Fourth-Order Compact Schemes for Solving Multidimensional Heat Problems with Neumann Boundary Conditions

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In this article, two sets of fourth-order compact finite difference schemes are constructed for solving heat-conducting problems of two or three dimensions, respectively. Both problems are with Neumann boundary conditions. These works are extensions of our earlier work (Zhao et al., Fourth order compact schemes of a heat conduction problem with Neumann boundary conditions, Numerical Methods Partial Differential Equations, to appear) for the one-dimensional case. The local one-dimensional method is employed to construct these two sets of schemes, which are proved to be globally solvable, unconditionally stable, and convergent. Numerical examples are also provided. © 2007 Wiley Periodicals, Inc. Numer Methods Partial Differential Eq 24: 165–178, 2008

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I. INTRODUCTION

In this article, two sets of fourth-order compact finite difference schemes for heat-conducting problems of two or three dimensions are studied, respectively. Both problems are with Neumann boundary conditions. These works are extensions of our earlier work reported in [1].

What makes these two sets of schemes different from many others, such as those reported in [2] and [3–14], is that they are uniformly fourth-order at both interior and boundary points. The LOD method is used so that the schemes are constructed through a sequence of two or three one-dimensional equations. Moreover, they are proved to be globally solvable, unconditionally stable with respect to initial data, and convergent. Numerical examples are also provided.

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The two sets of schemes are derived based on the following two-dimensional problem:

$$\begin{aligned} U_t &= U_{xx} + U_{yy} + F(x,y,t), \quad 0 < x,y < 1, \ t > 0, \\ U(x,y,0) &= U_0(x,y), \\ U_x(0,y,t) &= \alpha_1(y,t), \quad U_x(1,y,t) = \alpha_2(y,t), \\ U_y(x,0,t) &= \beta_1(x,t), \quad U_y(x,1,t) = \beta_2(x,t); \end{aligned} \tag{1}$$

and the following three-dimensional problem:

$$\begin{aligned} U_t &= U_{xx} + U_{yy} + U_{zz} + F(x,y,z,t), \quad 0 < x,y,z < 1, \ t > 0, \\ U(x,y,z,0) &= U_0(x,y,z), \\ U_x(0,y,z,t) &= \alpha_1(y,z,t), \quad U_x(1,y,z,t) = \alpha_2(y,z,t), \\ U_y(x,0,z,t) &= \beta_1(x,z,t), \quad U_y(x,1,z,t) = \beta_2(x,z,t), \\ U_z(x,y,0,t) &= \gamma_1(x,y,t), \quad U_z(x,y,1,t) = \gamma_2(x,y,t), \end{aligned} \tag{2}$$

where $\alpha_1(\cdot,t), \alpha_2(\cdot,t); \beta_1(\cdot,t), \beta_2(\cdot,t); \gamma_1(\cdot,t)$, and $\gamma_2(\cdot,t)$ are reasonably smooth functions of two or three space variables.

Here is the outline of the article. In Section II, a set of fourth-order compact schemes for the two-dimensional case is derived. Its solvability, stability, and convergence results are shown in Section III. Since the detail in proving these properties for the 2D and 3D cases is similar to each other, in Section IV, we only list the set of schemes for the 3D case. In Section V, numerical examples are provided to test the accuracy for the set of schemes in the 2D case.

II. A SET OF COMPACT SCHEMES FOR 2D CASE

Assume that the space meshes for both x and y directions are the same, which is denoted by h and assumed to satisfy $(M+1)h = 1$ for a positive integer M. $\triangle t$ denotes the time increment, and $u_{i,j}^m$, $(u_{xx})_{i,j}^m$, and $(u_{yy})_{i,j}^m$ are used to represent the approximations of $U(x_i, y_j, t^m)$, $U_{xx}(x_i, y_j, t^m)$, and $U_{yy}(x_i, y_j, t^m)$, respectively, where $U(x,y,t)$ is the exact solution of (1). i, j, and m are used to denote the discrete x, y space, and time indexes, respectively, where $0 \le i, j \le M+1$ and $m \ge 0$. Please take a note that m represents a positive constant, which may not be an integer.

Using the LOD method reported in [2], we first separate the following equation:

$$U_t = U_{xx} + U_{yy} + F(x,y,t)$$

into the following two one-dimensional equations:

$$\frac{1}{2}U_t = U_{xx} + \frac{1}{2}F(x,y,t); \quad \frac{1}{2}U_t = U_{yy} + \frac{1}{2}F(x,y,t). \tag{3}$$

We then apply the well-known Crank–Nicolson method to the above two equations and obtain the following two discrete equations:

$$\frac{1}{2}\frac{u_{i,j}^{m+\frac{1}{2}}-u_{i,j}^{m}}{\frac{\triangle t}{2}}=\frac{1}{2}\left((u_{xx})_{i,j}^{m+\frac{1}{2}}+(u_{xx})_{i,j}^{m}\right)+\frac{1}{2}F_{i,j}^{m+\frac{1}{4}}, \tag{4}$$

$$\frac{1}{2}\frac{u_{i,j}^{m+1}-u_{i,j}^{m+\frac{1}{2}}}{\frac{\triangle t}{2}}=\frac{1}{2}\left((u_{yy})_{i,j}^{m+1}+(u_{yy})_{i,j}^{m+\frac{1}{2}}\right)+\frac{1}{2}F_{i,j}^{m+\frac{3}{4}}, \tag{5}$$

where

$$F_{i,j}^{m+\frac{1}{4}}=\frac{1}{2}\left(F(x_i,y_j,t^m)+F(x_i,y_j,t^{m+\frac{1}{2}})\right), \tag{6}$$

or

$$\begin{aligned} F_{i,j}^{m+\frac{1}{4}}&=F\left(x_i,y_j,t^{m+\frac{1}{4}}\right),\\ F_{i,j}^{m+\frac{3}{4}}&=\frac{1}{2}\left(F\left(x_i,y_j,t^{m+\frac{1}{2}}\right)+F(x_i,y_j,t^{m+1})\right), \end{aligned} \tag{7}$$

or

$$F_{i,j}^{m+\frac{3}{4}}=F\left(x_i,y_j,t^{m+\frac{3}{4}}\right).$$

According to the result of Crank–Nicolson method, the truncation errors of (4) and (5) are order of $\triangle t^2$ in time.

