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A CLASS OF TWO-LEVEL COMPACT IMPLICIT SCHEMES FOR THREE-DIMENSIONAL UNSTEADY CONVECTION-DIFFUSION PROBLEMS

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Abstract

We derive a class of two-level high-order compact (HOC) finite difference schemes for solving three-dimensional unsteady convection-diffusion problems. The schemes are fourth-order accurate in space and second- or lower-order accurate in time depending on the choice of a weighted average parameter μ. It is shown through a discrete Fourier analysis that the schemes are unconditionally stable for $0.5 \leq \mu \leq 1$. Numerical experiments are conducted for the case $\mu = 0.5$ and the corresponding $(19, 19)$ scheme is compared to the standard Crank-Nicolson $(7, 7)$ scheme.

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1. Introduction

Partial differential equations are the basis of many models of physical, chemical and biological phenomena, and their use has also spread into economics, financial forecasting and many other fields. It is essential to approximate the solutions of these partial differential

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equations numerically in order to investigate the predictions of the mathematical models, as the exact solutions are usually unavailable.

In this paper, we shall consider the three-dimensional unsteady convection-diffusion problem for a transport variable u,

$$\alpha \frac{\partial u}{\partial t} - \Delta u + c_x \frac{\partial u}{\partial x} + c_y \frac{\partial u}{\partial y} + c_z \frac{\partial u}{\partial z} = f, \quad \text{in} \quad \Omega \times (0, T], \tag{1a}$$

$$u(x, y, z, t) = g(x, y, z, t), \quad (x, y, z) \in \partial\Omega, \quad t \in (0, T], \tag{1b}$$

$$u(x, y, z, 0) = u_0(x, y, z), \quad (x, y, z) \in \Omega, \tag{1c}$$

where $\Omega \subset \mathbb{R}^3$ is a rectangular domain, $(0, T]$ is the time interval, and f, g and u_0 are given functions of sufficient smoothness. In (1a), α is a constant and c_x, c_y and c_z are speeds of convection in the x-, y- and z-directions, respectively.

Equation (1a) may be seen in many applications to model convection-diffusion of quantities such as mass, heat, energy, vorticity etc. [21]. For example, it has been used to describe heat transfer in a draining film [10], water transfer in soils and groundwater [9, 18], flow in porous media [5, 14], the intrusion of salt water into fresh water aquifers, the spread of pollutants in rivers and streams [2, 3], and transport of pollutants in the atmosphere [29].

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Various numerical finite difference schemes have been proposed to solve convection-diffusion problems approximately. Most of these schemes are either first-order or second-order accurate in space, and have poor quality for convection dominated flows if the mesh is not sufficiently refined. Higher order discretizations are generally associated with large (non-compact) stencils which increase the bandwidth of the resulting matrix and lead to a large number of arithmetic operations, especially for higher dimensional problems.

To obtain satisfactory higher order numerical results with reasonable computational cost, there have been attempts to develop high-order compact (HOC) schemes, which utilize only the grid nodes directly adjacent to the central node. After deriving several higher order implicit schemes for unsteady one-dimensional convection-diffusion equations [16], Noye and Tan [17] proposed a compact nine-point HOC implicit scheme for unsteady 2-D convection-diffusion equations with constant coefficients. The scheme is third-order accurate in space and second-order accurate in time, and has a large zone of stability. Two other classes of compact difference schemes of order 2 in time and order 4 in space have been derived in [19, 20], with different choices of weighting parameters.

The 2-D HOC scheme proposed in [8] for solving steady-state equations was extended by Spotz and Carey to solve unsteady 1-D convection-diffusion equations with variable coefficients and 2-D diffusion equations [27]. Based on [27], classes of HOC schemes with weighted time discretization have been derived in [13] and [12] for solving unsteady 2-D convection-diffusion problems and 2-D parabolic problems with mixed derivatives, respectively. Recently, Karaa and Zhang [13] proposed a high-order ADI method for solving 2-D convection-diffusion problems. The proposed ADI method is fourth-order in space and second-order in time, and numerical experiments have been presented to test its high accuracy and to show its superiority over the standard second-order Peaceman-Rachford ADI method and the spatial third-order scheme by Noye and Tan [16].

