Numerical Gradient Schemes for Heat Equations Based on the Collocation Polynomial and Hermite Interpolation

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Abstract

It is a well-known fact that the convergence order of high-order compact difference schemes (H-OCD) for heat conduction problems with the first kind boundary conditions is $O(\tau^2 + h^4)$. However, when the spatial step size $h$ is too small, it will take longer time to get the approximate solutions. In addition, the changes of the errors of the difference terms are also small along with the reduction of $h$. In order to deal with these problems, this article presents a new numerical gradient method based on the collocation polynomial and Hermite interpolation. The analysis of truncation errors shows that the convergence order of this kind of numerical gradient is also $O(\tau^2 + h^4)$ in the discrete maximum norm, but there exists a more better approximate on the difference terms. Moreover, The Richardson extrapolation technique is also considered. Finally, some numerical experiments are given to confirm our theoretical analysis.

Key words: Heat equation, compact difference schemes, numerical gradient, collocation polynomial, bi-cubic Hermite interpolation, Richardson extrapolation

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1 Introduction

Recently, a great deal of efforts have been devoted to the development of numerical approximation of heat equation problems (see, [1,3,8,9]). It is well known that the traditional numerical schemes have low accuracy, and thus need fine discretization to obtain desired accuracy, which will present many computational challenges due to the prohibitive computer memory and CPU time requirements (see, [3]).

For heat equations, the forward Euler methods, backward Euler methods and Crank-Nicolson methods were presented in [1]. In addition, three layer implicit schemes also appeared in Ref. [8]. The forward Euler method and backward method only have one-order accuracy in time and two-order accuracy in space. Also, the forward Euler method is not stable when $c\tau/h^2 \leq 1/2$. The three layer implicit compact format can reach $O(\tau^2 + h^4)$, but the format is complex. The Crank-Nicolson method has two-order accuracy in time and two-order accuracy in space, which is not good compared to the high-order compact difference scheme (see, [3]) with two-order accuracy in time and four-order accuracy in space. The high-order compact difference format (H-OCD) has many advantages, such as using less grid backplane point, high accuracy, good stability. This scheme plays more and more important role in the numerical solution of partial differential equations and the computational fluid mechanics field. But the calculation will be increased rapidly with the increase of grid points. In addition, in the experimental process for the large problems, we found that the changes of the truncation errors of high-order compact difference schemes are large at first, and then very small along with the increase of the grid points.

This article will give a new numerical gradient method based on the collocation polynomial and Hermite interpolation to overcome the above problems on the high-order compact difference schemes. First, we obtain the intermediate points of the grids by cubic and bi-cubic Hermite interpolation. And then, based on these intermediate points, one can deduce new explicit schemes for the gradient of the discrete solutions of heat equations, which will greatly reduce the amount of calculation in the same accuracy with the high-order compact difference schemes.

The outline of the article is organized as follows. In Section 2, a linearized compact difference scheme is derived for one-dimensional heat equations. And then the numerical gradient method is presented and its convergence is analyzed in detail in Section 3. In addition, the local Hermit interpolation and refinement are also introduced in Section 3. Finally, some numerical results are reported in Section 4.
2 The High-Order Compact Difference

Firstly, for convenience, let us consider the following one-dimensional heat equation problem

\[
\begin{aligned}
\frac{\partial u}{\partial t}(x, t) &= c \frac{\partial^2 u}{\partial x^2}(x, t), \\
(x, t) &\in (0, 1) \times (0, T), \\
u(x, 0) &= \varphi(x), \\
u(0, t) &= g_1(t), \\
u(1, t) &= g_2(t), \\
u(t, t) &= g_2(t), \\
u(1, t) &= g_2(t), & t \in (0, T),
\end{aligned}
\]

where \(T\) is a positive number. Denote \(\Omega = (0, 1) \times (0, T)\). In addition, the solution \(u(x, t)\) is assumed to be sufficiently smooth and has the required continuous partial derivative.

Next, let us recall the linearized compact difference scheme, which has been introduced in Ref. [2].