Applying the results in [1] to $\{(u_{xx})_{i,j}^{m}\}$, $\{(u_{xx})_{i,j}^{m+\frac{1}{2}}\}$, $\{(u_{yy})_{i,j}^{m+\frac{1}{2}}\}$, $\{(u_{yy})_{i,j}^{m+1}\}$ in (4) and (5), we obtain the following three schemes for both interior and boundary points, which provide fourth-order approximations to $\{(u_{xx})_{i,j}^{m+\frac{1}{2}}\}$ and $\{(u_{xx})_{i,j}^{m}\}$ in (4)

$$\frac{1}{10}(u_{xx})_{i-1,j}^{m}+(u_{xx})_{i,j}^{m}+\frac{1}{10}(u_{xx})_{i+1,j}^{m}=\frac{6}{5h^2}\left(u_{i-1,j}^{m}-2u_{i,j}^{m}+u_{i+1,j}^{m}\right),\quad 2\le i\le M-1,\ 1\le j\le M; \tag{8}$$

$$\frac{11}{6}(u_{xx})_{1,j}^{m}-\frac{1}{3}(u_{xx})_{2,j}^{m}=-\frac{\alpha_1(y_j,t^m)}{h}+\frac{u_{2,j}^{m}-u_{1,j}^{m}}{h^2},\quad 1\le j\le M; \tag{9}$$

$$\frac{11}{6}(u_{xx})_{M,j}^{m}-\frac{1}{3}(u_{xx})_{M-1,j}^{m}=\frac{\alpha_2(y_j,t^m)}{h}+\frac{u_{M-1,j}^{m}-u_{M,j}^{m}}{h^2},\quad 1\le j\le M; \tag{10}$$

and the next three schemes for both interior and boundary points, which provide fourth-order approximations to $\{(u_{yy})_{i,j}^{m+1}\}$ and $\{(u_{yy})_{i,j}^{m+\frac{1}{2}}\}$ in (5)

$$\frac{1}{10}(u_{yy})_{i,j-1}^{m}+(u_{yy})_{i,j}^{m}+\frac{1}{10}(u_{yy})_{i,j+1}^{m}=\frac{6}{5h^2}\left(u_{i,j-1}^{m}-2u_{i,j}^{m}+u_{i,j+1}^{m}\right),\quad 1\le i\le M,\ 2\le j\le M-1; \tag{11}$$

$$\frac{11}{6}(u_{yy})_{i,1}^{m}-\frac{1}{3}(u_{yy})_{i,2}^{m}=-\frac{\beta_1(x_i,t^m)}{h}+\frac{u_{i,2}^{m}-u_{i,1}^{m}}{h^2},\quad 1\le i\le M; \tag{12}$$

$$\frac{11}{6}(u_{yy})_{i,M}^{m}-\frac{1}{3}(u_{yy})_{i,M-1}^{m}=\frac{\beta_2(x_i,t^m)}{h}+\frac{u_{i,M-1}^{m}-u_{i,M}^{m}}{h^2},\quad 1\le i\le M. \tag{13}$$

From the above derivation, it can be seen that the new set of schemes, (4)–(13), has a truncation error of order $\triangle t^2 + h^4$ in time and space, and hence, it is consistent with the original differential equations.

To express the set of schemes (4)–(13) into vector forms, we first define the following six vectors of M^2 dimensions; and the two block matrices of $M^2 \times M^2$ dimensions:

$$\begin{aligned}
\vec{u}^m &= \left(u^m_{1,1}, u^m_{2,1}, \ldots, u^m_{M,1}; \quad \ldots; \quad u^m_{1,M}, u^m_{2,M}, \ldots, u^m_{M,M}\right)^T, \\
\vec{u}^m_{xx} &= \left((u_{xx})^m_{1,1}, (u_{xx})^m_{2,1}, \ldots, (u_{xx})^m_{M,1}; \quad \ldots; \quad (u_{xx})^m_{1,M}, (u_{xx})^m_{2,M}, \ldots, (u_{xx})^m_{M,M}\right)^T, \\
\vec{u}^m_{yy} &= \left((u_{yy})^m_{1,1}, (u_{yy})^m_{1,2}, \ldots, (u_{yy})^m_{1,M}; \quad \ldots; \quad (u_{yy})^m_{M,1}, (u_{yy})^m_{M,2}, \ldots, (u_{yy})^m_{M,M}\right)^T,
\end{aligned} \tag{14}$$

$$\begin{aligned}
\vec{\alpha}(t^m) &= \left(-\frac{\alpha_1(y_1, t^m)}{h}, \ldots, -\frac{\alpha_2(y_M, t^m)}{h}; \quad \ldots; \quad -\frac{\alpha_1(y_1, t^m)}{h}, \ldots, -\frac{\alpha_2(y_M, t^m)}{h}\right)^T, \\
\vec{\beta}(t^m) &= \left(-\frac{\beta_1(x_1, t^m)}{h}, \ldots, -\frac{\beta_2(x_M, t^m)}{h}; \quad \ldots; \quad -\frac{\beta_1(x_1, t^m)}{h}, \ldots, -\frac{\beta_2(x_M, t^m)}{h}\right)^T,
\end{aligned}$$

$$\vec{F}^m = \left(F^m_{1,1}, F^m_{2,1}, \ldots, F^m_{M,1}; \quad \ldots; \quad F^m_{1,M} F^m_{2,M} \ldots, F^m_{M,M}\right)^T,$$