In this paper, we propose a class of implicit high-order compact schemes for solving 3-D convection-diffusion problems. The schemes are fourth-order accurate in space and second- or lower-order accurate in time depending on the choice of a weighted average parameter μ. The case with $\mu = 0.5$ is given special attention and numerical experiments are presented to test the high accuracy of the resulting scheme and to compare it with the standard Crank-Nicolson $(7, 7)$ scheme. We mention that some numerical schemes with at most a second-order accuracy in time and in space have been examined in [4].

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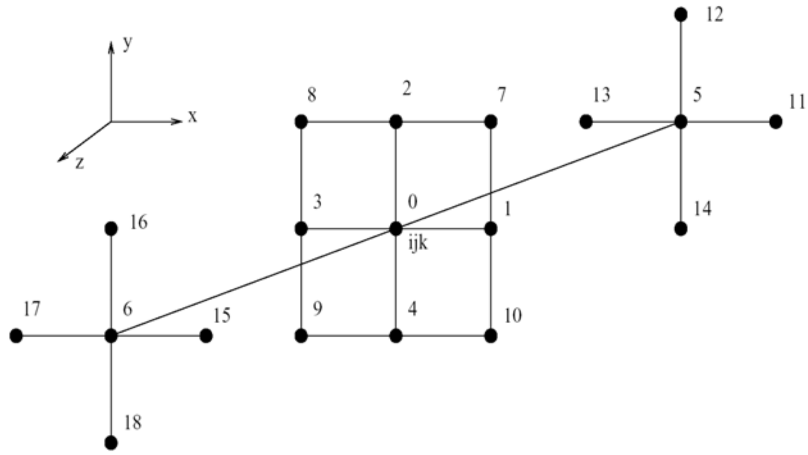

Figure 1. The 19-point stencil of the 3-D grid points in a reference cube.

2. High-order Implicit Discretization

We start by briefly discussing the derivation of HOC formulation for the steady-state form of equation (1a), which is obtained when u, the convection terms and f are independent of t. Under these conditions, (1a) becomes

$$-\Delta u + c_x \frac{\partial u}{\partial x} + c_y \frac{\partial u}{\partial y} + c_z \frac{\partial u}{\partial z} = f. \tag{2}$$

Assuming that the discretization is carried out on a uniform three-dimensional grid with a uniform mesh size h, the standard central difference approximation to equation (2) at the grid point (i, j, k) is given by

$$-\delta_x^2 u_{i,j,k} - \delta_y^2 u_{i,j,k} - \delta_z^2 u_{i,j,k} + c_x \delta_x u_{i,j,k},$$

$$+ c_y \delta_y u_{i,j,k} + c_z \delta_z u_{i,j,k} - \tau_{i,j,k} = f_{i,j,k}, \tag{3}$$

where δ_x, δ_x^2, δ_y, δ_y^2 and δ_z, δ_z^2 are the first- and second-order central difference operators in the x-, y- and z-directions, respectively. The truncation error $\tau_{i,j,k}$ is given by

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$$\tau_{i,j,k} = \frac{h^2}{12}\left[\left(2c_x \frac{\partial^3 u}{\partial x^3} - \frac{\partial^4 u}{\partial x^4}\right) + \left(2c_y \frac{\partial^3 u}{\partial y^3} - \frac{\partial^4 y}{\partial y^4}\right) + \left(2c_z \frac{\partial^3 u}{\partial z^3} - \frac{\partial^4 z}{\partial z^4}\right)\right] + O(h^4). \quad (4)$$

One way to derive high-order compact schemes is to operate on the partial differential equation (2) as an auxiliary relation to obtain second-order finite difference approximations for higher order derivatives in the truncation error. Inclusion of these expressions in the central difference approximation (3) increases the order of accuracy, typically to $O(h^4)$ while retaining a compact stencil defined by nodes surrounding the reference grid point (i, j, k). This approach was advocated by Spotz and Carey and has been used (without any symbolic computation procedure) to derive fourth-order compact approximations for 2-D convection-diffusion and 3-D Poisson equations [25, 26].

