Deferred Correction Technique to Construct High-Order Schemes for the Heat Equation with Dirichlet and Neumann Boundary Conditions

Damrongsak Yambangwai and Nikolay Moshkin

***Abstract*—A deferred correction method is utilized to increase the order of spatial accuracy of the Crank-Nikolson scheme for the numerical solution of the one-dimensional heat equation. Numerical examples are given for both Neumann and Dirichlet initial boundary value problems. The fourth-order methods proposed are compared with high-order compact schemes. The set of methods proposed demonstrate a better performance compared with high-order compact schemes in the case of the Neumann boundary conditions.**

***Index Terms*—high-order difference scheme; deferred correction scheme; high-order compact scheme; heat equation.**

I. Introduction

THE desired properties of finite difference schemes are stability, accuracy and efficiency. These requirements are in conflict with each other. In many applications a high-order accuracy is required in the spatial discretization. To reach better stability, implicit approximation is desired. For a high-order method of traditional type (not a high-order compact (HOC)), the stencil becomes wider with increasing order of accuracy. For a standard centered discretization of order p, the stencil is $p+1$ points wide. This inflicts problems at the fictional boundaries, and using an implicit method results in the solution of an algebraic system of equations with large bandwidth. In light of conflict requirements of stability, accuracy and computational efficiency, it is desired to develop schemes that have a wide range of stability, high-order of accuracy and lead to the solution of the system of linear equations with a tridiagonal matrix, i.e. the system of linear equations arising from a standard second order discretization of heat equation.

The development of high order compact schemes (HOC) [2-12, 14-19, 21, 22] is one approach to overcome the antagonism among stability, accuracy and computational cost. Most existing HOCs are constructed for problems with Dirichlet boundary conditions (Dbc) [2-12, 14-19, 22, 23]. Only few HOCs have been constructed for problems with Neumann (or insulated) boundary conditions (Nbc) [4,5,11, 12, 14-19, 22, 23]. Even for these less popular compact difference schemes involving Neumann boundary conditions, very often, the schemes are fourth-order, sixth-order or higher order at the interior points, but of lower order at the boundary [1, 4, 5, 11, 22, 23]. In the paper by Zhao *et al.* [22], a set of fourth-order one dimensional compact finite difference schemes is developed to solve a heat conduction problem with Neumann boundary conditions.

Another way of preserving a compact stencil at higher time level and reaching high-order spatial accuracy is the deferred correction approach [13]. A classical deferred correction procedure is developed in [20, 21].

In this paper we use the deferred correction technique to obtain fourth-order accurate schemes in space for the one dimensional heat conducting problem with Dirichlet and Neumann boundary conditions. The linear system that needs to be solved at each time step is similar to the standard Crank-Nicolson method of second order which can be solved by using Thomas algorithms. The fourth-order deferred-correction schemes are compared with the fourth-order compact schemes for the Dirichlet and Neumann boundary value problems.

A set of schemes are constructed for the one dimensional heat conducting problem with Dirichlet boundary conditions and Neumann boundary conditions and initial data,

$$u_t = \beta u_{xx} + f(x,t), \quad 0 < x < l, \quad t > 0, \tag{1}$$

$$u(x,0) = u_0(x), \quad 0 < x < l, \tag{2}$$

$$\text{Dbc: } u(0,t) = \alpha_1(t), u(l,t) = \alpha_2(t), t > 0, \tag{3}$$

$$\text{Nbc: } u_x(0,t) = \gamma_1(t), u_x(l,t) = \gamma_2(t), t > 0, \tag{4}$$

where the diffusion coefficient β is positive, $u(x,t)$ represents the temperature at point (x,t) and $f(x,t)$, $\alpha_1(t)$, $\alpha_2(t)$, $\gamma_1(t)$, $\gamma_2(t)$ are sufficiently smooth functions.

The rest of this paper is organized as follows: Section 2.1 presents a list of fourth-order deferred correction schemes. Section 2.2 presents briefly the high-order compact difference schemes, which we use to compare performance of proposed schemes and HOC schemes. Section 3 provides examples of comparisons. Although having a higher computational cost than HOC schemes, it is evident from these examples that the deferred correction schemes have the advantage of accuracy in the uniform norm (the accuracy at the internal points and at the boundary points are the same) and robustness. We conclude the paper in Section 4.

II. The Proposed Schemes

Let Δt denote the temporal mesh size. For simplicity, we consider a uniform mesh consisting of N points: $x_1, x_2, \ldots, x_N$ where $x_i = (i-1)\Delta x$ and the mesh size is $\Delta x = l/(N-1)$. Below we use the notations u_i^n and $(u_{xx})_i^n$ to represent the numerical approximations of $u(x_i, t^n)$ and

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D. Yambangwai is with the Department of Mathematics, School of Science, University of Phayao, Phayao 56000, Thailand, e-mail: damrong.sut@gmail.com.

N.P. Moshkin is with the School of Mathematics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, 30000, Thailand e-mail: nikolay.moshkin@gmail.com.