$$\text{and } A_b = \begin{bmatrix} A & & & \\ & A & & \\ & & \ddots & \\ & & & A \end{bmatrix}_{M^2 \times M^2}, \quad B_b = \begin{bmatrix} B & & & \\ & B & & \\ & & \ddots & \\ & & & B \end{bmatrix}_{M^2 \times M^2},$$

where A and B are the following two $M \times M$ matrices obtained in [1]:

$$A = \begin{bmatrix} 22 & -4 & & & \\ 1 & 10 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 10 & 1 \\ & & & -4 & 22 \end{bmatrix}_{M \times M}, \quad B = \begin{bmatrix} 6 & -6 & & & \\ -6 & 12 & -6 & & \\ & \ddots & \ddots & \ddots & \\ & & -6 & 12 & -6 \\ & & & -6 & 6 \end{bmatrix}_{M \times M}. \tag{15}$$

Furthermore, we let matrix P denote the $M^2 \times M^2$ permutation matrix such that:

$$\begin{aligned}
P\vec{u}^m &= P\left(u^m_{1,1}, u^m_{2,1}, \ldots, u^m_{M,1}; \quad \ldots; \quad u^m_{1,M}, u^m_{2,M}, \ldots, u^m_{M,M}\right)^T \\
&= \left(u^m_{1,1}, u^m_{1,2}, \ldots, u^m_{1,M}; \quad \ldots; \quad u^m_{M,1}, u^m_{M,2}, \ldots, u^m_{M,M}\right)^T.
\end{aligned} \tag{16}$$

It should be pointed out that the elements of vectors $\vec{u}^m$ and $\vec{u}^m_{xx}$ are arranged in M sectors according to their rows, while elements of $\vec{u}^m_{yy}$ and $P\vec{u}^m$ are arranged in the same number of sectors according to their columns.

Thus, the set of schemes (4)–(13) can be expressed into the following vector forms at a time level t^m:

$$\vec{u}^{m+\frac{1}{2}} = \vec{u}^m + \frac{\triangle t}{2}\left(\vec{u}_{xx}^m + \vec{u}_{xx}^{m+\frac{1}{2}}\right) + \frac{\triangle t}{2}\vec{F}^{m+\frac{1}{4}}, \tag{17}$$

$$\frac{1}{10}A_{\mathrm{b}}\vec{u}_{xx}^m = -\frac{1}{5h^2}B_{\mathrm{b}}\vec{u}^m + \frac{6}{5}\vec{\alpha}(t^m), \tag{18}$$

$$\frac{1}{10}A_{\mathrm{b}}\vec{u}_{xx}^{m+\frac{1}{2}} = -\frac{1}{5\,h^2}B_{\mathrm{b}}\vec{u}^{m+\frac{1}{2}} + \frac{6}{5}\vec{\alpha}\left(t^{m+\frac{1}{2}}\right), \tag{19}$$

and

$$\frac{1}{10}A_{\mathrm{b}}\vec{u}_{yy}^{m+\frac{1}{2}} = -\frac{1}{5\,h^2}B_{\mathrm{b}}P\vec{u}^{m+\frac{1}{2}} + \frac{6}{5}\vec{\beta}\left(t^{m+\frac{1}{2}}\right), \tag{20}$$

$$\frac{1}{10}A_{\mathrm{b}}\vec{u}_{yy}^{m+1} = -\frac{1}{5h^2}B_{\mathrm{b}}P\vec{u}^{m+1} + \frac{6}{5}\vec{\beta}(t^{m+1}), \tag{21}$$

$$P\vec{u}^{m+1} = P\vec{u}^{m+\frac{1}{2}} + \frac{\triangle t}{2}\left(\vec{u}_{yy}^{m+1} + \vec{u}_{yy}^{m+\frac{1}{2}}\right) + \frac{\triangle t}{2}\vec{F}^{m+\frac{3}{4}}. \tag{22}$$

Here A_{b} is invertible since A_{b} is a block-matrix of A, and A is invertible which is shown in [1](see the Appendix).

III. SOLVABILITY, STABILITY AND CONVERGENCE FOR THE 2D CASE

A. Solvability

Assume that $\left\{u_{i,j}^m\right\}$ have been obtained for $0 \le m \le n$. The following two steps show that they can be advanced to the next level $\left\{u_{i,j}^{n+1}\right\}$.

Step 1. $\left\{u_{i,j}^n\right\} \to \left\{u_{i,j}^{n+\frac{1}{2}}\right\}$

We substitute $\left\{u_{i,j}^n\right\}$ into (17), (18), and (19), which can be combined into the following vector form:

$$\vec{u}^{n+\frac{1}{2}} = \vec{u}^n + \frac{\triangle t}{2}\left(-\frac{2}{h^2}A_{\mathrm{b}}^{-1}B_{\mathrm{b}}\right)\left(\vec{u}^{n+\frac{1}{2}} + \vec{u}^n\right) + \frac{\triangle t}{2}12A_{\mathrm{b}}^{-1}\left(\vec{\alpha}\left(t^{n+\frac{1}{2}}\right) + \vec{\alpha}(t^n)\right) + \frac{\triangle t}{2}\vec{F}^{n+\frac{1}{4}}. \tag{23}$$

(23) can be further simplified to the next form:

$$\left(I + rA_{\mathrm{b}}^{-1}B_{\mathrm{b}}\right)\vec{u}^{n+\frac{1}{2}} = \left(I - rA_{\mathrm{b}}^{-1}B_{\mathrm{b}}\right)\vec{u}^n + 6\triangle tA_{\mathrm{b}}^{-1}\left(\vec{\alpha}(t^{n+\frac{1}{2}}\right) + \vec{\alpha}(t^n)) + \frac{\triangle t}{2}\vec{F}^{n+\frac{1}{4}}, \tag{24}$$

where $r = \frac{\triangle t}{h^2}$.