Another popular approach advocated by Gupta et al. [8], consists of expanding $u(x, y, z)$ in Taylor series at the grid point 0 as

$$u(x, y, z) = \sum_{i,j,k} a_{i,j,k} x^i y^j z^k. \quad (5)$$

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Here, we use a local truncation coordinate system where the unit grids are labeled in Fig. 1. The approximate value of a function $u(x, y, z)$ at an internal grid point (i, j, k) is denoted by u_0. The approximate values of its immediate 18 neighboring mesh points are denoted by u_l, $l = 1, 2, ..., 18$, as in Fig. 1. The convection coefficients c_x, c_y, c_z and the forcing function f are expanded in Taylor series analogously. The expansions are substituted into equation (2) to obtain a finite difference approximation of order 4. This is achieved by truncating the Taylor series to power 4 (by setting all the Taylor series coefficients $a_{i,j,k}$ to zero for $i + j + k > 4$). The procedure is straightforward but extremely tedious and requires substantial symbolic manipulations for three-dimensional problems. Some fourth-order compact finite difference schemes for the 3-D elliptic differential equations were obtained by Anantha-Krishnaiah et al. [1] using a lot of pencil and paper analysis. Several implementations with the symbolic computation packages, Mathematica and Maple, have been reported in [6, 7, 28]. The fourth-order 19-point approximation for equation (2) obtained in [28] is given by

$$\sum_{l=0}^{18} w_l u_l = F_0, \tag{6}$$

where the coefficients w_l, $l = 0, \ldots, 18,$ are given by

$$w_0 = [24 + h^2(c_{x_0}^2 + c_{y_0}^2 + c_{z_0}^2) - h(c_{x_1} - c_{x_3} + c_{y_2} - c_{y_4} + c_{z_5} c_{z_6})],$$

$$w_1 = -2 - \frac{h}{4}(2c_{x_0} - 3c_{x_1} - c_{x_2} + c_{x_3} - c_{x_4} - c_{x_5} - c_{x_6})$$

$$- \frac{h^2}{8}[4c_{x_0}^2 + c_{x_0}(c_{x_1} - c_{x_3}) + c_{y_0}(c_{x_2} - c_{x_4}) + c_{z_0}(c_{x_5} - c_{x_6})],$$

$$w_2 = -2 - \frac{h}{4}(2c_{y_0} - c_{y_1} - 3c_{y_2} - c_{y_3} + c_{y_4} - c_{y_5} - c_{y_6})$$

$$- \frac{h^2}{8}[4c_{y_0}^2 + c_{x_0}(c_{y_1} - c_{y_3}) + c_{y_0}(c_{y_2} - c_{y_4}) + c_{z_0}(c_{y_5} - c_{y_6})],$$

$$w_3 = -2 + \frac{h}{4}(2c_{x_0} + c_{x_1} - c_{x_2} - 3c_{x_3} - c_{x_4} - c_{x_5} - c_{x_6})$$

$$- \frac{h^2}{8}[4c_{x_0}^2 - c_{x_0}(c_{x_1} - c_{x_3}) - c_{y_0}(c_{x_2} - c_{x_4}) - c_{z_0}(c_{x_5} - c_{x_6})],$$

$$w_4 = -2 + \frac{h}{4}(2c_{y_0} - c_{y_1} + c_{y_2} - c_{y_3} - 3c_{y_4} - c_{y_5} - c_{y_6})$$

$$- \frac{h^2}{8}[4c_{y_0}^2 - c_{x_0}(c_{y_1} - c_{y_3}) - c_{y_0}(c_{y_2} - c_{y_4}) - c_{z_0}(c_{y_5} - c_{y_6})],$$

$$w_5 = -2 - \frac{h}{4}(2c_{z_0} - c_{z_1} - c_{z_2} - c_{z_3} - c_{z_4} - 3c_{z_5} + c_{z_6})$$

