

OPTIMAL POINT-WISE ERROR ESTIMATE OF TWO SECOND-ORDER ACCURATE FINITE DIFFERENCE SCHEMES FOR THE HEAT EQUATION WITH CONCENTRATED CAPACITY*

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Abstract

In this paper, we propose and analyze two second-order accurate finite difference schemes for the one-dimensional heat equation with concentrated capacity on a computational domain $\Omega = [a, b]$. We first transform the target equation into the standard heat equation on the domain excluding the singular point equipped with an inner interface matching (IIM) condition on the singular point $x = \xi \in (a, b)$, then adopt Taylor's expansion to approximate the IIM condition at the singular point and apply second-order finite difference method to approximate the standard heat equation at the nonsingular points. This discrete procedure allows us to choose different grid sizes to partition the two sub-domains $[a, \xi]$ and $[\xi, b]$, which ensures that $x = \xi$ is a grid point, and hence the proposed schemes can be generalized to the heat equation with more than one concentrated capacities. We prove that the two proposed schemes are uniquely solvable. And through in-depth analysis of the local truncation errors, we rigorously prove that the two schemes are second-order accurate both in temporal and spatial directions in the maximum norm without any constraint on the grid ratio. Numerical experiments are carried out to verify our theoretical conclusions.

Mathematics subject classification: 65M06, 65M12.

Key words: Heat equation with concentrated capacity, Finite difference scheme, Inner interface matching condition, Unconditional convergence, Optimal error estimate.

1. Introduction

In this paper, we consider the one-dimensional heat equation with concentrated capacity (the heat system) [1, 3, 8, 12, 13]

$$[1 + K\delta(x - \xi)]\partial_t u(x, t) - \partial_{xx}u(x, t) = f(x, t), \quad (x, t) \in (a, b) \times (0, T] \quad (1.1)$$

with boundary condition

$$u(a, t) = 0, \quad u(b, t) = 0, \quad t \in (0, T], \quad (1.2)$$

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and initial condition

$$u(x, 0) = u_0(x), \quad x \in [a, b], \quad (1.3)$$

where $u(x, t)$ is the unknown real-valued function, $\delta(x)$ is the Dirac delta function, the positive constant K is the coefficient of the heat concentrated capacity at $x = \xi$ with $\xi \in (a, b)$ being an interior point, $u_0(x)$ and $f(x, t)$ are given real-valued functions, the terminal time T is in $(0, T^*)$ with T^* being the maximal existence time of the solution $u(x, t)$ to the heat system (1.1)-(1.3). The heat equation with concentrated capacity is a special kind of heat equation, in which the heat capacity coefficient contains a Dirac delta function. In other words, the heat capacity coefficient has the property that the jump of heat flow at the singular point is proportional to the time derivative of the temperature [7, 12]. The heat system is an important class of mathematical model widely used in fluid dynamics and chemistry, including chemical reactor theory and colloid chemistry [2, 21].

Extensive mathematical and numerical studies have been carried out for the heat system (1.1) in the literature. Along the mathematical front, we refer to the derivation [5], well-posedness [3, 9] and stability [10] of the heat system. Along the numerical front, different efficient and accurate numerical methods are proposed. By treating the Dirac delta function either as a single point discontinuity, or a smooth function with small support, one can modify the standard finite difference scheme by using the properties of the heat capacity coefficient. Therefore, many of the finite difference schemes [3–6, 8, 9, 18–20] and the finite element approximations [5, 14–16] have been proposed. Javanović and Vulkov [8, 9] derived a finite difference scheme on the uniform grid stencil and proved the convergence order of $(\tau + h^2)$ in the discrete L^2 norm but with the order of $(\tau + h^2 + h^2\sqrt{|\ln \tau|})$ in the discrete H^1 norm, besides the first-order accurate scheme, they also proposed a second-order accurate one for the heat system at the end of their paper [8]. If the exact solution of the original problem on the nonsingular points is smooth enough, Sun and Zhu [20] proposed another second-order accurate finite difference scheme (a box scheme) by using the method of order reduction on non-uniform meshes, and established the optimal error estimate in the maximum norm. Their box scheme possesses three distinct advantages: firstly, no local truncation error is introduced in discretizing the IIM condition; secondly, the scheme features overall second-order accuracy in space; thirdly, non-uniform grids can be employed in the scheme, as ensures that the singular points align precisely with grid nodes. However, the box scheme given in [20] was proposed by using an indirect method, and even at those nonsingular points with a uniform grid, enhancing the precision of the numerical solution is quite challenging. At such times, a compact finite difference scheme instead of the box scheme can be employed to improve the accuracy of the numerical solutions.