From Lemma 1 in [1] (see the Appendix), which shows that the eigenvalues of $A^{-1}B$ are real and non-negative, one may see that the eigenvalues of $A_{\mathrm{b}}^{-1}B_{\mathrm{b}}$ are real and non-negative since $A_{\mathrm{b}}^{-1}B_{\mathrm{b}}$ is a block-matrix of $A^{-1}B$. Hence, $I + rA_{\mathrm{b}}^{-1}B_{\mathrm{b}}$ is invertible because all its eigenvalues are real and in the form: $1 + r\lambda_{A_b^{-1}B_b}$, which are strictly positive. This proves that the system equations in (24) are solvable, and thus, $\{u_{i,j}^{n+\frac{1}{2}}\}$ can be obtained from $\{u_{i,j}^n\}$.

Step 2. $\{u_{i,j}^{n+\frac{1}{2}}\} \to \{u_{i,j}^{n+1}\}$

Once $\{u_{i,j}^{n+\frac{1}{2}}\}$ are obtained in Step 1, we substitute them into (20)–(22), which are combined into the following vector form:

$$\left(I + rA_b^{-1}B_b\right)P\vec{u}^{n+1} = \left(I - rA_b^{-1}B_b\right)P\vec{u}^{n+\frac{1}{2}} + 6\triangle t A_b^{-1}\left(\vec{\beta}(t^{n+\frac{1}{2}}) + \vec{\beta}(t^n)\right) + \frac{\triangle t}{2}\vec{F}^{n+\frac{3}{4}}. \quad (25)$$

Because $I + rA_b^{-1}B_b$ is invertible, (25) shows that the system equations in (25) are solvable. That is to say that $\{u_{i,j}^{n+1}\}$ can be obtained from $\{u_{i,j}^{n+\frac{1}{2}}\}$. These two steps show that $\{u_{i,j}^m\}$, $(0 \le m \le n)$, can be advanced to $\{u_{i,j}^{n+1}\}$.

B. Stability

Assume that $\vec{u}_1^m, \vec{u}_2^m$ are two solutions of (4)–(13) with different initial data sets, but the same function F and same boundary conditions. Then, $\vec{\theta}^m = \vec{u}_1^m - \vec{u}_2^m, \vec{\theta}^{m+\frac{1}{2}} = \vec{u}_1^{m+\frac{1}{2}} - \vec{u}_2^{m+\frac{1}{2}}$, and $\vec{\theta}^{m+1} = \vec{u}_1^{m+1} - \vec{u}_2^{m+1}$ satisfy the following relations:

$$\begin{aligned}\left(I + rA_b^{-1}B_b\right)\vec{\theta}^{m+\frac{1}{2}} &= \left(I - rA_b^{-1}B_b\right)\vec{\theta}^m,\\ \left(I + rA_b^{-1}B_b\right)P\vec{\theta}^{m+1} &= \left(I - rA_b^{-1}B_b\right)P\vec{\theta}^{m+\frac{1}{2}}. \end{aligned} \quad (26)$$

By eliminating the intermedium term $\vec{\theta}^{m+\frac{1}{2}}$ in (26), we obtain that:

$$\vec{\theta}^{m+1} = P^{-1}\left(I + rA_b^{-1}B_b\right)^{-1}\left(I - rA_b^{-1}B_b\right)P\left(I + rA_b^{-1}B_b\right)^{-1}\left(I - rA_b^{-1}B_b\right)\vec{\theta}^m. \quad (27)$$

Theorem 1. *The set of schemes,* (4)–(13)*, is unconditionally stable with respect to the initial data. This implies that no restriction on the ratio r is required.*

Proof. Since P, P^{-1} are permutation matrices obtained from the identity matrix I, they satisfy the following results:

$$\lambda_\sigma(P) = 1, \quad \lambda_\sigma(P^{-1}) = 1. \quad (28)$$

Here, $\lambda_\sigma(C)$ represents the spectral radius of a matrix C. According to the result obtained in [1], the following result is true.

$$\lambda_\sigma\left(\left(I + rA_b^{-1}B_b\right)^{-1}\left(I - rA_b^{-1}B_b\right)\right) \le 1. \quad (29)$$

According to a result stated in [15] (see the Appendix), we have the following results:

$$\|P\|_\epsilon \le 1 + \epsilon, \quad \|P^{-1}\|_\epsilon \le 1 + \epsilon, \quad (30)$$

$$\left\|\left(I + rA_b^{-1}B_b\right)^{-1}\left(I - rA_b^{-1}B_b\right)\right\|_\epsilon \le 1 + \epsilon, \quad (31)$$

where ϵ is a positive constant, and $\|\cdot\|_\epsilon$ represents a matrix norm corresponding to ϵ.

Thus, by applying (30) and (31), we obtain the next result: At any fixed time level t^n, where $t^n \le T$, we have that:

$$\begin{aligned}\|\vec{\theta}^n\|_\epsilon &\le \|P^{-1}\|_\epsilon \left\| \left(I + rA_b^{-1}B_b\right)^{-1}\left(I - rA_b^{-1}B_b\right)\right\|_\epsilon^2 \|P\|_\epsilon \|\vec{\theta}^{n-1}\|_\epsilon \\ &\le (1+\epsilon)^4 \|\vec{\theta}^{n-1}\|_\epsilon \\ &\quad\vdots \\ &\le (1+\epsilon)^{4n}\|\vec{\theta}^0\|_\epsilon. \end{aligned} \tag{32}$$

If ϵ is taken to be $\triangle t$, we then obtain from (32) that:

$$\begin{aligned}\|\vec{\theta}^n\|_{\triangle t} &\le [(1+\triangle t)^n]^4 \|\vec{\theta}^0\|_{\triangle t} \\ &\le e^{4n\triangle t}\|\vec{\theta}^0\|_{\triangle t} \\ &\le e^{4T}\|\vec{\theta}^0\|_{\triangle t}, \quad t^n \le T. \end{aligned} \tag{33}$$

(33) does not mean that the difference between the two solutions, $\|\vec{\theta}^n\|_{\triangle t}$, increases with n. Instead, it shows that for a given time $T > 0$, the difference between the two solutions, $\|\vec{\theta}^n\|_{\triangle t}$, is bounded by the initial difference between the two solutions for any $t^n \le T$. This indicates that the new set of schemes is stable. ■

C. Convergence

According to the theory for the finite difference method stated in [3], a set of consistent and stable finite difference schemes is convergent to the exact solution of the original differential equations. Thus, we conclude that the stability and consistency results for the set of schemes, (4)–(13), imply its convergence.