$$- \frac{h^2}{8}[4c_{z_0}^2 + c_{x_0}(c_{z_1} - c_{z_3}) + c_{y_0}(c_{z_2} - c_{z_4}) + c_{z_0}(c_{z_5} - c_{z_6})],$$

$$w_6 = -2 + \frac{h}{4}(2c_{z_0} - c_{z_1} - c_{z_2} - c_{z_3} - c_{z_4} + c_{z_5} - 3c_{z_6})$$

$$- \frac{h^2}{8}[4c_{z_0}^2 - c_{x_0}(c_{z_1} - c_{z_3}) - c_{y_0}(c_{z_2} - c_{z_4}) - c_{z_0}(c_{z_5} - c_{z_6})],$$

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$$w_7 = -1 + \frac{h}{2}(c_{x_0} + c_{y_0}) + \frac{h}{8}(c_{x_2} - c_{x_4} + c_{y_1} - c_{y_3}) - \frac{h^2}{4}c_{x_0}c_{y_0},$$

$$w_8 = -1 - \frac{h}{2}(c_{x_0} - c_{y_0}) - \frac{h}{8}(c_{x_2} - c_{x_4} + c_{y_1} - c_{y_3}) + \frac{h^2}{4}c_{x_0}c_{y_0},$$

$$w_9 = -1 - \frac{h}{2}(c_{x_0} + c_{y_0}) + \frac{h}{8}(c_{x_2} - c_{x_4} + c_{y_1} - c_{y_3}) - \frac{h^2}{4}c_{x_0}c_{y_0},$$

$$w_{10} = -1 + \frac{h}{2}(c_{x_0} - c_{y_0}) - \frac{h}{8}(c_{x_2} - c_{x_4} + c_{y_1} - c_{y_3}) + \frac{h^2}{4}c_{x_0}c_{y_0},$$

$$w_{11} = -1 + \frac{h}{2}(c_{x_0} + c_{z_0}) + \frac{h}{8}(c_{x_5} - c_{x_6} + c_{z_1} - c_{z_3}) - \frac{h^2}{4}c_{x_0}c_{z_0},$$

$$w_{12} = -1 + \frac{h}{2}(c_{x_0} + c_{z_0}) + \frac{h}{8}(c_{x_5} - c_{x_6} + c_{z_2} - c_{z_4}) - \frac{h^2}{4}c_{x_0}c_{z_0},$$

$$w_{13} = -1 - \frac{h}{2}(c_{x_0} - c_{z_0}) - \frac{h}{8}(c_{x_5} - c_{x_6} + c_{z_1} - c_{z_3}) + \frac{h^2}{4}c_{x_0}c_{z_0},$$

$$w_{14} = -1 - \frac{h}{2}(c_{x_0} - c_{z_0}) - \frac{h}{8}(c_{x_5} - c_{x_6} + c_{z_2} - c_{z_4}) + \frac{h^2}{4}c_{x_0}c_{z_0},$$

$$w_{15} = -1 + \frac{h}{2}(c_{y_0} - c_{z_0}) - \frac{h}{8}(c_{y_5} - c_{y_6} + c_{z_1} - c_{z_3}) + \frac{h^2}{4}c_{y_0}c_{z_0},$$

$$w_{16} = -1 + \frac{h}{2}(c_{y_0} - c_{z_0}) - \frac{h}{8}(c_{y_5} - c_{y_6} + c_{z_2} - c_{z_4}) + \frac{h^2}{4}c_{y_0}c_{z_0},$$

$$w_{17} = -1 - \frac{h}{2}(c_{y_0} + c_{z_0}) + \frac{h}{8}(c_{y_5} - c_{y_6} + c_{z_1} - c_{z_3}) - \frac{h^2}{4}c_{y_0}c_{z_0},$$

$$w_{18} = -1 - \frac{h}{2}(c_{y_0} + c_{z_0}) + \frac{h}{8}(c_{y_5} - c_{y_6} + c_{z_2} - c_{z_4}) - \frac{h^2}{4}c_{y_0}c_{z_0},$$

$$F_0 = \frac{h^2}{2}(6f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6)$$

$$- \frac{h^3}{4}[c_{x_0}(f_1 - f_3) + c_{y_0}(f_2 - f_4) + c_{z_0}(f_5 - f_6)].$$