In the literature, the heat capacity coefficient containing a Dirac delta function can be viewed as an IIM condition [4, 10, 11]. Many numerical methods have been carried out to solve the interface problems, such as immersed interface method [17], explicit jump immersed interface method and Peskin's immersed boundary method [11]. In this paper, we first rewrite the heat equation with concentrated capacity as an equivalent interface problem, i.e. we split the computational domain into two sub-domains, and take different mesh sizes for the two sub-domains, which ensures that the singular point is a grid node. Then, we deal with the IIM condition by Taylor's expansion at the singular point, while adopting the standard discretization at the nonsingular points, resulting in two finite difference schemes. The main difference between the two schemes is to adopt different approximations of the IIM condition. In particular, we establish the optimal point-wise error estimates of the two proposed schemes by using the H^1 -technique, which differs from the convergence result given in [8] where the error estimate in

the discrete H^1 norm is mere “almost” optimal. The convergence order of the two proposed schemes are proved to be of $\mathcal{O}(\tau^2 + h_1^2 + h_2^2)$ without any constraints on the grid ratio, where h_1 and h_2 are the grid sizes defined on the subdomains $[a, \xi]$ and $[\xi, b]$, respectively. Lastly, we extend the numerical methods and their convergence results to the heat equation with multiple concentrated capacities.

The rest of the paper is arranged as follows. In Section 2, we reformulate the heat equation with concentrated capacity into an interface problem, then derive two second-order accurate finite difference schemes. In Section 3, we prove the unique solvability of the two proposed schemes and establish the optimal point-wise error estimates without any grid-ratio constraint. In Section 4, we extend the heat capacity coefficient with a single Dirac delta function to that with multiple Dirac delta functions. In Section 5, some numerical results are reported to test our theoretical analysis. Finally, we draw some concise conclusions and outlooks in Section 6. Throughout the paper, we use C to be a general positive constant with different values in different occurrences, but independent of the discrete parameters.

2. Two Crank-Nicolson Finite Difference Schemes

In this section, we shall derive two second-order accurate finite difference schemes for the heat system (1.1)-(1.3). Following the procedure of [20], one can reformulate the system (1.1)-(1.3) into the standard heat equation defined on two sub-domains (a, ξ) and (ξ, b) with the following IIM condition at $x = \xi$:

$$\partial_x u(\xi + 0, t) - \partial_x u(\xi - 0, t) = K \partial_t u(\xi, t), \quad 0 < t \leq T. \quad (2.1)$$

The above interface condition can be also formally derived by integrating the Eq. (1.1) over the interval $[\xi - \varepsilon, \xi + \varepsilon]$ and then taking the limit as $\varepsilon \rightarrow 0$, i.e.

$$\lim_{\varepsilon \rightarrow 0} \int_{\xi - \varepsilon}^{\xi + \varepsilon} (1 + K \delta(x - \xi)) \partial_t u(x, t) dx - \lim_{\varepsilon \rightarrow 0} \int_{\xi - \varepsilon}^{\xi + \varepsilon} \partial_{xx} u(x, t) dx = \lim_{\varepsilon \rightarrow 0} \int_{\xi - \varepsilon}^{\xi + \varepsilon} f(x, t) dx \quad (2.2)$$

for $0 < t \leq T$. This together with the continuity of $\partial_t u$ and f with respect to x and the definition of the functional (Dirac delta function) $\delta(x)$ give (2.1).

Utilizing the IIM condition (2.1), the initial-boundary value problem (1.1)-(1.3) can be rewritten as the following interface problem:

$$\partial_t u(x, t) - \partial_{xx} u(x, t) = f(x, t), \quad (x, t) \in (a, \xi) \cup (\xi, b) \times (0, T], \quad (2.3)$$

$$\partial_x u(\xi + 0, t) - \partial_x u(\xi - 0, t) = K \partial_t u(\xi, t), \quad t \in (0, T], \quad (2.4)$$