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$u_{xx}(x_i, t^n)$ where $t^n = n\Delta t$ and $u^{(p)}$ is the value of the p-th derivative of the given function u.

A. Deferred correction schemes

A set of high order deferred correction schemes (HOD) is based on the well-known Crank-Nikolson type of scheme in the following form,

$$\frac{u_i^{n+1,s+1} - u_i^n}{\Delta t} = \frac{\beta}{2}\left[(u_{xx})_i^{n+1,s+1} + (u_{xx})_i^n\right] + f_i^{n+1/2}, \quad f_i^{n+1/2} = \frac{f_i^{n+1} + f_i^n}{2} \tag{5}$$

the second superscript "s" denotes the number of iterations $s = 0, \ldots, \hat{S}$ and $i = 2, \ldots, N-1$.

The deferred correction technique [13] is utilized to approximate the second-order derivatives at higher time levels $(u_{xx})_i^{n+1,s+1}$, $i = 2, \ldots, N-1$ by the iterative method

$$(u_{xx})_i^{n+1,s+1} = (u_{xx}^l)_i^{n+1,s+1} + \left[(u_{xx}^h)_i^{n+1,s} - (u_{xx}^l)_i^{n+1,s}\right], \tag{6}$$

where

$$(u_{xx}^h)_i^{n+1,s}, i = 2, \ldots, N-1, s = 0, \ldots, \widehat{S}$$

is high-order approximation on wide stencil, and

$$(u_{xx}^l)_i^{n+1,k}, k = s, s+1, i = 2, \ldots, N-1$$

is the lower order approximation on compact stencil (usually three point stencil). The expression in the square brackets of (6) is evaluated explicitly using the values known from the previous iteration. When $s = 0$ we use the solution from the time level n (so $u^{n+1,0} = u^n$ and $(u_{xx})_i^{n+1,0} = (u_{xx})_i^n$). Once the iterations converge, the lower order approximation terms drop out and the approximation of $(u_{xx})_i^{n+1,s+1}$ obtained has the same order of approximation as $(u_{xx}^h)_i^{n+1,\widehat{S}}$. There are no difficulties to construct high-order approximation for interior points.

To preserve a compact 3 using wide stencil in the finite difference scheme at higher time level $(n+1, s+1)$, we use the central second-order finite difference approximation to approximate the lower order term in (6)

$$(u_{xx}^l)_i^{n+1,k} = \frac{1}{\Delta x^2}\Lambda_l u_i^{n+1,k}, k = s, s+1, \tag{7}$$

$$\Lambda_l u_i^{n+1,k} = u_{i-1}^{n+1,k} - 2u_i^{n+1,k} + u_{i+1}^{n+1,k}, i = 3, \ldots, N-2.$$

For the high-order approximation term in (6), we use a symmetric five point wide stencil for the inner points to reach the fourth-order of approximation

$$(u_{xx}^h)_i^{n+1,s} = \frac{1}{\Delta x^2}\Lambda_h u_i^{n+1,s}, \quad i = 3, \ldots, N-2, \tag{8}$$

$$\Lambda_h u_i^{n+1,s} = \frac{1}{12}\big(-u_{i-2}^{n+1,s} + 16u_{i-1}^{n+1,s} - 30u_i^{n+1,s} + 16u_{i+1}^{n+1,s} - u_{i+2}^{n+1,s}\big).$$

Case $s = 0$ in equations (8) gives the fourth-order of approximation to approximate the second-order derivatives at the time level n, $(u_{xx})_i^n$, $i = 3, \ldots, N-2$ in (5).

Stability analysis

To study the stability of scheme (1)-(8), we use the Von-Neumann stability analysis. For simplicity, we assume that $f_i^{n+1/2} \equiv 0$ in (5), and u is periodic in x.

Let us recast scheme (5) in the following form,

$$[E + (\alpha/2)\Lambda_l]\, u_i^{n+1,s+1} = (\alpha/2)\,[\Lambda_l - \Lambda_h]\, u_i^{n+1,s} + [E - (\alpha/2)\Lambda_l]\, u_i^n, \tag{9}$$

where $\alpha = \beta\Delta t/\Delta x^2$. If we define the following operators: $A = E + (\alpha/2)\Lambda_l$, $B = E - (\alpha/2)\Lambda_h$, $C = E + (\alpha/2)\Lambda_h$, where E is the identity operator, then (9) can be rewritten as follows

$$Au_i^{n+1,s+1} = (A - C)u_i^{n+1,s} + Bu_i^n. \tag{10}$$

Assuming that the operators commute (for example in the case of uniform grid),

$$(A - C)A = A(A - C),$$

it is easy to demonstrate that if $u_i^{n+1,\widehat{S}+1} = u_i^{n+1}$ and $u_i^{n+1,0} = u_i^n$ we get

$$A^{\widehat{S}+1}u_i^{n+1} = \left(\sum_{k=0}^{\widehat{S}} A^{\widehat{S}-k}(A - C)^k\right) Bu_i^n + (A - C)^{\widehat{S}+1}u_i^n. \tag{11}$$