Writing (6) in the operator form

$$Au_{i,j,k} = Lf_{i,j,k}, \tag{7}$$

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where A and L are, respectively, 19-point and 7-point finite difference operators, the HOC approach can be extended directly to the 3-D unsteady equation by simply replacing f by $f - \alpha(\partial u / \partial t)$ to yield

$$Au_{i,j,k} = L\left(f - \alpha \frac{\partial u}{\partial t}\right)_{i,j,k}.$$

This generates the semi-discrete problem

$$\alpha L \frac{\partial u}{\partial t}\bigg|_{i,j,k} = -Au_{i,j,k} + Lf_{i,j,k}. \tag{8}$$

Clearly any time integrator can be implemented to solve (8). Since the discretization in space is high-order, one can elect to implement high-order time integrators like the fourth-order Runge-Kutta family. But since our focus is to extend the HOC formulation to 3-D time-depending problems, a simpler time-stepping scheme would be instructive. Following [27], and differentiating at $t_\mu = (1-\mu)t^n + \mu t^{n+1}$, where $0 \leq \mu \leq 1$ and the superscript n denotes the time level, yields a class of integrators that includes the forward Euler $(\mu = 0)$, the Crank-Nicolson $(\mu = 1/2)$, and the backward Euler $(\mu = 1)$ schemes. The resulting fully discrete difference scheme for grid point (i, j, k) at time level n then becomes

$$\left(L + \mu \frac{\Delta t}{\alpha} A\right) u_{i,j,k}^{n+1} = \left(L - (1-\mu)\frac{\Delta t}{\alpha} A\right) u_{i,j,k}^{n} + \frac{\Delta t}{\alpha}((1-\mu)Lf_{i,j,k}^{n} + \mu Lf_{i,j,k}^{n+1}). \tag{9}$$

The accuracy of the scheme is $O((\Delta t)^s, h^4)$, with $s \leq 2$, and it should be noted that for $\mu = 0.5$, the difference stencil requires 19 points in both the nth and $(n+1)$th time levels resulting in what may be called a $(19, 19)$ scheme. Similarly, a $(19, 7)$ and a $(7, 19)$ schemes are obtained for $\mu = 0$ and $\mu = 1$, respectively.

The high-order implicit discretization (9) results in a system of linear equations of the form

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$$BU = b, \tag{10}$$

where B is the coefficient matrix, U is the solution vector at time level $(n+1)$, and b is the right hand side including boundary condition information. The implementation of Dirichlet boundary conditions is straightforward due to the compactness of the schemes. Each row of B corresponding to an interior node away from the boundary contains at most 19 nonzero elements. Those rows corresponding to the nodes next to the boundary contain fewer than 19 nonzero elements. Neumann boundary conditions can also be implemented as is done in [27] and [11] for the 1-D and 2-D cases, respectively. In general, the matrix B is of large size and has at most 19 nonzero diagonals, so it is very sparse.

In order to compute a numerical solution for the three-dimensional convection-diffusion problem, the sparse linear system (10) is solved at each time step with the same coefficient matrix and a different right hand side. Thus, the total computational cost is dominated by the way this linear system is solved. Direct solution methods based on Gaussian elimination are usually not practical for large size problems due to the excessive requirements on computer memory and CPU time. We propose then to use a Krylov subspace method coupled with a robust preconditioner so that (10) can be solved in a few iterations at each time. We mainly focus on GMRES, a minimal residual algorithm based on the use of the Arnoldi process [22, 23], coupled with an incomplete LU factorization based preconditioner. Incomplete LU factorization has been one of the best known preconditioning techniques used to improve the convergence of GMRES [15, 22].