$$u(\xi + 0, t) = u(\xi - 0, t), \quad t \in (0, T], \quad (2.5)$$

$$u(a, t) = 0, \quad u(b, t) = 0, \quad t \in (0, T], \quad (2.6)$$

$$u(x, 0) = u_0(x), \quad x \in [a, b]. \quad (2.7)$$

Choosing a positive integer N , we define the step size $\tau := T/N$ and denote time steps as $t_n := n\tau$ for $n = 0, 1, 2, \dots, N$ on the time interval $[0, T]$. Choosing two positive integers m and J such that $0 < m < J$, then we define mesh sizes $h_1 := (\xi - a)/m$, $h_2 := (b - \xi)/(J - m)$ on the two subintervals $[a, \xi]$ and $[\xi, b]$, then we denote grid points as $x_j := a + jh_1$ for $j = 0, 1, 2, \dots, m$ and $x_j := x_m + (j - m)h_2$ for $j = m + 1, m + 2, \dots, J$. Denote

$$\Omega_h := \{x_j \mid j = 0, 1, \dots, J\}, \quad \Omega_\tau := \{t_n \mid n = 0, 1, \dots, N\},$$

then the computational domain $[a, b] \times [0, T]$ is partitioned by $\Omega_{h,\tau} := \Omega_h \times \Omega_\tau$. Define the grid function space

$$Z_h^0 := \{u := (u_0, u_1, \dots, u_J)^\top \mid u_0 = u_J = 0\} \subseteq \mathbb{C}^{J+1},$$

and index sets

$$\begin{aligned} \mathcal{T}_h &:= \{j \mid j = 1, 2, \dots, J-1\}, \\ \mathcal{T}_h^0 &:= \{j \mid j = 0, 1, 2, \dots, J\}, \\ \mathcal{T}_h^m &:= \{j \mid j = 1, 2, \dots, m-1, m+1, \dots, J-1\}. \end{aligned}$$

We use u_j^n and U_j^n to denote the approximation and exact value of u at the point $(x_j, t_n) \in \Omega_{h,\tau}$ respectively, and we denote the exact solution vector $U^n \in Z_h^0$ and numerical solution vector $u^n \in Z_h^0$ as

$$U^n := (U_0^n, U_1^n, \dots, U_m^n, \dots, U_J^n)^\top, \quad u^n := (u_0^n, u_1^n, \dots, u_m^n, \dots, u_J^n)^\top, \quad n = 0, 1, \dots, N.$$

Besides, for simplicity of notations, we introduce finite difference discretization operators for $u^n \in Z_h^0$ as follows:

$$\begin{aligned} D_x^+ u_j^n &:= \begin{cases} \frac{u_{j+1}^n - u_j^n}{h_1}, & j = 0, 1, 2, \dots, m-1, \\ \frac{u_{j+1}^n - u_j^n}{h_2}, & j = m, m+1, \dots, J-1, \\ 0, & j = J, \end{cases} \\ D_x^- u_j^n &:= \begin{cases} D_x^+ u_{j-1}^n, & j = 1, 2, \dots, J, \\ 0, & j = 0, \end{cases} \\ D_t^+ u_j^n &:= \frac{u_j^{n+1} - u_j^n}{\tau}, \quad u_j^{n+\frac{1}{2}} := \frac{u_j^n + u_j^{n+1}}{2}, \\ D_x^2 u_j^n &:= \begin{cases} \frac{D_x^+ u_j^n - D_x^- u_j^n}{h_1}, & j = 1, 2, \dots, m-1, \\ \frac{D_x^+ u_j^n - D_x^- u_j^n}{h_2}, & j = m+1, \dots, J-1, \\ \frac{D_x^+ u_m^n - D_x^- u_m^n}{(h_1 + h_2)/2}, & j = m, \\ 0, & j = 0, J. \end{cases} \end{aligned}$$

The discrete inner product, standard l^2 -norm, l^∞ -norm and H^1 -seminorm for $v^n, u^n \in Z_h^0$ are given as

$$\begin{aligned} (v^n, u^n) &:= h_1 \sum_{j=1}^{m-1} v_j^n u_j^n + h_2 \sum_{j=m+1}^{J-1} v_j^n u_j^n + \frac{1}{2} (h_1 + h_2) v_m^n u_m^n, \\ \langle D_x^+ v^n, D_x^+ u^n \rangle &:= h_1 \sum_{j=0}^{m-1} (D_x^+ v_j^n) (D_x^+ u_j^n) + h_2 \sum_{j=m}^{J-1} (D_x^+ v_j^n) (D_x^+ u_j^n), \\ \|v^n\| &:= \sqrt{(v^n, v^n)}, \quad |v^n|_1 := \sqrt{\langle D_x^+ v^n, D_x^+ v^n \rangle}, \quad \|v^n\|_\infty := \max_{0 \leq j \leq J} |v_j^n|. \end{aligned}$$