Let $u_i^n = \xi^n e^{I\Theta i}$, $I = \sqrt{-1}$, be the solution of (5)-(8), where $\Theta = 2\pi\triangle x/l$ is the phase angle with wavelength l. From (11), we can derive an equation for the amplification factor in the form

$$|\xi| = |\varphi(\Theta, \widehat{S}, \alpha)|, \tag{12}$$

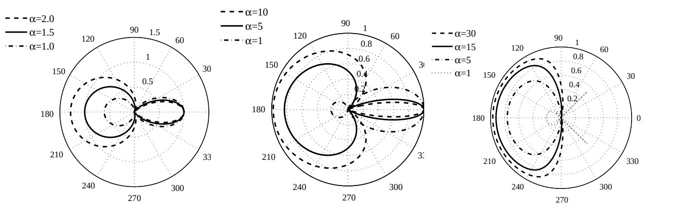
where $\widehat{S}$ is the number of iterations, and

$$|\varphi(\Theta, \widehat{S}, \alpha)| = \frac{\left|\left[\left(\sum_{k=0}^{\widehat{S}} A^{\widehat{S}-k}(A - C)^k\right) B + (A - C)^{\widehat{S}+1}\right] e^{I\Theta i}\right|}{|A^{\widehat{S}+1}e^{I\Theta i}|}.$$

For stability of the method it is necessary that the absolute values of the amplification factor is less than one, i.e.

$$|\xi| < 1. \tag{13}$$

Calculations are tedious and almost impossible to do by hand without mistake. We have therefore automated all calculations in a computer algebra environment based on REDUCE to obtain an explicit form of $|\varphi(\Theta, \widehat{S}, \alpha)|$. Figure 1 shows the values of $|\xi|^2$ in the polar coordinate system $(|\xi|^2, \Theta)$ for $\widehat{S} = 1, 3$ and 5. If only one iteration executes in (5), $\widehat{S} = 1$, inequality (13) holds if $\alpha < 1.5$, as can be seen from Figure 1 a). If 3 iterations are done in (5) (Figure 1 b) , $\widehat{S} = 3$, the amplification factor remains bounded by one at least for $\alpha \leq 10$. In case of $\widehat{S} = 5$, the stability criteria hold up to $\alpha = 30$ as can be seen from Figure 1 c). It can be seen that increasing the number of internal iterations results in increasing the range of α needed for stability. This tendency allows to assume that as $\widehat{S} \to \infty$, our method becomes the unconditionally stable Crank-Nikolson method for the heat equation.



(a) (b) (c)

Fig. 1. Variation of amplification factor with Θ. (a)–$\widehat{S}=1$, dashed line $\alpha = 2.0$, solid line $\alpha = 1.5$, dash-doted line $\alpha = 1.0$, (b)–$\widehat{S}=3$, dashed line $\alpha = 10.0$, solid line $\alpha = 5.0$, dash-doted line $\alpha = 1.0$, (c)–$\widehat{S}=5$, dashed line $\alpha = 30.0$, solid line $\alpha = 15$, dash-doted line $\alpha = 5.0$, doted line $\alpha = 1.0$

Fourth-order deferred correction scheme (Dirichlet boundary conditions)

Let us first consider the one dimensional heat conduction problem with initial data and Dirichlet boundary conditions (1)-(3),

$$u_1^{n+1} = u_1^{n+1,k} = \alpha_1(t^{n+1}), \quad u_N^{n+1} = u_N^{n+1,k} = \alpha_2(t^{n+1}).$$

The finite difference approximations at x_2 and x_{N-1}, which are the points next to the left and right boundaries, are straightforward

$$(u^l_{xx})_2^{n+1,k} = \frac{1}{\Delta x^2}\Big(\alpha_1(t^{n+1}) - 2u_2^{n+1,k} + u_3^{n+1,k}\Big), \quad (14)$$

$$(u^h_{xx})_2^{n+1,s} = \frac{1}{12\Delta x^2}\Big(10\alpha_1(t^{n+1}) - 15u_2^{n+1,s} - 4u_3^{n+1,s} + 14u_4^{n+1,s} - 6u_5^{n+1,s} + u_6^{n+1,s}\Big), \quad (15)$$

$$(u^l_{xx})_{N-1}^{n+1,k} = \frac{1}{\Delta x^2}\left(u_{N-2}^{n+1,k} - 2u_{N-1}^{n+1,k} + \alpha_2(t^{n+1})\right), \quad (16)$$

$$(u^h_{xx})_{N-1}^{n+1,s} = \frac{1}{12\Delta x^2}\Big(10\alpha_2(t^{n+1}) - 15u_{N-1}^{n+1,s} - 4u_{N-2}^{n+1,s} + 14u_{N-3}^{n+1,s} - 6u_{N-4}^{n+1,s} + u_{N-5}^{n+1,s}\Big), \quad (17)$$

where $k = s, s+1$. Cases $s = 0$ or $k = 0$ give formulae to approximate $(u^n_{xx})_i$. Substituting equations (7), (8), (14)–(17) into equation (6) the following fourth-order deferred correction approximations of $(u_{xx})_i^{n+1,s+1}$, $i = 2,\dots,N-1$ are