Let \(\Omega_h = \{x_j | x_j = jh, \ 0 \leq j \leq N\}\) be a uniform partition of \([0, 1]\) with the mesh size \(h = 1/N\) and \(\Omega_\tau = \{t_k | t_k = k\tau, \ 0 \leq k \leq M\}\) be a uniform partition of \([0, T]\) with the temporal step size \(\tau = T/M\). We denote \(\Omega_{h\tau} = \Omega_h \times \Omega_\tau\). Let \(\{u_j^k | 0 \leq j \leq N, \ 0 \leq k \leq M\}\) be a mesh function defined on \(\Omega_{h\tau}\). For convenience, some other notations are introduced below.

\[
\begin{aligned}
[u]_j^k &= u(x_j, t_k), \\
u_j^k &\approx u(x_j, t_k), \\
u_j^{k+\frac{1}{2}} &= \frac{u_j^k + u_{j+1}^k}{2}, \\
\delta_t u_j^{k+\frac{1}{2}} &= u_j^{k+1} - u_j^k, \\
\delta_t u_j^{k-\frac{1}{2}} &= \frac{u_j^k - u_{j-1}^k}{2}, \\
\delta_x u_j^{k+\frac{1}{2}} &= u_j^k - u_{j-1}^k, \\
\delta_x u_j^{k-\frac{1}{2}} &= 2u_j^k - u_{j-1}^k - u_{j+1}^k.
\end{aligned}
\]

In the sequel, we sometimes use the index pair \((j, k)\) to represent the mesh point \((x_j, t_k)\).

Lemma 2.1 ([2]). Suppose \(g(x) \in C^6[x_{i-1}, x_{i+1}]\), then

\[
\begin{aligned}
\frac{1}{12}[g''(x_{i-1}) + 10g''(x_i) + g''(x_{i+1})] - \\
\frac{1}{12}[g(x_{i-1}) - 2g(x_i) + g(x_{i+1})] &= \frac{h^4}{240}g^{(6)}(\omega_i),
\end{aligned}
\]

where \(\omega_i \in (x_{i-1}, x_{i+1})\).
In order to obtain the high-order compact difference schemes on the equation (1), let us firstly consider it at the point \((x_j, t_{k+\frac{1}{2}})\)

\[
\frac{\partial u}{\partial t}(x_j, t_{k+\frac{1}{2}}) = c \frac{\partial^2 u}{\partial x^2}(x_j, t_{k+\frac{1}{2}}), \quad 0 \leq i \leq N, \quad 0 \leq k \leq M - 1. \tag{3}
\]

Next, for \(g(x) = [g_0(x), g_1(x), \ldots, g_N(x)]\), we introduce the operator \(\beta\) with the help of Lemma 2.1. We denote

\[
\beta g_j(x) = \frac{1}{12} [g_{j-1}(x) + 10g_j(x) + g_{j+1}(x)], \quad 1 \leq j \leq N - 1. \tag{4}
\]

By the famous Taylor formula, we have

\[
\delta t u_{k+\frac{1}{2}}^j - \frac{1}{2} \delta t u_{k+1}^j + 10 \delta t u_{k}^j + \delta t u_{k+1}^j = \frac{6c \tau}{h^2} \delta_x^2 u(x_j, t_{k+\frac{1}{2}}) + R_k^j, \tag{5}
\]

and

\[
R_k^j = \tau^2 \beta r_j^k + \frac{c \tau h^4}{40} \left[ \frac{\partial^6 u}{\partial x^6}(\theta_j^k, t_k) + \frac{\partial^6 u}{\partial x^6}(\theta_j^{k+1}, t_{k+1}) \right], \tag{6}
\]

where

\[
r_j^k = \frac{1}{24} \frac{\partial^4 u}{\partial x^2}(x_j, \xi_j^k) - \frac{c}{8} \frac{\partial^4 u}{\partial x^2 \partial t^2}(x_j, \eta_j^k), 1 \leq j \leq N - 1, 0 \leq k \leq M - 1. \]

Noting the initial and boundary conditions in the equation (1), we obtain the following high-order compact difference scheme.