Inspired by the assumption on the exact solution of the problem (2.3)-(2.7) given in [20], here we similarly assume that

$$u(\xi, \cdot) \in C^3([0, T]), \quad u \in C^{0,3}(\bar{Q}_l) \cap C^{2,2}(\bar{Q}_l) \cap C^{4,0}(\bar{Q}_l), \quad l = 1, 2, \quad (2.8)$$

where

$$Q_1 = (a, \xi) \times (0, T], \quad Q_2 = (\xi, b) \times (0, T].$$

Then under the assumption (2.8), we use the Taylor's expansion for $D_x^- u(x_m, t_{n+1/2})$ at the singular point $x = x_m - 0$ and (2.3) to obtain

$$\begin{aligned} D_x^- U_m^{n+\frac{1}{2}} &= D_x^- u(x_m, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) - \frac{h_1}{2!} \partial_{xx} u(x_m - 0, t_{n+\frac{1}{2}}) \\ &\quad + \frac{h_1^2}{3!} \partial_{xxx} u(\tilde{\theta}_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) - \frac{h_1}{2!} [\partial_t u(x_m, t_{n+\frac{1}{2}}) - f(x_m, t_{n+\frac{1}{2}})] \\ &\quad + \frac{h_1^2}{3!} \partial_{xxx} u(\tilde{\theta}_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) - \frac{h_1}{2!} \left[D_t^+ u(x_m, t_n) - f(x_m, t_{n+\frac{1}{2}}) - \frac{\tau^2}{24} \partial_{ttt} u(x_m, \tilde{\eta}_{n_m}) \right] \\ &\quad + \frac{h_1^2}{3!} \partial_{xxx} u(\tilde{\theta}_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) - \frac{h_1}{2} [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] + \frac{\tau^2 h_1}{48} \partial_{ttt} u(x_m, \tilde{\eta}_{n_m}) \\ &\quad + \frac{h_1^2}{6} \partial_{xxx} u(\tilde{\theta}_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}), \end{aligned} \quad (2.9)$$

where

$$U_m^{n+\frac{1}{2}} = \frac{1}{2} (U_m^n + U_m^{n+1}), \quad \theta_{m_n}, \tilde{\theta}_{m_n} \in (x_{m-1}, x_m), \quad \eta_{n_m}, \tilde{\eta}_{n_m} \in (t_n, t_{n+1}).$$

Similarly, we have

$$\begin{aligned} D_x^+ U_m^{n+\frac{1}{2}} &= \partial_x u(x_m + 0, t_{n+\frac{1}{2}}) + \frac{h_2}{2} [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] - \frac{\tau^2 h_2}{48} \partial_{ttt} u(x_m, \tilde{\eta}_{n_m}) \\ &\quad + \frac{h_2^2}{6} \partial_{xxx} u(\tilde{\vartheta}_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\vartheta_{m_n}, \eta_{n_m}), \end{aligned} \quad (2.10)$$

where $\vartheta_{m_n}, \tilde{\vartheta}_{m_n} \in (x_m, x_{m+1}), \eta_{n_m}, \tilde{\eta}_{n_m} \in (t_n, t_{n+1})$. Subtracting (2.9) from (2.10) and using

$$\begin{aligned} &\partial_x u(x_m + 0, t_{n+\frac{1}{2}}) - \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) \\ &= K \partial_t u(x_m, t_{n+\frac{1}{2}}) = K D_t^+ u(x_m, t_n) - \frac{\tau^2}{24} K \partial_{ttt} u(x_m, \tilde{\eta}_{n_m}), \quad \tilde{\eta}_{n_m} \in (t_n, t_{n+1}), \end{aligned} \quad (2.11)$$

where the assumption $u(\xi, \cdot) \in C^3([0, T])$ was used, we obtain

$$\begin{aligned} &D_x^+ U_m^{n+\frac{1}{2}} - D_x^- U_m^{n+\frac{1}{2}} - \frac{h_1 + h_2}{2} [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] \\ &= K D_t^+ u(x_m, t_n) + r_m^n, \quad n = 0, 1, \dots, N-1, \end{aligned} \quad (2.12)$$