IV. A SET OF COMPACT SCHEMES FOR 3D CASE

The detail for constructing the set of schemes for the three-dimensional case is very similar to that of the two-dimensional case derived in the previous two sections. Therefore, only the set of schemes is listed here.

As in the two-dimensional case, we let h and $\triangle t$ be the space mesh and time increment, respectively. The space meshes for all three directions, x, y and z, are assumed to be h and satisfy $(M+1)h = 1$ for a positive integer M. $u^m_{i,j,k}$, $(u_{xx})^m_{i,j,k}$, $(u_{yy})^m_{i,j,k}$, and $(u_{zz})^m_{i,j,k}$ are used to represent the approximations of $U(x_i, y_j, z_k, t^m)$, $U_{xx}(x_i, y_j, z_k, t^m)$, $U_{yy}(x_i, y_j, z_k, t^m)$, and $U_{zz}(x_i, y_j, z_k, t^m)$, where $U(x, y, z, t)$ is the exact solution of (2).

By using the LOD method, the heat equation

$$U_t = U_{xx} + U_{yy} + U_{zz} + F(x, y, z, t)$$

can be separated into the following three one-dimensional equations:

$$\begin{aligned}\frac{1}{3}U_t &= U_{xx} + \frac{1}{3}F(x, y, z, t), \\ \frac{1}{3}U_t &= U_{yy} + \frac{1}{3}F(x, y, z, t), \\ \frac{1}{3}U_t &= U_{zz} + \frac{1}{3}F(x, y, z, t). \end{aligned} \tag{34}$$

Applying the Crank–Nicolson method to the equations in (34) sequentially, we obtain that:

$$\frac{u_{i,j,k}^{m+\frac{1}{3}} - u_{i,j,k}^{m}}{3\,\frac{\triangle t}{3}} = \frac{1}{2}\left((u_{xx})_{i,j,k}^{m+\frac{1}{3}} + (u_{xx})_{i,j,k}^{m}\right) + \frac{1}{3}F_{i,j,k}^{m+\frac{1}{6}}, \tag{35}$$

$$\frac{u_{i,j,k}^{m+\frac{2}{3}} - u_{i,j,k}^{m+\frac{1}{3}}}{3\frac{\triangle t}{3}} = \frac{1}{2}\left((u_{yy})_{i,j,k}^{m+\frac{2}{3}} + (u_{yy})_{i,j,k}^{m+\frac{1}{3}}\right) + \frac{1}{3}F_{i,j,k}^{m+\frac{1}{2}}, \tag{36}$$

$$\frac{u_{i,j,k}^{m+1} - u_{i,j,k}^{m+\frac{2}{3}}}{3\frac{\triangle t}{3}} = \frac{1}{2}\left((u_{zz})_{i,j,k}^{m+1} + (u_{zz})_{i,j,k}^{m+\frac{2}{3}}\right) + \frac{1}{3}F_{i,j,k}^{m+\frac{5}{6}}, \tag{37}$$

where

$$F_{i,j,k}^{m+\frac{1}{6}} = \frac{1}{2}\left(F(x_i, y_j, z_k, t^m) + F\left(x_i, y_j, z_k, t^{m+\frac{1}{3}}\right)\right), \tag{38}$$

or

$$F_{i,j,k}^{m+\frac{1}{6}} = F\left(x_i, y_j, z_k, t^{m+\frac{1}{6}}\right), \tag{39}$$

$$F_{i,j,k}^{m+\frac{1}{2}} = \frac{1}{2}\left(F\left(x_i, y_j, z_k, t^{m+\frac{1}{3}}\right) + F\left(x_i, y_j, z_k, t^{m+\frac{2}{3}}\right)\right), \tag{40}$$

or

$$F_{i,j,k}^{m+\frac{1}{2}} = F\left(x_i, y_j, z_k, t^{m+\frac{1}{2}}\right), \tag{41}$$

$$F_{i,j,k}^{m+\frac{5}{6}} = \frac{1}{2}\left(F\big(x_i, y_j, z_k, t^{m+1}\big) + F\big(x_i, y_j, z_k, t^{m+\frac{2}{3}}\big)\right), \tag{42}$$

or

$$F_{i,j,k}^{m+\frac{5}{6}} = F\left(x_i, y_j, z_k, t^{m+\frac{5}{6}}\right). \tag{43}$$

By using a similar argument as that in the 2D case, we obtain the following three schemes, which provide fourth-order approximations to $\left\{(u_{xx})_{i,j,k}^{m+\frac{1}{3}}\right\}$, $\left\{(u_{xx})_{i,j,k}^{m}\right\}$ in (35).