\[
(u_{j-1}^{k+\frac{1}{2}} - u_{j-1}^k) + 10(u_{j}^{k+\frac{1}{2}} - u_{j}^k) + (u_{j+1}^{k+\frac{1}{2}} - u_{j+1}^k) = \frac{6c \tau}{h^2} \delta_x^2 (u_{j}^k + u_{j}^{k+1}), \tag{7}
\]

where \(1 \leq j \leq N - 1, 0 \leq k \leq M - 1, \)

\[
u_j^0 = \varphi(x_j), \quad 0 \leq j \leq N, \tag{8}
\]

\[
u_0^k = g_1(k \tau), \quad u_N^k = g_2(k \tau), \quad 0 \leq k \leq M. \tag{9}
\]

Denoting \(u_h^k = [u_1^k, u_2^k, \ldots, u_{N-1}^k]^T, \quad k = 0, 1, 2, \ldots, M - 1, \) the above equation (7)-(9) can be written as

\[
(T_{10} - \frac{6c \tau}{h^2} T_2) u_h^{k+1} = (T_{10} + \frac{6c \tau}{h^2} T_2) u_h^k + F_0, \tag{10}
\]
where

\[
T_{10} = \begin{pmatrix}
10 & 1 & 0 & \ldots & 0 & 0 \\
1 & 10 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 1 & -10
\end{pmatrix}
\quad \text{and} \quad
T_2 = \begin{pmatrix}
-2 & 1 & 0 & \ldots & 0 & 0 \\
1 & -2 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 1 & -2
\end{pmatrix}.
\]

Obviously, by (6), we know that the truncation error of the compact difference scheme (7) is \(O(\tau^2 + h^4)\).

### 3 A Numerical Gradient Method Based on the Local Hermite Interpolation and Collocation Polynomial

The truncation errors of compact difference methods talked about in section 2 are \(O(\tau^2 + h^4)\) in [2]. However, the calculation will be increased rapidly with the increase of grid points. In addition, in the experimental process for the large problems, we found that the changes of the truncation errors of high-order compact difference scheme are large at first, and then very small along with the increase of the grid points (see Table 2,3,4 in Section 4).

In order to deal with those problems, we will give a new numerical gradient method based on the collocation polynomial and Hermite interpolation.

Let \(U_h\) be the vector space of the grid function on \(\Omega_{\tau h}\). The \(u_h\) denotes the discrete solution satisfying the formula (7)-(9). Denote

\[
P = \frac{\partial u(x, t)}{\partial x},
\]

(11)

Our improvements are as follows:

(1) First, get the values of points \(u_j^T\) by H-OCD scheme (7)-(9) in Section 2;
(2) Based on (1), we obtain the formula of \(P_j\) with the help of collocation polynomial; i.e, \(P_j = \frac{1}{12h}[8u(x_{j+1}, T) - 8u(x_{j-1}, T) + u(x_{j-2}, T) - u(x_{j+2}, T)]\);
(3) Then, get the intermediate points based on the Hermite interpolation; i.e., \(u_{j+\frac{1}{2}} = \frac{1}{2}(u_j^T + u_{j+1}^T) + \frac{h}{8}(P_j - P_{j+1})\).

Through the above improvements, one can deduce a new explicit numerical gradient scheme for the gradient term of the discrete solutions of heat equa-
tions, which will greatly reduce the amount of calculation in the same accuracy with the high-order compact difference format.

Next, according to our improvement scheme, let us analysis the convergence orders of $u$ and its partial derivative on the refinement and collocation parts in the internal $[0,1]$.

### 3.1 The Local Hermite Interpolation and Refinement

For convenience, we just consider Hermite cubic and bi-cubic interpolation function $u_H(x, T)$ on the interval $[x_j, x_{j+1}] \subset \Omega_h$, and its vertexes are as follows:

$$z_1(x_j, T), \quad z_2(x_{j+1}, T) \in \Omega_{\tau h}.$$

On the segment $z_1 - z_2$, let the cubic interpolation function satisfy the condition

$$u_H(z_1) = u(z_1), \quad u_H(z_2) = u(z_2),$$

$$(u_H)_x(z_1) = u_x(z_1), \quad (u_H)_x(z_2) = u(z_2).$$

Based on [5], we can get the Hermite interpolation polynomial as follows

$$u_H(x_{j+\frac{1}{2}}, T) = \frac{1}{2}[u(z_1) + u(z_2)] + \frac{h}{8}[u_x(z_1) - u_x(z_2)], \quad (12)$$