where

$$\begin{aligned} r_m^n := & \frac{\tau^2}{8} \partial_{xtt} [u(\vartheta_{m_n}, \eta_{m_n}) - u(\theta_{m_n}, \eta_{m_n})] - \frac{\tau^2}{48} (h_1 + h_2) \partial_{ttt} u(x_m, \tilde{\eta}_{m_n}) \\ & + \frac{1}{6} \partial_{xxx} [h_2^2 u(\tilde{\vartheta}_{m_n}, t_{n+\frac{1}{2}}) - h_1^2 u(\tilde{\theta}_{m_n}, t_{n+\frac{1}{2}})] - \frac{K}{24} \tau^2 \partial_{ttt} u(x_m, \tilde{\eta}_{m_n}). \end{aligned} \quad (2.13)$$

Then, under assumption (2.8), we obtain the following estimate of r_m^n :

$$|r_m^n| \leq C (\tau^2 + h_1^2 + h_2^2). \quad (2.14)$$

Dividing both sides of (2.12) by $(h_1 + h_2)/2$ and recalling the definition of the operator D_x^2 , we obtain

$$\left(1 + \frac{2K}{h_1 + h_2}\right) D_t^+ U_m^n - D_x^2 U_m^{n+\frac{1}{2}} = f(x_m, t_{n+\frac{1}{2}}) + R_m^n, \quad 0 \leq n < N, \quad (2.15)$$

where

$$R_m^n := -\frac{2r_m^n}{h_1 + h_2}. \quad (2.16)$$

Then we obtain from (2.14) and (2.16) the following estimate of R_m^n :

$$|R_m^n| \leq C (h_1 + h_2)^{-1} (\tau^2 + h_1^2 + h_2^2). \quad (2.17)$$

Omitting the small term R_m^n in (2.15), we derive the following approximation to the heat equation at $x = x_m$:

$$\left(1 + \frac{2K}{h_1 + h_2}\right) D_t^+ u_m^n - D_x^2 u_m^{n+\frac{1}{2}} = f(x_m, t_{n+\frac{1}{2}}), \quad n = 0, 1, \dots, N-1. \quad (2.18)$$

Similarly, under the assumption (2.8), by using Taylor's expansion on the heat equation (2.3) at the point $x = x_j \in \Omega_h \setminus \{x_m\}$, we can obtain that

$$D_t^+ U_j^n - D_x^2 U_j^{n+\frac{1}{2}} = f(x_j, t_{n+\frac{1}{2}}) + R_j^n, \quad j \in \mathcal{T}_h^m, \quad n = 0, 1, \dots, N-1, \quad (2.19)$$

where

$$R_j^n := \frac{\tau^2}{24} \partial_{ttt} u(x_j, \eta_{n_j}) - \frac{h_j^2}{12} \partial_{xxxx} u(\theta_{j_n}, t_{n+\frac{1}{2}}) - \frac{\tau^2}{8} \partial_{xtt} u(\tilde{\theta}_{j_n}, \tilde{\eta}_{n_j}) \quad (2.20)$$

with

$$\theta_{j_n}, \tilde{\theta}_{j_n} \in (x_{j-1}, x_{j+1}), \quad \eta_{n_j}, \tilde{\eta}_{n_j} \in (t_n, t_{n+1}), \quad h_j = \begin{cases} h_1, & j < m, \\ h_2, & j > m. \end{cases} \quad (2.21)$$

Then, under the assumption (2.8), we obtain from (2.20) the following estimate of R_j^n :

$$|R_j^n| \leq C (\tau^2 + h_1^2 + h_2^2), \quad j \in \mathcal{T}_h^m, \quad n = 0, 1, \dots, N-1. \quad (2.22)$$

Omitting the small term R_j^n in (2.19), we derive the following approximation to the heat equation (2.3):

$$D_t^+ u_j^n - D_x^2 u_j^{n+\frac{1}{2}} = f(x_j, t_{n+\frac{1}{2}}), \quad j \in \mathcal{T}_h^m, \quad n = 0, 1, \dots, N-1. \quad (2.23)$$