$$\begin{aligned}(u_{xx})_2^{n+1,s+1} &= \frac{5}{6\Delta x^2}\alpha_1(t^{n+1}) + \frac{1}{\Delta x^2}\Big(-2u_2^{n+1,s+1} + u_3^{n+1,s+1}\Big)\\ &+ \frac{1}{12\Delta x^2}\Big(9u_2^{n+1,s} - 16u_3^{n+1,s} + 14u_4^{n+1,s} - 6u_5^{n+1,s} + u_6^{n+1,s}\Big),\end{aligned} \quad (18)$$

$$\begin{aligned}(u_{xx})_i^{n+1,s+1} &= \frac{1}{\Delta x^2}\Big(u_{i-1}^{n+1,s+1} - 2u_i^{n+1,s+1} + u_{i+1}^{n+1,s+1}\Big)\\ &+ \frac{1}{12\Delta x^2}\Big(-u_{i-2}^{n+1,s} + 4u_{i-1}^{n+1,s} - 6u_i^{n+1,s} + 4u_{i+1}^{n+1,s} - u_{i+2}^{n+1,s}\Big), i = 3,\dots,N-2,\end{aligned} \quad (19)$$

$$\begin{aligned}(u_{xx})_{N-1}^{n+1,s+1} &= \frac{5}{6\Delta x^2}\alpha_2(t^{n+1}) + \frac{1}{\Delta x^2}\Big(-2u_{N-1}^{n+1,s+1} + u_N^{n+1,s+1}\Big)\\ &+ \frac{1}{12\Delta x^2}\Big(9u_{N-1}^{n+1,s} - 16u_{N-2}^{n+1,s} + 14u_{N-3}^{n+1,s} - 6u_{N-4}^{n+1,s} + u_{N-5}^{n+1,s}\Big).\end{aligned} \quad (20)$$

The scheme including equations (5), (18)–(20) is called the fourth-order deferred correction scheme for Dirichlet boundary value problem (we will use the abbreviation **DHOD**). The order of approximation is $O(\Delta t^2, \Delta x^4)$ in the uniform norm.

Fourth-order deferred correction scheme (Neumann boundary conditions)

Next, we develop the fourth-order approximations (based on principle of deferred corrections) of $(u_{xx})^{n+1,s+1}$ at the near boundary points x_2 and x_{N-1}. We do not approximate the first derivatives using one side wide stencil. The main idea is to use the given Neumann boundary conditions (value of the first derivative) in the approximation of the second-order derivatives at the points near the boundary. A similar approach has used [16] to construct a high-order compact scheme.

To preserve a compact stencil (two points) at level $(n+1, s+1)$, we use the first-order finite difference formula for the lower order approximation term in (6) $(u^l_{xx})_i^{n+1,k}$, $i = 2, N-1$, $k = s, s+1$

$$(u^l_{xx})_2^{n+1,k} = \frac{a_1}{\Delta x}(u_x)_1^{n+1,k} + \frac{1}{\Delta x^2}\left[a_2 u_2^{n+1,k} + a_3 u_3^{n+1,k}\right], \quad (21)$$

$$(u^l_{xx})_{N-1}^{n+1,k} = -\frac{a_1}{\Delta x}(u_x)_N^{n+1,k} + \frac{1}{\Delta x^2}\left[a_2 u_{N-1}^{n+1,k} + a_3 u_{N-2}^{n+1,k}\right], \quad (22)$$

where the coefficients can be found by matching the Taylor series expansion of left-hand side up to the term $O(\Delta x)u^{(3)}$ which gives the following values of coefficients

$$a_1 = -\frac{2}{3}, \quad a_2 = -\frac{2}{3}, \quad a_3 = \frac{2}{3}.$$

Substituting coefficients into (21) and (22), the second-order derivatives $(u^l_{xx})_i^{n+1,k}$, $i = 2, N-1$, $k = s, s+1$ are approximated with first-order by the following formula

$$(u^l_{xx})_2^{n+1,k} = -\frac{2}{3\Delta x}\gamma_1(t^{n+1}) - \frac{2}{3\Delta x^2}\left(u_2^{n+1,k} - u_3^{n+1,k}\right), \quad (23)$$

$$(u^l_{xx})_{N-1}^{n+1,k} = \frac{2}{3\Delta x}\gamma_2(t^{n+1}) - \frac{2}{3\Delta x^2}\left(u_{N-1}^{n+1,k} - u_{N-2}^{n+1,k}\right). \quad (24)$$

The absolute truncation errors of equations (23) and (24) are $(2\Delta x)/9\left|u^{(3)}\right|$.