where $j = 1, 2, ..., N - 1$. The interpolation errors are

$$u_H(x_{j+\frac{1}{2}}, T) - u(x_{j+\frac{1}{2}}, T) = \frac{h^4}{4!}u_{xxxx}(\xi_j)(x_{j+\frac{1}{2}} - x_j)^2(x_{j+\frac{1}{2}} - x_{j+1})^2$$

$$= \frac{h^4}{24 \times 16}u_{xxxx}(\xi_j), \quad j = 1, 2, ..., N - 1, \quad (13)$$

where $\xi_j$ is between $z_1$ and $z_2$ (see, [5]). So we have, by (11), the refinement computation format

$$u_{j+\frac{1}{2}}^T = \frac{1}{2}(u_j^T + u_{j+1}^T) + \frac{h}{8}(P_j - P_{j+1}), \quad j = 2, 3, ..., N - 1. \quad (14)$$

From (13), we know that the refinement schemes also have the four-order accuracy in terms of spacial.
3.2 The Collocation Polynomial

From the above analysis, we know that we must obtain the express of $P_j$ in order to get the specific formula of the intermediate points. Here, we choose the collocation polynomial method. For convenience, we just consider the sub-domain $[x_{j-1}, x_{j+1}] \subset \Omega, (j = 1, 2, ..., N - 1)$.

Then, we denote

$$\xi = x - x_j, \quad x \subset \Omega, \quad (j = 1, 2, ..., N - 1).$$

In order to get the approximation polynomial of $u$, we consider the polynomial space

$$H_4 = \text{span}\{1, \xi, \xi^2, \xi^3, \xi^4\}. \quad (15)$$

Because $T$ are freely chosen, we can just think about the approximation polynomial of $u$ when $t = T$. So we denote $t = M\tau = T$, then

$$H = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + a_4\xi^4. \quad (16)$$

Then we can obtain the following numerical gradients by means of the collocation polynomial.

$$H(x_{j-1}) = u_h(x_{j-1}, T), \quad H(x_j) = u_h(x_{j-1}, T), \quad H(x_{j+1}) = u_h(x_{j+1}, T), \quad j = 2, 3, \ldots, N.$$

By the above conditions and Eq. (1), we get

$$P_j = \frac{1}{2h}[u(x_{j+1}, T) - u(x_{j-1}, T)] + \frac{1}{12h} [\frac{\partial u}{\partial t}(x_{j-1}, T) - \frac{\partial u}{\partial t}(x_{j+1}, T)]
= \frac{1}{12h}[8u(x_{j+1}, T) - 8u(x_{j-1}, T) + u(x_{j-2}, T) - u(x_{j+2}, T)] \quad (17)$$

$$P_0 = P_N = 0.$$

where $j = 2, 3, \ldots, N.$
Next, let us analyze the accuracy of $P_j$. For convenience, we first introduce some basic operators as follows:

Let $n$ be a positive number, and $h = 1/(n - 1)$, then the region $[a, b]$ can be discretized as

$$\Omega_h = \{x_j | x_j = a + jh, \ j = 0, 1, 2, ... n - 1\}.$$  

- **The shift operator**: $Eu(x_j) = Eu(x_{j+1})$

  We suppose that the arbitrary order derivatives of $u(x)$ is existing, then using Taylor expansion to shift operators, we get

  $$u(x_j + h) = \sum_{k=0}^{\infty} \frac{1}{k!} h^k \frac{d^k}{dx^k} u(x_j).$$ (18)

  If we denote $D = \frac{d}{dx}$, then

  $$u(x_{j+1}) = \sum_{k=0}^{\infty} \frac{1}{k!} (hD)^k u(x_j).$$ (19)

  So the shift operator can be written as

  $$E = \sum_{k=0}^{\infty} \frac{1}{k!} (hD)^k = \exp(hD).$$ (20)

- **The inverse shift operator**: $E^{-1}u(x_j) = u(x_{j-1})$.

Thus, we get the following theorems:

**Theorem 3.1** If $u(x, t) \in C^6 (\Omega)$ and $u(x, t) \in C^3 (\Omega)$, then we have

$$\|P - P_j\|_\infty \leq \frac{h^4}{30} \|u\|_{C^5(\Omega)},$$ (21)

where $j = 2, 3, 4, ... N$.