$$\frac{1}{10}(u_{xx})_{i-1,j,k}^{m} + (u_{xx})_{i,j,k}^{m} + \frac{1}{10}(u_{xx})_{i+1,j,k}^{m} = \frac{6}{5h^2}\big(u_{i-1,j,k}^{m} - 2u_{i,j,k}^{m} + u_{i+1,j,k}^{m}\big),$$
$$2 \le i \le M-1,\ \ 1 \le j,\ k \le M, \tag{44}$$

$$\frac{11}{6}(u_{xx})_{1,j,k}^{m} - \frac{1}{3}(u_{xx})_{2,j,k}^{m} = -\frac{\alpha_1(y_j, z_k, t^m)}{h} + \frac{u_{2,j,k}^{m} - u_{1,j,k}^{m}}{h^2}, \quad i = 1,\ \ 1 \le j,k \le M \tag{45}$$

$$\frac{11}{6}(u_{xx})_{M,j,k}^{m} - \frac{1}{3}(u_{xx})_{M-1,j,k}^{m} = \frac{\alpha_2(y_j, z_k, t^m)}{h} + \frac{u_{M-1,j,k}^{m} - u_{M,j,k}^{m}}{h^2}, \quad i = M,\ \ 1 \le j,k \le M. \tag{46}$$

The next three schemes provide fourth-order approximations to $\{(u_{yy})_{i,j,k}^{m+\frac{2}{3}}\}$ and $\{(u_{yy})_{i,j,k}^{m+\frac{1}{3}}\}$ in (36).

$$\frac{1}{10}(u_{yy})_{i,j-1,k}^{m} + (u_{yy})_{i,j,k}^{m} + \frac{1}{10}(u_{yy})_{i,j+1,k}^{m} = \frac{6}{5h^2}\left(u_{i,j-1,k}^{m} - 2u_{i,j,k}^{m} + u_{i,j+1,k}^{m}\right),$$
$$2 \le j \le M-1,\ 1 \le i,k \le M, \quad (47)$$

$$\frac{11}{6}(u_{yy})_{i,1,k}^{m} - \frac{1}{3}(u_{yy})_{i,2,k}^{m} = -\frac{\beta_1(x_i, z_k, t^m)}{h} + \frac{u_{i,2,k}^{m} - u_{i,1,k}^{m}}{h^2}, \quad j = 1,\ 1 \le i,k \le M, \quad (48)$$

$$\frac{11}{6}(u_{yy})_{i,M,k}^{m} - \frac{1}{3}(u_{yy})_{i,M-1,k}^{m} = \frac{\beta_2(x_i, z_k, t^m)}{h} + \frac{u_{i,M-1,k}^{m} - u_{i,M,k}^{m}}{h^2}, \quad j = M,\ 1 \le i,k \le M. \quad (49)$$

The last three schemes provide fourth-order approximations to $\{(u_{zz})_{i,j,k}^{m+1}\}$ and $\{(u_{zz})_{i,j,k}^{m+\frac{2}{3}}\}$ in (37).

$$\frac{1}{10}(u_{zz})_{i,j,k-1}^{m} + (u_{zz})_{i,j,k}^{m} + \frac{1}{10}(u_{zz})_{i,j,k+1}^{m} = \frac{6}{5h^2}\left(u_{i,j,k-1}^{m} - 2u_{i,j,k}^{m} + u_{i,j,k+1}^{m}\right),$$
$$2 \le k \le M-1,\ 1 \le i,j \le M, \quad (50)$$

$$\frac{11}{6}(u_{zz})_{i,j,1}^{m} - \frac{1}{3}(u_{zz})_{i,j,2}^{m} = -\frac{\gamma_1(x_i, y_j, t^m)}{h} + \frac{u_{i,j,2}^{m} - u_{i,j,1}^{m}}{h^2}, \quad k = 1,\ 1 \le i,j \le M, \quad (51)$$

$$\frac{11}{6}(u_{zz})_{i,j,M}^{m} - \frac{1}{3}(u_{zz})_{i,j,M-1}^{m} = \frac{\gamma_2(x_i, y_j, t^m)}{h} + \frac{u_{i,j,M-1}^{m} - u_{i,j,M}^{m}}{h^2}, \quad k = M,\ 1 \le i,j \le M. \quad (52)$$

It can be seen that the set of schemes, (35)–(52), has truncation error of order $\triangle t^2 + h^4$ in time and space.

V. NUMERICAL EXAMPLES

The numerical examples provided in this section are based on equations of two dimensions. The new set of schemes obtained in Section II is compared to the following set of Crank–Nicolson schemes, which has truncation error of order $\triangle t^2 + h^2$ at interior points, but only order h at the boundary points.

$$\frac{u_{i,j}^{m+1} - u_{i,j}^{m}}{\triangle t} = \delta_x^2\left(\frac{u_{i,j}^{m+1} + u_{i,j}^{m}}{2}\right) + \delta_y^2\left(\frac{u_{i,j}^{m+1} + u_{i,j}^{m}}{2}\right) + F_{i,j}^{m+\frac{1}{2}}, \quad 1 \le i,j \le M,\ m \ge 0, \quad (53)$$

$$\frac{u_{1,j}^{m} - u_{0,j}^{m}}{h} = \alpha_1(y_j, t^m), \quad \frac{u_{M+1,j}^{m} - u_{M,j}^{m}}{h} = \alpha_2(y_j, t^m), \quad 1 \le j \le M,\ m \ge 0,$$
$$\frac{u_{i,1}^{m} - u_{i,0}^{m}}{h} = \beta_1(x_i, t^m), \quad \frac{u_{i,M+1}^{m} - u_{i,M}^{m}}{h} = \beta_2(x_i, t^m), \quad 1 \le i \le M,\ m \ge 0,$$

where

$$\delta_x^2\theta_{i,j} = \frac{\theta_{i+1,j} - 2\theta_{i,j} + \theta_{i-1,j}}{h^2}, \quad \delta_y^2\theta_{i,j} = \frac{\theta_{i,j+1} - 2\theta_{i,j} + \theta_{i,j-1}}{h^2}.$$