To approximate $(u^h_{xx})_i^{n+1,s}$, $i = 2, N-1$ with ***fourth-order*** we use five points stencil and given Neumann boundary conditions

$$(u^h_{xx})^{n+1,s}_2 = \frac{a_1}{\Delta x}\gamma_1(t^{n+1}) + \frac{1}{\Delta x^2}\Big(a_2 u^{n+1,s}_2 + a_3 u^{n+1,s}_3 + a_4 u^{n+1,s}_4 + a_5 u^{n+1,s}_5 + a_6 u^{n+1,s}_6\Big), \quad (25)$$

$$(u^h_{xx})^{n+1,s}_{N-1} = -\frac{a_1}{\Delta x}\gamma_2(t^{n+1}) + \frac{1}{\Delta x^2}\Big(a_2 u^{n+1,s}_{N-1} + a_3 u^{n+1,s}_{N-2} + a_4 u^{n+1,s}_{N-3} + a_5 u^{n+1,s}_{N-4} + a_6 u^{n+1,s}_{N-5}\Big), \quad (26)$$

where the coefficients are found by matching the Taylor series expansion of the left-hand side terms up to the term $O(\Delta x^4)|u^{(6)}|$ which gives us the following values of coefficients

$$a_1 = -\frac{50}{137}, a_2 = \frac{315}{548}, a_3 = -\frac{887}{411},$$
$$a_4 = \frac{653}{274}, a_5 = -\frac{131}{137}, a_6 = \frac{257}{1644}.$$

Substituting coefficients into (25) and (26), the second-order derivatives $(u^h_{xx})^{n+1,s}_i$ $i = 2, N-1$ are approximated with the fourth-order approximation by the following formula

$$(u^h_{xx})^{n+1,s}_2 = -\frac{50}{137\Delta x}\gamma_1(t^{n+1}) + \frac{1}{\Delta x^2}\Big(\frac{315}{548}u^{n+1,s}_2 - \frac{887}{411}u^{n+1,s}_3 + \frac{653}{274}u^{n+1,s}_4 - \frac{131}{137}u^{n+1,s}_5 + \frac{257}{1644}u^{n+1,s}_6\Big), \quad (27)$$

$$(u^h_{xx})^{n+1,s}_{N-1} = \frac{50}{137\Delta x}\gamma_2(t^{n+1}) + \frac{1}{\Delta x^2}\Big(\frac{315}{548}u^{n+1,s}_{N-1} - \frac{887}{411}u^{n+1,s}_{N-2} + \frac{653}{274}u^{n+1,s}_{N-3} - \frac{131}{137}u^{n+1,s}_{N-4} + \frac{257}{1644}u^{n+1,s}_{N-5}\Big). \quad (28)$$

The absolute truncation errors of equations (27) and (28) are $(\Delta x^4/15)\left|u^{(6)}\right|$. In (5) second-order derivatives at time level n, $(u_{xx})^n_i$ are approximated by equations (27) and (28) with $s = 0$. Substituting equations (23), (24), (27) and (28) into equation (6), the following fourth-order deferred correction approximations of $(u_{xx})^{n+1,s+1}_i$, $i = 2, N-1$ are

$$(u_{xx})^{n+1,s+1}_2 = -\frac{50}{137\Delta x}\gamma_1(t^{n+1}) - \frac{2}{3\Delta x^2}\Big(u^{n+1,s+1}_2 - u^{n+1,s+1}_3\Big) + \frac{1}{\Delta x^2}\Big(\frac{2041}{1644}u^{n+1,s}_2 - \frac{387}{137}u^{n+1,s}_3 + \frac{653}{274}u^{n+1,s}_4 - \frac{131}{137}u^{n+1,s}_5 + \frac{257}{1644}u^{n+1,s}_6\Big), \quad (29)$$

$$(u_{xx})^{n+1,s+1}_{N-1} = \frac{50}{137\Delta x}\gamma_2(t^{n+1}) - \frac{2}{3\Delta x^2}\Big(u^{n+1,s+1}_{N-1} - u^{n+1,s+1}_{N-2}\Big) + \frac{1}{\Delta x^2}\Big(\frac{2041}{1644}u^{n+1,s}_{N-1} - \frac{387}{137}u^{n+1,s}_{N-2} + \frac{653}{274}u^{n+1,s}_{N-3} - \frac{131}{137}u^{n+1,s}_{N-4} + \frac{257}{1644}u^{n+1,s}_{N-5}\Big). \quad (30)$$

When the iterations converge the absolute truncation error of (29) and (30) is $(\Delta x^4/15)\left|u^{(6)}\right|$. We will use the abbreviation **NHOD** to denote the deferred correction scheme of fourth-order with Neumann boundary conditions (5), (19) and (27)–(30).

B. Fourth-order compact scheme

Let us briefly represent the main idea and final formulae of compact schemes. Spatial derivatives in the Crank-Nikolson scheme are evaluated by the fourth-order compact of implicit finite differences schemes [5, 7, 8, 13, 14, 20].