**Proof.** First, we use the Taylor expansion to shift operators, and we get

$$E_x - E_x^{-1} = 2hD_x + \frac{h^3}{3} D_x^3 + \frac{h^5}{60} D_x^5 + O(h^7),$$

$$E_x + E_x^{-1} = 2 + h^2 D_x^2 + \frac{h^4}{12} D_x^4 + O(h^6).$$
Then

\[ P_j = \frac{1}{2h}[u(x_{j+1}, T) - u(x_{j-1}, T) + \frac{h}{12c}[\frac{\partial u}{\partial t}(x_{j-1}, T) - \frac{\partial u}{\partial t}(x_{j+1}, T)] \]

\[ = \frac{1}{12h}[8u(x_{j+1}, T) - 8u(x_{j-1}, T) + u(x_{j-2}, T) - u(x_{j+2}, T)] \]

\[ = \frac{1}{12h}[8E_x - 8E_x^{-1} + E_x^{-1}E_x - E_x E_x]u(x_j, T) \]

\[ = \frac{1}{12h}(E_x - E_x^{-1})(8 - E_x - E_x^{-1})u(x_j, T) \]

\[ = \frac{1}{12h}(2hD_x + \frac{h^3}{3}D_x^3 + \frac{h^5}{60}D_x^5 + O(h^7))(6 - h^2D_x - \frac{h^4}{12}D_x^4 - O(h^6))u(x_j, T) \]

\[ = (D_x + \frac{h^2}{6}D_x^3 + \frac{h^4}{120}D_x^5 - \frac{h^2}{6}D_x^3 - \frac{h^4}{30}D_x^5 - \frac{h^4}{12}D_x^5)u(x_j, T) + O(h^6) \]

\[ = D_x u(x_j, T) - \frac{h^4}{30}D_x^5 u(x_j, T) + O(h^6), \]

where \( j = 2, 3, ..., N \). So

\[ P_j - P = P_j - u_x(x_j, T) = -\frac{1}{30}h^4D_x^5 u(x_j, T) + O(h^6). \]

Thus the proof is completed. □

Through the above theorem, we know that the accuracy of the partial derivative of \( u \) (i.e., \( P_j \)) is \( O(h^4) \) when \( t = T \). In fact, due to (14), it is easy to prove that the accuracy of the intermediate points is \( O(h^4) \), too. The analysis is as follows.

**Theorem 3.2** If \( u(x, t) \in C^6_x(\Omega) \) and \( u(x, t) \in C^4_t(\Omega) \), and \( u(x, t) \) satisfies (1), then

\[ \| u - u^T_{j+\frac{1}{2}} \| \leq \frac{h^4}{384} \| u \|_{C^4(\Omega)} \tag{22} \]

where \( j = 1, 2, ..., N - 1 \).

**Proof.** First, we use the Taylor expansion to shift operators, and we get

\[ E_x - E_x^{-1} = 2hD_x + \frac{h^3}{3}D_x^3 + \frac{h^5}{60}D_x^5 + O(h^7), \]

\[ E_x = 1 + hD_x + \frac{h^3}{2}D_x^3 + \frac{h^5}{6}D_x^5 + \frac{h^4}{24}D_x^4 + \frac{h^5}{120}D_x^5 + O(h^7), \]

\[ E_x^{\frac{1}{2}} = 1 + \frac{h^2}{8}D_x^2 + \frac{h^3}{24}D_x^3 + \frac{h^4}{384}D_x^4 + O(h^5). \]
and then with the help of (14) and (17), we can make the derivations as follows:

\[ u^T_{j+\frac{1}{2}} = \frac{a_{j+1}^T + a_j^T}{2} + \frac{h}{8}(P_j - P_{j+1}) \]

\[ = \frac{u(x_{j+1}, T) + u(x_{j+1}, T)}{2} + \frac{h}{16}[u(x_{j+1}, T) - u(x_{j-1}, T)] - \frac{h^2}{10}[u(x_{j+2}, T) - u(x_j, T)] \]

\[ + \frac{h^3}{96}[\frac{\partial^2 u}{\partial x^2}(x_{j-1}, T) - \frac{\partial^2 u}{\partial x^2}(x_{j+1}, T)] - \frac{h^3}{96}[\frac{\partial^2 u}{\partial x^2}(x_j, T) - \frac{\partial^2 u}{\partial x^2}(x_{j+2}, T)] \]