To study the stability of the two-level difference scheme (9), we use the von Neumann linear stability analysis assuming that the convection terms to be constants and the forcing function f to be zero in (1a). If we let $u_{i,j,k}^n = b^n e^{I\theta_x i} e^{I\theta_y j} e^{I\theta_z k}$ to be the value of u^n at node (i, j, k), where $I = \sqrt{-1}$, b^n is the amplitude at time level n, and $\theta_x (= 2\pi\Delta x/\Lambda_1)$, $\theta_y (= 2\pi\Delta y/\Lambda_2)$ and $\theta_z (= 2\pi\Delta z/\Lambda_3)$ are phase angles with wavelengths Λ_1, Λ_2 and Λ_3, respectively, the amplification factor $\xi(\theta_x, \theta_y, \theta_z) =$

b^{n+1}/b^n, for stability, has to satisfy the relation

$$|\xi(\theta_x, \theta_y, \theta_z)| \le 1,$$

for all θ_x, θ_y and θ_z in $[-\pi, \pi]$. The amplification factor ξ can then be found by substituting the expressions for u_{ij}^n and u_{ij}^{n+1} in (9), and following the approach used in [27] and [11], the stability criterion of the scheme becomes

$$(1 - 2\mu) \le \frac{2h^2\alpha}{\Delta t[(4 + h^2c_x^2) + (4 + h^2c_y^2) + (4 + h^2c_z^2)]}. \tag{11}$$

This shows that the scheme is unconditionally stable for $0.5 \le \mu \le 1$, since the left-hand side in (11) becomes negative, but conditionally stable for $0 \le \mu < 0.5$.

3. Numerical Experiments

In this section, two numerical examples are carried out. We fix our attention on the case where $\mu = 0.5$ and compare the resulting $(19, 19)$ scheme with the classical second-order $(7, 7)$ difference scheme, which uses central difference in space and Crank-Nicolson type integration in time.

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We first consider a three-dimensional diffusion problem in the cubic region $[0, 1] \times [0, 1] \times [0, 1]$. We set $c_x = c_y = c_z = 0$ and properly select the forcing function f so that the exact solution for this test problem is

$$u(x, y, z, t) = e^{-\pi^2 t} \sin(\pi x)\sin(\pi y)\sin(\pi z).$$

The initial and Dirichlet boundary conditions are set to satisfy this solution. We consider uniform grids with different mesh sizes and compare the accuracy of the computed solutions from the present $(19, 19)$ scheme and the classical $(7, 7)$ difference scheme. The quantity that we compare is the L^2-norm error of the computed solution with respect to the exact solution. We choose a time step $\Delta t = 0.001$ and $T = 1$ for the entire simulation process.

In Fig. 2, we plot the L^2-norm errors at each time step in each case. The figure shows the superiority of the present scheme over the $(7, 7)$ scheme. The error obtained on an 11×11 grid is much smaller than the one obtained using $(7, 7)$ scheme on a 41×41 grid.

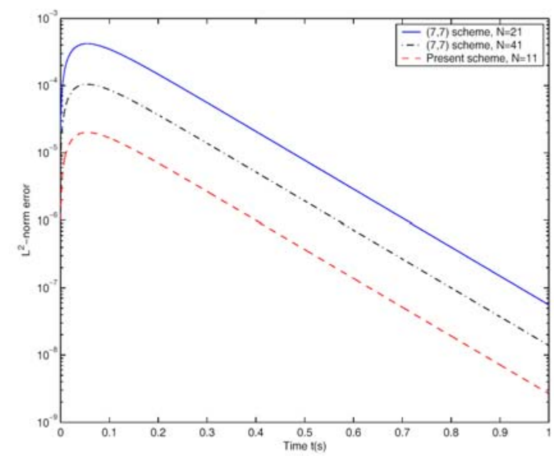

Figure 2. Comparison of the L^2-norm errors produced by the present $(19, 19)$ scheme and the $(7, 7)$ scheme at each time step.