Fourth-order compact scheme (Dirichlet boundary conditions)

In [8, 14], the Dirichlet boundary conditions $u(0, m\Delta t) = \alpha_1(t^m) = u^m_1$, and $u(l, m\Delta t) = \alpha_2(t^m) = u^m_N$ are used to derive the following fourth-order schemes

$$\begin{aligned}(u_{xx})^m_2 + \alpha(u_{xx})^m_3 &= \frac{1}{\Delta x^2}(a_1 u^m_1 + a_2 u^m_2 + a_3 u^m_3 + a_4 u^m_4 + a_5 u^m_5 + a_6 u^m_6) \\ &= \frac{a_1}{\Delta x^2}\alpha_1(t^m) + \frac{1}{\Delta x^2}(a_2 u^m_2 + a_3 u^m_3 + a_4 u^m_4 + a_5 u^m_5 + a_6 u^m_6),\end{aligned} \quad (31)$$

$$(u_{xx})^m_{i-1} + 10(u_{xx})^m_i + (u_{xx})^m_{i+1} = \frac{2}{\Delta x^2}(6u^m_{i-1} - 12u^m_i + 6u^m_{i+1}), i = 2, \ldots, N-1, \quad (32)$$

$$\begin{aligned}(u_{xx})^m_{N-1} + \alpha(u_{xx})^m_{N-2} &= \frac{1}{\Delta x^2}(a_1 u^m_N + a_2 u^m_{N-1} + a_3 u^m_{N-2} + a_4 u^m_{N-3} + a_5 u^m_{N-4} + a_6 u^m_{N-5}) \\ &= \frac{a_1}{\Delta x^2}\alpha_2(t^m) + \frac{1}{\Delta x^2}(a_2 u^m_{N-1} + a_3 u^m_{N-2} + a_4 u^m_{N-3} + a_5 u^m_{N-4} + a_6 u^m_{N-5}),\end{aligned} \quad (33)$$

where the coefficients can be found by matching the Taylor series expansion of left-hand side terms up to order $O(\Delta x^4)|u^{(6)}|$ which gives the following values of coefficients [10]

$$\alpha = \frac{1}{2}, a_1 = \frac{19}{24}, a_2 = -\frac{7}{12}, \quad a_3 = -\frac{19}{12}, a_4 = \frac{11}{6}, a_5 = -\frac{13}{24}, a_6 = \frac{1}{12}. \quad (34)$$

The scheme (5), (31)–(34) is a fourth-order compact finite difference scheme for the Dirichlet boundary value problem. In (5) one has to replace the index $n+1, s+1$ by the index m. We will use the abbreviation **DHOC** for this scheme.

Fourth-order compact scheme (Neumann boundary conditions)

In [22], the Neumann boundary conditions (4), $u_x(0, m\Delta t) = \gamma_1(t^m)$ and $u_x(l, m\Delta t) = \gamma_2(t^m)$ are used to derive the following fourth-order approximations at the near boundary points (x_2, t^m), (x_3, t^m), (x_{N-2}, t^m) and (x_{N-1}, t^m)

$$22(u_{xx})^m_2 - 4(u_{xx})^m_3 = -\frac{12\gamma_1(t^m)}{\Delta x} + \frac{12}{\Delta x^2}(u^m_3 - u^m_2), \quad (35)$$

$$22(u_{xx})^m_{N-1} - 4(u_{xx})^m_{N-2} = \frac{12\gamma_2(t^m)}{\Delta x} + \frac{12}{\Delta x^2}(u^m_{N-2} - u^m_{N-1}). \quad (36)$$

The scheme (5), (32), (35) and (36) has the order $O(\Delta t^2, \Delta x^4)$ at the interior grid points $i = 3, \ldots, N-2$, (see for example [22]) and the order of $O(\Delta t^2, \Delta x^2)$ at the grid points x_2 and x_{N-1} [11]. We will use abbreviation **NHOC** to denote this scheme.

Updated fourth-order compact scheme (Neumann boundary conditions)

To increase the order of accuracy of the **NHOC** scheme, we suggest to use the fourth-order deferred correction approximation (29) and (30) for the Neumann boundary conditions and the compact finite difference scheme (32) at interior points. Thus, the updated fourth-order compact scheme with Neumann boundary conditions is as follows. At the interior points the second-order derivatives at higher $n+1, s+1$ and lower n levels are approximated by standard compact schemes

$$(u_{xx})_{i-1}^{n+1,s+1} + 10(u_{xx})_i^{n+1,s+1} + (u_{xx})_{i+1}^{n+1,s+1} = \frac{12}{\Delta x^2}(u_{i-1}^{n+1,s+1} - 2u_i^{n+1,s+1} + u_{i+1}^{n+1,s+1}), \quad (37)$$

$$(u_{xx})_{i-1}^{n} + 10(u_{xx})_i^{n} + (u_{xx})_{i+1}^{n} = \frac{12}{\Delta x^2}(u_{i-1}^{n} - 2u_i^{n} + u_{i+1}^{n}), i = 2, \ldots, N-1. \quad (38)$$

The fourth-order deferred approximations (29) and (30) are used at the near boundary points at the higher time level and equations (27) and (28) are used to approximate the second-order derivatives at the lower time level n. Together with equation (5) we get the fourth-order compact scheme for the Neumann boundary value problem (1), (2) and (4). We are use the abbreviation **NHODC** to denote this scheme. The NHODC scheme has the order of approximation O$(\Delta t^2, \Delta x^4)$ in the uniform norm.

III. Numerical examples

In this section, several numerical examples are carried to verify and compare the accuracy of the DHOC, DHOD, NHOC, NHOD, and NHODC schemes.