\[ = \left[ 1 + E_x + \frac{E_x - E_x^{-1}}{16} \right] - \frac{h^2}{16}(E_x + 1) + \frac{h^3}{96}(E_x - E_x^{-1}) + \frac{h^2}{96}(E_x - 1)(E_x + 1) \]

\[ u^T_{j+\frac{1}{2}} = [1 + \frac{1}{2}hD_x + \frac{1}{8}h^2D_x^2 + \frac{1}{48}h^3D_x^3 + O(h^5)]u(x_j, T). \]

So

\[ u^T_{j+\frac{1}{2}} - u(x_{j+\frac{1}{2}}, T) = -\frac{h^4}{384}D_x^4u(x_j, T) + O(h^5). \]

The theorem has been proved. \( \square \)

In addition, according to the constitution of \( P_j \) and \( u^T_{j+\frac{1}{2}} \), they are obviously two-order in terms of time, so we do not talk about the time term in details here.

4 Numerical Experiments

Example 4.1 When \( u(x, 0) = \sin(\pi x), u(0, t) = u(1, t) = 0 \) for the equation (1) with \((x, t) \in (0, 1) \times (0, 1)\), the exact solution of the problem (1) is

\[ u(x, t) = \exp(-\pi^2 t)\sin(\pi x). \]

Next, let us compare the different numerical solutions in the same number of grid points (note that the numerical gradient scheme need only the half of these grid points before the interpolation) with the exact solution as follows.

Table 1 lists the computational results (where Rate\((h) = \log_2(\frac{Error(h)}{Error(\frac{h}{2})})\), and Error\((h) = \max_{x_k=x_0+k h, k=0, 1, \ldots, N} \{ | u(x_k, T) - u(x_k, T) | \} \), \( u(x_k, T) \) represents the exact solution and \( u(x_k, T) \) is the numerical solution.) and Error\((P) = \max_{x_k=x_0+k h, k=0, 1, \ldots, N} \{ | P(x_k, T) - P_k | \} \) with different temporal step sizes when spatial step size is fixed as \( h = 1/10000 \). In order to make sure that the dominated error is from temporal discretization, we use a very small \( h \). From the table, we can draw the conclusion that the convergence orders of backward methods, Crank-Nicolson methods, the compact difference methods and the intermediate points (see Eq. (14)) which are obtained by the numerical gradient scheme in temporal are all \( O(h^2) \).
Table 2 lists the errors for a small and fixed $\tau = 1/100000$, where $h$ is different. The reason why we use a very small $\tau$ is to make sure that the dominated error is from spatial discretization. Obviously, the convergence orders in space are $O(h^4)$.

Table 3 lists the computational results of the intermediate points and $u_x$ with different temporal step sizes when spatial step size is fixed as $h = 1/10000$. We can see that the convergence orders in time can also reach $O(\tau^2)$.

Table 1
Errors and rate of backward, C-N, H-OCD scheme (7-9) and intermediate points in time direction with $h = 1/10000$.

| $\tau$ | Backward method | C-N Compact difference | intermediate points |
|--------|----------------|------------------------|-------------------|
|        | Error     | Rate  | Error | Rate   | Error | Rate |
| 1/10   | 9.9085e-004 | 1.8420 | 3.1587e-005 | 1.7017 | 3.1587e-005 | 1.7017 |
| 1/20   | 2.7638e-004 | 1.5280 | 9.7107e-006 | 1.9297 | 9.7107e-006 | 1.9297 |
| 1/40   | 9.5835e-005 | 1.2936 | 2.5489e-006 | 1.9827 | 2.5487e-006 | 1.9827 |
| 1/80   | 3.9095e-005 | 1.1539 | 6.4490e-007 | 1.9957 | 6.4490e-007 | 1.9957 |
| 1/160  | 1.7570e-005 | 1.0786 | 1.6170e-007 | 1.9989 | 1.6171e-007 | 1.9989 |
| 1/320  | 3.8191e-006 | *     | 4.0453e-008 | 2.0002 | 4.0457e-008 | 1.9997 |
| 1/640  | *     | 1.0112e-008 | *     | 1.0116e-008 | *     |

Figure 1 and 2 display errors curves with different step sizes of the grids and intermediate points when $t = 1$. We can know that, with the changes of $h$ and $\tau$, the changes of the truncation errors in the grid points and intermediate points are large. That means the scheme are good.