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To further study the validity and effectiveness of the new high-order scheme, we solve a convection-diffusion problem defined in the cubic region $[0, 2] \times [0, 2] \times [0, 2]$, with an analytical solution given, as in [4], by

$$u(x, y, z, t)$$

$$= \frac{1}{(4t+1)^{3/2}} \exp\left[-\frac{(x - \tilde{c}_x t - 0.5)^2}{\alpha^{-1}(4t+1)} - \frac{(y - \tilde{c}_y t - 0.5)^2}{\alpha^{-1}(4t+1)} - \frac{(z - \tilde{c}_z t_z - 0.5)^2}{\alpha^{-1}(4t+1)}\right],$$

where $\tilde{c}_x = c_x/\alpha$, $\tilde{c} = c_y/\alpha$ and $\tilde{c}_z = c_z/\alpha$. The Dirichlet boundary and the initial conditions are directly taken from this exact solution. We choose $\alpha = 100$, $c_x = c_y = c_z = 80$ as in [16] and [4], and we let $T = 1.25$ for the entire simulation process.

Table 1. Errors at $t = 1.25s$ and CPU times delivered by the difference schemes, with $\Delta t = 0.001$ and $\Delta x = \Delta y = \Delta z = 0.05$

Scheme	L^2-norm error	Maximum |error|	CPU time (s)
(7, 7) scheme	2.17×10^{-3}	1.41×10^{-2}	1708
(9, 9) scheme	3.19×10^{-4}	2.29×10^{-3}	4293

Table 1 presents the L^2-norm errors and the maximum absolute errors evaluated at $t = 1.25$ for the present scheme and the (7, 7) scheme, with the total elapsed time (CPU) in seconds delivered in each case. The results show that the present scheme provides high accuracy solution. The detail of the convergence history of each scheme is shown in Fig. 3, where we plot the L^2-norm errors at each time step for the entire simulation process. It is seen that the two errors show similar behaviors with the error of the present scheme remaining smaller than the other error at every time step.

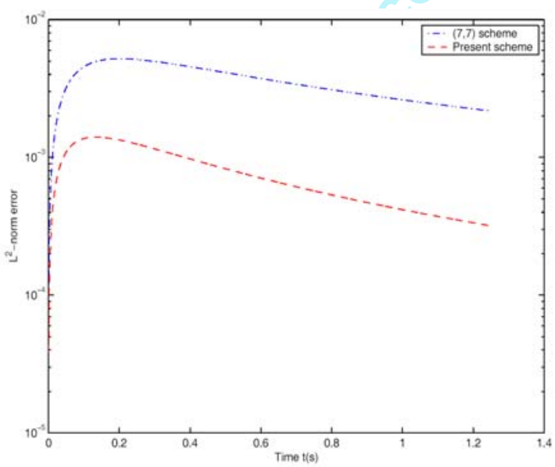

Figure 3. Comparison of the L^2-norm errors produced by the difference schemes at each time step.

We also remark that the improvement in accuracy comes at a higher cost of computations and storage. This is due in part to the fact that, since the sparse matrix arising from the $(7, 7)$ scheme has only 7 nonzero diagonals, performing a matrix-vector product using the present $(19, 19)$ scheme is almost three times expensive as using the $(7, 7)$ scheme. We have also observed that, at each time level, the iterative solver took six iterations to converge in the case of present $(19, 19)$ scheme compared to three iterations in the other case. We believe that developing an ADI solution method in the case of the $(9, 9)$ scheme would significantly decrease the overall execution time and produce a very efficient solver. We finally notice that the sparse linear systems arising from both discretization schemes are solved using GMRES coupled with the ILU(1) preconditioner. At each time level, the iterations are terminated when the 2-norm of the relative residual is reduced by a factor of 10^7, and we did not take the advantage of using the current solution on each time level as an initial guess for the next time level.

4. Concluding Remarks

In this paper, we present a class of implicit high-order compact schemes for solving 3-D convection-diffusion problems. The schemes are fourth-order accurate in space and second- or lower-order accurate in time depending on the choice of a weighted average parameter μ. It is shown through a discrete Fourier analysis that the schemes are unconditionally stable for $0.5 \leq \mu \leq 1$. Numerical examples supporting our theoretical analysis are provided. The improvement in accuracy comes at a higher cost of computations and storage. Developing an ADI solution method would significantly decrease the overall execution time and produce a very efficient solver.

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