In all computations, we used $\Delta t = \Delta x^2/4$ and $\epsilon = 10^{-10}$. The following stopping criterion is used

$$\max_{1 \le i \le N} \mid u_i^{n+1,\widehat{S}+1} - u_i^{n+1,\widehat{S}} \mid < \epsilon, \quad s = 0, \ldots, \widehat{S},$$

where “$\widehat{S}$” denotes the number of the last iteration.

In the first part of this section, numerical examples are provided to compare the accuracy of DHOC and DHOD schemes with zero and non-zero Dirichlet boundary conditions. The computations are performed using uniform grids of $11, 21, 41, 81$ and 161 nodes. The initial and boundary conditions are obtained based on the exact solutions. For the testing purpose only, all computations are performed for $0 \le t \le 1$.

Example I (The homogeneous heat equation with the homogeneous Dirichlet boundary conditions.)

$$u_t = u_{xx}, \quad 0 \le x \le 1, \quad t > 0,$$
$$u(x,0) = sin(\pi x), \quad u(0,t) = 0, \quad u(1,t) = 0. \quad (39)$$

The exact solution is $u(x,t) = e^{-\pi^2 t}\sin(\pi x)$. The results of performance over the time interval $t \in [0,1]$ for the DHOC and DHOD schemes are represented in Table I, where the maximum error and the rate of convergence at time instant $t = 1$ are shown.

TABLE I
Maximum absolute error, Rate of convergence, Average number of iterations and CPU time in seconds of the DHOC and DHOD schemes for problem (39) at time instant $t = 1$.

Types of scheme	Grid points	Maximum absolute error	Rate of conv.	Average number of itr.	CPU time
DHOC	11	1.541×10^{-5}	–	1	0.006
	21	8.335×10^{-7}	4.209	1	0.047
	41	6.221×10^{-8}	3.743	1	0.374
	81	3.968×10^{-9}	3.970	1	2.992
	161	2.479×10^{-10}	4.001	1	23.938
DHOD	11	4.565×10^{-5}	–	5	0.017
	21	2.065×10^{-6}	4.466	3	0.118
	41	1.662×10^{-7}	3.635	2	0.944
	81	1.069×10^{-8}	3.959	2	6.471
	161	6.714×10^{-10}	3.994	2	51.766

Example II (The non-homogeneous heat equation with non-homogeneous Dirichlet boundary conditions)

$$u_t = u_{xx} + (\pi^2 - 1)e^{-t}\cos(\pi x) + 4x - 2,$$
$$0 \le x \le 1, t > 0,$$
$$u(x,0) = \cos(\pi x) + x^2, \quad u(0,t) = e^{-t},$$
$$u(1,t) = -e^{-t} + 4t + 1. \quad (40)$$

The exact solution is $u(x,t) = e^{-t}\cos(\pi x) + x^2 + 4xt$. The results of performance over the time domain $t \in [0,1]$ for the DHOC and DHOD schemes are represented in Table II, where the maximum error and the rate of convergence at time instant $t = 1$ are shown.

TABLE II
Maximum absolute error, the rate of convergence, Average number of iterations and CPU time in seconds of the DHOC and DHOD schemes for problem (40) at time instant $t = 1$.

Types of scheme	Grid points	Maximum absolute error	Rate of conv.	Average number of itr.	CPU time
DHOC	11	1.847×10^{-5}	–	1	0.007
	21	3.690×10^{-7}	5.645	1	0.058
	41	7.559×10^{-9}	5.609	1	0.460
	81	6.643×10^{-10}	3.508	1	3.678
	161	4.809×10^{-11}	3.787	1	29.422
DHOD	11	2.852×10^{-5}	–	8	0.024
	21	6.961×10^{-7}	5.356	7	0.166
	41	2.047×10^{-8}	5.087	7	1.326
	81	1.839×10^{-9}	3.476	6	9.092
	161	1.264×10^{-10}	3.862	6	72.735

The two last columns of Tables I and II demonstrate the average number of iterations in DHODs at one time step and the CPU time required to obtain the solution at time instant $t = 1$. The average number of iterations means the total number of iterations divided by the number of time steps. As a rule, at the initial stage the convergence of deferred correction requires more iterations. For larger instants of time, the convergence occurs after $2 \sim 8$ iterations as can be seen from Tables I and II. Clearly, the DHOC scheme provides a more accurate solution. Both schemes are seen to be the fourth-order of accuracy, as the error is reduced approximately by a factor four when the mesh is refined by half. The better computational efficiency of DHOC schemes obvious from the results in Tables I and II (DHOC is almost three times better than DHOD in the sense of the CPU time). At the same time, it is worth to note that construction of the DHOD scheme is easy and require only a regular three point stencil at higher time level which can be solved similar to the standard second-order Crank-Nicolson method to give higher order results. There is no need to store the inverse of coefficient matrices before the time-marching in the implementation of DHOC scheme.

In the second part of this section, numerical examples are provided to verify and compare the accuracy of the NHOC, NHOD, and NHODC schemes with zero and non-zero Neumann boundary. The computations are performed using the uniform grids of $11, 21, 41$, and 81 nodes.