Figure 3 shows the numerical solutions and exact solutions of all the points when $h = 1/8$, $\tau = 1/100$, $t = 1$. In order to make the figure more clearly, we choose $h = 1/8$. It is easy to find that the second curve are more smooth.

Figure 4 and 5 show the errors surface maps with different step sizes in both spatial and temporal directions of the mesh grids and intermediate points.

Through these figures, one knows that combination of the compact difference and numerical gradient method in sparse grids is more better than other methods.
Table 2
Errors and rate of backward, C-N and H-OCD scheme (7-9) in space direction with \( \tau = 1/100000. \)

| \( h \)   | Backward method Error | Rate  | C-N Error | Rate  | Compact difference Error | Rate  |
|----------|-----------------------|-------|-----------|-------|--------------------------|-------|
| 1/4      | 3.3338e-005           | 2.2550| 3.3300e-005 | 2.2591| 8.3491e-007              | 4.0355|
| 1/8      | 6.9842e-006           | 2.0471| 6.9563e-006 | 2.0635| 5.0915e-008              | 4.0073|
| 1/16     | 1.6900e-006           | 1.9518| 1.6642e-006 | 2.0158| 3.1660e-009              | 4.0045|
| 1/32     | 4.3687e-007           | 1.7729| 4.1151e-007 | 2.0039| 1.9725e-010              | 4.0466|
| 1/64     | 1.2783e-007           | 1.3303| 1.0260e-007 | 2.0010| 1.1936e-011              | 5.0602|
| 1/128    | 5.0838e-008           | 0.6857| 2.5632e-008 | 2.003 | 3.5776e-013              | *     |
| 1/256    | 3.1605e-008           | 0.2380| 6.4065e-009 | 2.003 | 3.6559e-013              | *     |
| 1/512    | 2.6798e-008           | *     | 1.6012e-009 | *     | 4.1063e-013              | *     |

Table 3
Errors and rate of intermediate points and numerical gradient \( P \) (17) in space direction with \( \tau = 1/100000. \)

| \( h \) | intermediate points Error | Rate  | P Error | Rate  |
|---------|---------------------------|-------|---------|-------|
| 1/4     | 6.9238e-007              | 3.9015| 8.5132e-007 | 3.500 |
| 1/8     | 4.6330e-008              | 3.9759| 7.5242e-008 | 3.8837|
| 1/16    | 2.9444e-009              | 3.9970| 5.0975e-009 | 3.9767|
| 1/32    | 1.8411e-010              | 4.0479| 3.2379e-010 | 4.0820|
| 1/64    | 1.1149e-011              | 5.1740| 1.9119e-011 | 9.7195|
| 1/128   | 3.0883e-013              | *     | 2.2679e-014 | *     |
| 1/256   | 3.6864e-013              | *     | 1.2201e-012 | *     |

**Example 4.2** For \( u(x, 0) = \exp(x), u(0, t) = \exp(t), u(1, t) = \exp(1 + t) \) with \((x, t) \in (0, 1) \times (0, 1)\), the exact solution of the problem (1) is

\[
u(x, t) = \exp(x + t).
\]
Next, let us compare the numerical solution with the exact solution as follows.

From Tables 4 and 5, we know that the numerical results are consistent to our theoretical results.
Fig. 3. The numerical solutions by numerical gradient scheme and exact solutions of all the points when $h = 1/8, \tau = 1/100, t = 1$.

Fig. 4. The errors surface maps with different step sizes in both spatial and temporal directions of the compact difference scheme.