The maximum absolute errors of these two sets of schemes are computed and compared with each other. The computations are performed for $0 < t < 1$ using $\Delta t = 0.0001$ and $h = 0.02, 0.04$, and 0.1, respectively. It is worth reiterating at this point that no restriction on h and Δt for either set of schemes is required. The choices of h and Δt in this section are for testing purpose only. The convergent criterion for time level $m + 1$ is:

$$\text{Max}_{1\le i,j\le M}\left|\left(u_{i,j}^{m+1}\right)^{\text{new}} - \left(u_{i,j}^{m+1}\right)^{\text{old}}\right| < 10^{-8}.$$

The first example is described below:

$$\begin{aligned} &U_t = U_{xx} + U_{yy}, \quad 0 < x, y < 1; \; t > 0, \\ &U(x, y, 0) = \cos(\pi x)\cos(\pi y), \\ &U_x(0, y, t) = U_x(1, y, t) = 0, \\ &U_y(x, 0, t) = U_y(x, 1, t) = 0, \end{aligned} \tag{54}$$

where the exact solution is $U(x, y, t) = e^{-2\pi^2 t}\cos(\pi x)\cos(\pi y)$. In application, the homogeneous boundary conditions imply that the boundaries are insulated. The maximum absolute errors at each time level are plotted in Fig. 1, which shows that the maximum absolute error of

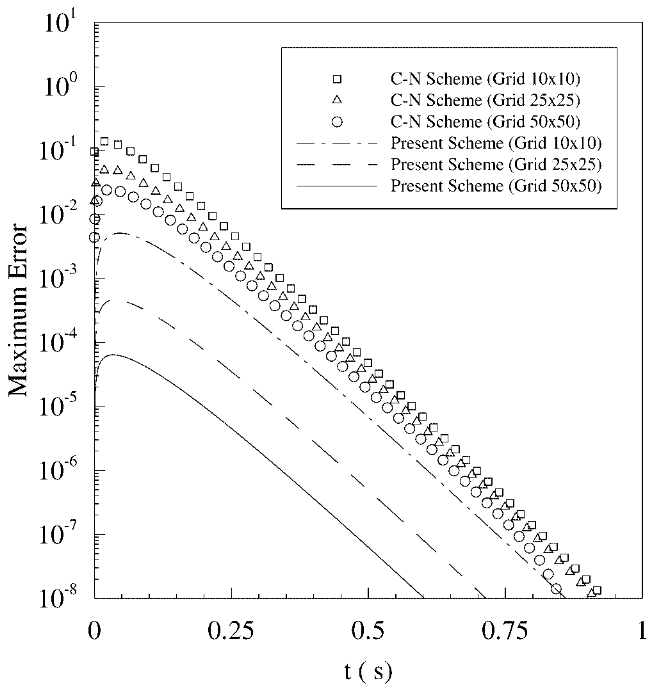

FIG. 1. Comparison results for Example 1.

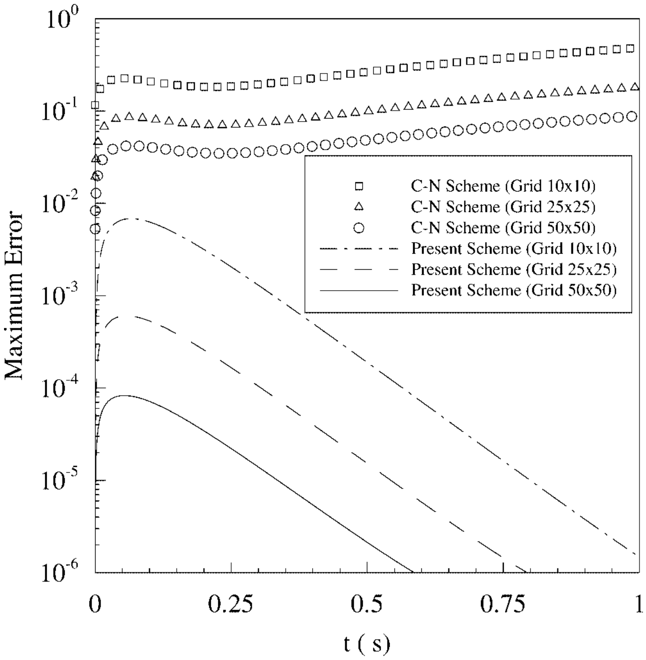

FIG. 2. Comparison results for Example 2.

the new set of schemes is about the square of the maximum absolute error of the Crank–Nicolson scheme. Noted that the truncation error of the Crank–Nicolson schemes is order $O(h^2)$ is space, the numerical result indicates that our set of schemes has much higher order of accuracy than the Crank–Nicolson scheme.

The second example is the following nonhomogeneous one:

$$
\begin{aligned}
&U_t = U_{xx} + U_{yy} + F(x, y, t), \quad 0 < x, y < 1; \; t > 0,\\
&F(x, y, t) = \pi^2 e^{-\pi^2 t} \cos(\pi x)\cos(\pi y) - 4 + x + y,\\
&U(x, y, 0) = \cos(\pi x)\cos(\pi y) + x^2 + y^2,\\
&U_x(0, y, t) = t, \quad U_x(1, y, t) = t + 2,\\
&U_y(x, 0, t) = t, \quad U_y(x, 1, t) = t + 2,
\end{aligned}
\tag{55}
$$

where the exact solution is

$$U(x, y, t) = e^{-\pi^2 t} \cos(\pi x)\cos(\pi y) + x^2 + y^2 + (x + y)t.$$

The nonhomogeneous boundary conditions imply that there is a heat exchange through the boundaries. The comparison results are plotted in Fig. 2. Again, we see significant improvement in accuracy of the current set of schemes over the Crank–Nicolson schemes.