Example III (The homogeneous heat equation with homogeneous Neumann boundary conditions)

$$\begin{aligned} u_t =& u_{xx}, \quad 0 \le x \le 1, \quad t > 0, \\ u(x,0) =& \cos(\pi x), \quad u_x(0,t) = 0, \quad u_x(1,t) = 0. \end{aligned} \tag{41}$$

The exact solution is $u(x,t) = e^{-\pi^2 t}\cos(\pi x)$. The results of performance over the time interval $t \in [0,1]$ for the NHOC, NHOD and NHODC schemes are represented in Table III, where the maximum error and the rate of convergence at $t = 1$ are shown.

TABLE III
THE MAXIMUM ABSOLUTE ERROR, RATE OF CONVERGENCE, AVERAGE NUMBER OF ITERATIONS AND THE CPU TIME IN SECONDS OF THE NHOC, NHOD AND NHODC SCHEMES FOR PROBLEM (41) AT TIME INSTANT $t = 1$.

Types of scheme	Grid points	Maximum absolute error	Rate of conv.	Average number of itr.	CPU time
NHOC	11	7.060×10^{-6}	–	1	0.004
	21	9.363×10^{-7}	2.915	1	0.033
	41	1.196×10^{-7}	2.969	1	0.262
	81	1.503×10^{-8}	2.989	1	2.094
NHOD	11	3.808×10^{-7}	–	5	0.014
	21	1.361×10^{-8}	4.807	3	0.068
	41	3.907×10^{-10}	5.122	2	0.361
	81	8.748×10^{-12}	5.481	2	2.890
NHODC	11	5.546×10^{-7}	–	5	0.014
	21	2.2241×10^{-8}	4.640	3	0.068
	41	7.456×10^{-10}	4.899	2	0.363
	81	2.429×10^{-11}	4.940	2	2.906

Example IV (The non-homogeneous heat equation with non-homogeneous Neumann boundary conditions)

$$\begin{aligned} & u_t = u_{xx} + (\pi^2/2)e^{-(\pi^2/2)t}\cos(\pi x) + x - 2, \\ & 0 \le x \le 1, \quad t > 0, \\ & u(x,0) = \cos(\pi x) + x^2, \quad u_x(0,t) = t, \\ & u_x(1,t) = 2 + t. \end{aligned} \tag{42}$$

The exact solution is $u(x,t) = e^{-(\pi^2/2)t}\cos(\pi x) + x^2 + xt$. The results of performance over the time interval $t \in [0,1]$ for the NHOC, NHOD and NHODC schemes are compared in Table IV, where the maximum error and the rate of convergence at the time instant $t = 1$ are shown.

TABLE IV
THE MAXIMUM ABSOLUTE ERROR, RATE OF CONVERGENCE, AVERAGE NUMBER OF ITERATIONS AND THE CPU TIME IN SECONDS OF THE NHOC, NHOD AND NHODC SCHEMES FOR PROBLEM (42) AT TIME INSTANT $t = 1$.

Types of scheme	Grid points	Maximum absolute error	Rate of conv.	Average number of itr.	CPU time
NHOC	11	1.940×10^{-4}	–	1	0.005
	21	2.743×10^{-5}	2.823	1	0.042
	41	3.584×10^{-6}	2.936	1	0.332
	81	4.562×10^{-7}	2.974	1	2.656
NHOD	11	1.039×10^{-5}	–	8	0.023
	21	3.684×10^{-7}	4.818	7	0.161
	41	1.002×10^{-8}	5.201	6	1.102
	81	1.670×10^{-10}	5.906	5	7.344
NHODC	11	1.533×10^{-5}	–	8	0.021
	21	6.254×10^{-7}	4.616	7	0.150
	41	2.052×10^{-8}	4.930	6	1.029
	81	6.187×10^{-10}	5.051	5	6.859

It can be seen from Tables III and IV that the convergence rate of the NHOC scheme is about 3.0, while the NHODC scheme gives a higher convergence rate of about 5.0. This observation confirms that high-order compact schemes are very sensitive to the approximation of Neumann boundary conditions. The NHOD scheme demonstrates the highest convergence rate of more than 5.0. and provides a more accurate solution on the same grid compared with the both, the NHOC and NHODC schemes. Computational efficiency of the NHOD and NHODC schemes are very similar and they are more efficient than the NHOC scheme (in terms of the CPU time required to reach the same accuracy).

IV. CONCLUSION

In this article, a new set of high-order schemes for the one dimensional heat conduction problem with Dirichlet and Neumann boundary conditions is constructed using a deferred correction technique. The greatest significance of this set of deferred correction schemes, compared with high-order compact ones, is the easier development and better accuracy in the case of Neumann boundary conditions. Numerical examples confirm the order of accuracy. The construction of high-order deferred correction schemes require only a regular three point stencil at higher time level which is similar to the standard second-order Crank-Nicolson method. We could also apply such methods for multi-dimensional problem while splitting in simpler one dimensional problems.

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