**Remark 4.1** In fact, if we use the Richardson extrapolation [10], we can get that the errors of H-OCD scheme (7)-(9) are four-order in terms of time. However, by Table 6, we conclude that the Richardson extrapolation is good for Problem 4.1, while it is worse for Problem 4.2. That is to say, the Richardson extrapolation method has some limitations. But, according to the constitute forms of the
intermediate points, we know that their truncation errors of numerical gradient scheme can reach \(O(\tau^4)\). Therefore, one may choose different schemes according to the specific problems.
Table 5

Errors and rate of H-OCD scheme (7-9), intermediate points and numerical gradient $P$ (17) in time direction with $h = 1/10000$.

| $\tau$      | Compact difference | Intermediate points | P               |
|-------------|---------------------|---------------------|-----------------|
|             | Error               | Rate               | Error           | Rate           | Error           | Rate           |
| 1/10        | 4.3449e-004         | 1.9988             | 4.3449e-004     | 1.9988         | 2.0491e-003    | 1.9769         |
| 1/20        | 1.0871e-004         | 1.9998             | 1.0871e-004     | 1.9998         | 5.2055e-004    | 1.9887         |
| 1/40        | 2.7183e-005         | 1.9999             | 2.7183e-005     | 1.9999         | 1.3116e-004    | 1.9945         |
| 1/80        | 6.7960e-006         | 2.0005             | 6.7960e-006     | 2.0005         | 3.2914e-005    | 1.9987         |
| 1/160       | 1.6984e-006         | 2.0053             | 1.6984e-006     | 2.0053         | 8.2362e-006    | 2.0053         |
| 1/320       | 4.2303e-007         | 2.0246             | 4.2303e-007     | 2.0246         | 2.0515e-006    | 2.0259         |
| 1/640       | 1.0397e-007         | *                  | 1.0397e-007     | *              | 5.0375e-007    | *              |

Table 6

Errors and rate of H-OCD scheme (7-9) for Problem 4.1, 4.2 in temple direction with $h = 1/10000$.

| $\tau$ | Problem 4.1 |               | Problem 4.2 |               |
|--------|-------------|---------------|-------------|---------------|
|        | Error       | Rate          | Error       | Rate          |
| 1/10   | 2.4185e-006 | 3.9037        | 3.7940e-007 | 4.0358        |
| 1/20   | 1.6158e-007 | 3.9788        | 2.3132e-008 | 4.0350        |
| 1/40   | 1.0249e-008 | 3.9948        | 1.4111e-009 | 0.2075        |
| 1/80   | 6.4288e-008 | 3.9929        | 1.2220e-009 | *             |
| 1/160  | 4.0378e-011 | 3.8824        | 2.2340e-009 | *             |
| 1/320  | 2.7380e-012 | 2.7509        | *           | *             |
| 1/640  | 4.0675e-013 | *             | *           | *             |
5 Further work

Finally, the numerical gradient method can also be applied to the two-dimension heat equation

\[
\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}, \quad (x, y, t) \in (a, b) \times (c, d) \times (0, T),
\]

\[
\begin{align*}
  u(x, y, 0) &= \varphi(x, y), & (x, y) &\in [a, b] \times [c, d], \\
  u(a, y, t) &= g_1(y, t), & u(b, y, t) &= g_2(y, t), & (y, t) &\in [c, d] \times (0, T), \\
  u(x, c, t) &= g_3(x, t), & u(x, d, t) &= g_4(x, t), & (x, t) &\in [a, b] \times (0, T).
\end{align*}
\]

The intermediate points \(u(x_{i+1/2}, y_{j+1/2})\) can be expressed by the values \(u\) of the points and their partial derivatives \(P\) around it (see Fig. 6). \(P(x_i, y_j)\) is connected to the points \(u\) around \(u(x_i, y_j)\) (see Fig. 7).

Fig. 6. The relationships between \(u(x_{i+1/2}, y_{j+1/2})\) and the points \(u\), the partial derivatives \(P\) around \(u(x_{i+1/2}, y_{j+1/2})\).

For this problem, we will research in detail in the future.

6 Conclusions

Recently, many people devote themselves on the development of numerical approximation of heat equation problems. By the numerical comparisons, we can
say that the compact difference scheme is better than the traditional numerical schemes. However, when the space step size $h$ is too small, it will take longer time to get the approximate solution of problem. Also, the truncation errors of the compact difference method changes little along with the change of $h$. Fortunately, the method talked in this article can solve the problem to some extent. And from the last experiment, we know the Richardson extrapolation has some limitations. So we may choose it according to the practical problems. Finally, the numerical experiments showed that our theoretical analysis is true.

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