VI. CONCLUSIONS

In this article, two sets of fourth-order compact finite difference schemes are derived for heat-conducting problems of two or three dimensions with Neumann boundary conditions, respectively. What makes these two sets of schemes different from others is that they are uniformly fourth-order at both interior and boundary points. The LOD method is used so that both sets of schemes are constructed through a sequence of one-dimensional equations. Moreover, the set of schemes for the 2D case is shown to be globally solvable, unconditionally stable with respect to initial data, and convergent. The proofs of the same properties for the 3D case are very similar to those of 2D case, so the detail is omitted. Numerical examples for the 2D case are used to verify the accuracy of the set of the schemes.

APPENDIX

For review purpose, we list a few results obtained in [1].

Lemma 1. *Assume that λ is an eigenvalue of matrix $A^{-1}B$, and $\vec{x}$, a vector of dimension M, is a corresponding eigenvector. Then λ is real and satisfies:*

$$\lambda \geq 0.$$

Proof. Since λ and $\vec{x}$ are an eigenvalue and a corresponding eigenvector of matrix $A^{-1}B$, they satisfy the following conditions:

$$\lambda\,\vec{x} = A^{-1}B\vec{x} \quad \text{or} \quad \lambda\,\vec{x}^T A\vec{x} = \vec{x}^T B\vec{x}.$$

Since

$$\begin{aligned}
\vec{x}^T A\vec{x} &= [x_1, x_2, \ldots, x_M]\begin{bmatrix} 22 & -4 & & & \\ 1 & 10 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 10 & 1 \\ & & & -4 & 22 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_M \end{bmatrix} \\
&= 22x_1^2 - 4x_1x_2 + x_1x_2 + 10x_2^2 + 2x_2x_3 + 10x_3^3 + 2x_3x_4 + \cdots \\
&\quad + 2x_{M-2}x_{M-1} + 10x_{M-1}^2 - 4x_{M-1}x_M + x_{M-1}x_M + 22x_M^2 \\
&\geq 22x_1^2 - \frac{3}{2}\left(x_1^2 + x_2^2\right) + 10x_2^2 - \left(x_2^2 + x_3^2\right) + 10x_3^2 - \left(x_3^2 + x_4^2\right) + \cdots \\
&\quad + \left(x_{M-2}^2 + x_{M-1}^2\right) + 10x_{M-1}^2 - \frac{3}{2}\left(x_{M-1}^2 + x_M^2\right) + 22x_M^2 \\
&= \frac{41}{2}x_1^2 + \frac{15}{2}x_2^2 + 8x_3^2 + \cdots + 8x_{M-2}^2 + \frac{15}{2}x_{M-1}^2 + \frac{41}{2}x_M^2 \\
&> 0
\end{aligned}$$

and

$$
\begin{aligned}
\vec{x}^T B\vec{x} &= [x_1, x_2, \ldots, x_M]\begin{bmatrix} 6 & -6 & & & \\ -6 & 12 & -6 & & \\ & \ddots & \ddots & \ddots & \\ & & -6 & 12 & -6 \\ & & & -6 & 6 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_M \end{bmatrix} \\
&= 6x_1^2 - 6x_1x_2 - 6x_1x_2 + 12x_2^2 - 12x_2x_3 + 12x_3^2 - 12x_3x_4 - \cdots \\
&\quad - 12x_{M-2}x_{M-1} + 12x_{M-1}^2 - 6x_{M-1}x_M - 6x_{M-1}x_M + 6x_M^2 \\
&\geq 6x_1^2 - 6\big(x_1^2 + x_2^2\big) + 12x_2^2 - 6\big(x_2^2 + x_3^2\big) + 12x_3^2 - 6\big(x_3^2 + x_4^2\big) - \cdots \\
&\quad - 6\big(x_{M-2}^2 + x_{M-1}^2\big) + 12x_{M-1}^2 - 6\big(x_{M-1}^2 + x_M^2\big) + 6x_M^2 \\
&= 0,
\end{aligned}
$$

the above two results indicate that λ is real and $\lambda \geq 0$. ■

The following lemma is from [15].

Lemma 2. *Let A be an arbitrary square matrix. Then for any operator matrix norm $\|\cdot\|$, we have $\lambda_\sigma(A) \leq \|A\|$, here $\lambda_\sigma(A)$ represents the spectral radius of A. Moreover, if $\epsilon > 0$, then there exists an operator matrix norm, denoted here by $\|\cdot\|_\epsilon$, such that $\|A\|_\epsilon \leq \lambda_\sigma(A) + \epsilon$*

Theorem 1. *The set of schemes, consisting of* (2), (7), (19), *and* (20) *or their equivalent vector form* (25) *in* [1], *is unconditionally stable with respect to the initial data*

Proof. Lemma 1, (31) and (32) in [1] indicate the following result:

$$
\|(I + rA^{-1}B)^{-1}(I - r\,A^{-1}B)\|_\epsilon \leq \lambda_\sigma((I + rA^{-1}B)^{-1}\,(I - rA^{-1}B)) + \epsilon\ \leq\ 1 + \epsilon,
$$

where $\epsilon > 0$. From this, it can be concluded that:

$$
\begin{aligned}
\|\vec{\theta}^n\|_\epsilon &\leq \|[(I + rA^{-1}B)^{-1}(I - rA^{-1}B)]^n\|_\epsilon \|\vec{\theta}^0\|_\epsilon \\
&\leq (\|(I + rA^{-1}B)^{-1}(I - rA^{-1}B)\|_\epsilon)^n \|\vec{\theta}^0\|_\epsilon \\
&\leq (1 + \epsilon)^n \|\vec{\theta}^0\|_\epsilon \\
&\leq e^{n\epsilon}\|\vec{\theta}^0\|_\epsilon.
\end{aligned}
$$

If we take $\epsilon = \triangle t$, then the above relation yields the following result:

$$
\|\vec{\theta}^n\|_{\triangle t} \leq e^{n\triangle t}\|\vec{\theta}^0\|_{\triangle t} \leq e^T\|\vec{\theta}^0\|_{\triangle t},
$$

for $t^n \leq T$. This completes the proof. ■

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