.02	3.49e−4		37	0.03	2.03e−4	
1/16	137	1.28	2.20e−5	3.99	137	2.84	6.33e−6	5.00
1/32	513	41.53	1.37e−6	4.00	514	99.14	1.31e−7	5.59
1/64	1942	1330.25	8.61e−8	4.00	1947	3254.85	2.38e−9	5.78

Table 7
Comparison of the number of the ADI iterations, the maximum absolution errors and the CPU seconds of the FOC and the REC scheme for solving the Problems 2 with $Re = 100$.

h	Zhang's FOC scheme [19]				Present REC scheme			
	Num	CPU	Error	Order	Num	CPU	Error	Order
1/8	18	0.02	4.20e−3		17	0.02	3.70e−3	
1/16	58	0.55	3.00e−4	3.81	57	1.28	1.64e−4	4.50
1/32	209	17.25	1.92e−5	3.97	209	40.53	4.72e−6	5.12
1/64	785	540.69	1.21e−6	3.99	786	1523.25	9.71e−8	5.60

Table 8
Comparison of the number of the ADI iterations, the maximum absolution errors and the CPU seconds of the FOC and the REC scheme for solving the Problems 2 with $Re = 1000$.

h	Zhang's FOC scheme [19]				Present REC scheme			
	Num	CPU	Error	Order	Num	CPU	Error	Order
1/8	31	0.02	2.58e−2		33	0.03	2.40e−2	
1/16	42	0.41	3.32e−3	2.95	44	1.00	2.55e−3	3.24
1/32	43	4.02	2.63e−4	3.66	41	8.34	1.21e−4	4.40
1/64	115	88.02	1.74e−5	3.92	114	195.25	3.82e−6	4.98

accurate than the FOC scheme. In terms of computational cost (the CPU time) with the same mesh size h, the FOC scheme is the faster. The reason is that the FOC scheme is just performed in the single grid while REC scheme is in the two set of grids and the Richardson extrapolation and the operator interpolation also need extra time. However, if we compare a solution with comparable accuracy, the REC scheme by using a coarser mesh size is seen to be faster (in fewer CPU time) than the FOC scheme by using a finer mesh size. For instance, in Table 5, the computed solution with a maximum absolute error around 5.76×10^{-8} by the FOC scheme using $h = 1/64$, CPU time is 1411.25 s. For the REC scheme, a more accurate approximate solution with a maximum absolute error around 4.76×10^{-8}, can be computed with $h = 1/32$ and the corresponding computational cost is just 106.72 s. Similar comparison can be made other data to reach similar conclusions.

5. Concluding remarks

We extended the sixth order compact finite difference discretization strategy proposed in [24] for solving the 1D and 2D convection diffusion equations to 3D case. The present sixth order REC scheme is based on the fourth order compact difference scheme, Richardson extrapolation technique and operator interpolation scheme. ADI iteration process is designed for solving the resulting sparse linear systems. Numerical experiments are carried out to exhibit the superiority of present method, compared with the FOC scheme. When we compute a solution with comparable accuracy, the REC scheme by using a coarser mesh size is seen to be faster than the FOC scheme by using a finer mesh size.

It is worthy pointing out that the present method can be applied to solve the general 3D convection diffusion equation with Dirichlet boundary conditions. If a problem involves a derivative boundary condition such as Neumann boundary condition, we can use a one-sided finite difference approximation for the derivative as described in [35] i.e., in the approximations the odd order error terms are eliminated while the even order terms are left to be taken care of by Richardson extrapolation (more details, see [35]).

Recently, Wang and Zhang [36] proposed a sixth order finite difference discretization strategy with multigrid method and Richardson extrapolation to solve the 2D Poisson equation. They used a FOC scheme and a multiscale multigrid algorithm to compute the fourth order accurate solution on the fine and the coarse grids. Then, they applied the Richardson extrapolation technique combined an operator interpolation scheme to get the sixth order accurate solution on the fine grid. The strategy is much faster than ADI method and can also be extended to solve other partial differential equations, such as the 3D Poisson equation, 2D and 3D convection diffusion equations and incompressible Navier–Stokes equations. The research on these aspects will be reported in the future.

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