Based on the above preparations, setting $u_j^0 = u_0(x_j)$ for $j \in \mathcal{T}_h^0$, we propose the following Crank-Nicolson finite difference (CNFD-1) scheme for the problem (1.1)-(1.3):

$$(1 + K\delta_{m,j}) D_t^+ u_j^n - D_x^2 u_j^{n+\frac{1}{2}} = f(x_j, t_{n+\frac{1}{2}}), \quad j \in \mathcal{T}_h, \quad n = 0, 1, \dots, N-1, \quad (2.24a)$$

$$u_0^n = 0, \quad u_j^n = 0, \quad n = 0, 1, \dots, N, \quad (2.24b)$$

$$u_j^0 = u_0(x_j), \quad j \in \mathcal{T}_h^0, \quad (2.24c)$$

where

$$\delta_{m,j} := \begin{cases} 0, & j \neq m, \\ \frac{2}{h_1 + h_2}, & j = m \end{cases} \quad (2.25)$$

can be viewed as an approximation of the Dirac delta function $\delta(x - \xi)$ on Ω_h .

Furthermore, under the following assumption:

$$u(\xi, \cdot) \in C^3([0, T]), \quad u \in C^{1,3}(\bar{Q}_l) \cap C^{2,2}(\bar{Q}_l) \cap C^{4,0}(\bar{Q}_l), \quad l = 1, 2, \quad (2.26)$$

we try to improve the local truncation error of the approximation to the heat equation at the singular point $x = x_m$. To do this, we use again Taylor's expansion on the IIM condition (2.1) at the singular point $x = x_m$ to obtain that

$$\begin{aligned} D_x^- U_m^{n+\frac{1}{2}} &= D_x^- u(x_m, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) - \frac{h_1}{2!} \partial_{xx} u(x_m - 0, t_{n+\frac{1}{2}}) + \frac{h_1^2}{3!} \partial_{xxx} u(x_m - 0, t_{n+\frac{1}{2}}) \\ &\quad - \frac{h_1^3}{4!} \partial_{xxxx} u(\sigma_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) - \frac{h_1}{2!} [\partial_t u(x_m, t_{n+\frac{1}{2}}) - f(x_m, t_{n+\frac{1}{2}})] \\ &\quad + \frac{h_1^2}{3!} \partial_x [\partial_t u(x_m, t_{n+\frac{1}{2}}) - f(x_m, t_{n+\frac{1}{2}})] \\ &\quad - \frac{h_1^3}{4!} \partial_{xxxx} u(\sigma_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) - \frac{h_1}{2!} \left[D_t^+ u(x_m, t_n) - f(x_m, t_{n+\frac{1}{2}}) - \frac{\tau^2}{24} \partial_{ttt} u(x_m, \tilde{\eta}_{m_n}) \right] \\ &\quad + \frac{h_1^2}{3!} D_x^- [D_t^+ u(x_m, t_n) - f(x_m, t_{n+\frac{1}{2}})] - \frac{\tau^2 h_1^2}{144} \partial_{xttt} u(\tilde{\sigma}_{m_n}, \tilde{\eta}_{m_n}) \\ &\quad + \frac{h_1^3}{12} \partial_{xxxx} u(\hat{\sigma}_{m_n}, t_{n+\frac{1}{2}}) - \frac{h_1^3}{4!} \partial_{xxxx} u(\sigma_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m - 0, t_{n+\frac{1}{2}}) - \frac{h_1}{2!} [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] \\ &\quad + \frac{h_1^2}{3!} D_x^- [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] + \frac{\tau^2 h_1}{48} \partial_{ttt} u(x_m, \tilde{\eta}_{m_n}) \\ &\quad - \frac{\tau^2 h_1^2}{144} \partial_{xttt} u(\tilde{\sigma}_{m_n}, \tilde{\eta}_{m_n}) + \frac{h_1^3}{12} \partial_{xxxx} u(\hat{\sigma}_{m_n}, t_{n+\frac{1}{2}}) \\ &\quad - \frac{h_1^3}{4!} \partial_{xxxx} u(\sigma_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\theta_{m_n}, \eta_{n_m}), \end{aligned} \quad (2.27)$$

where $\theta_{m_n}, \sigma_{m_n}, \tilde{\sigma}_{m_n}, \hat{\sigma}_{m_n} \in (x_{m-1}, x_m), \eta_{m_n}, \tilde{\eta}_{m_n} \in (t_n, t_{n+1})$. Similarly, we have

$$\begin{aligned} D_x^+ U_m^{n+\frac{1}{2}} &= D_x^+ u(x_m, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\vartheta_{m_n}, \eta_{n_m}) \\ &= \partial_x u(x_m + 0, t_{n+\frac{1}{2}}) + \frac{h_2}{2!} [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] \\ &\quad + \frac{h_2^2}{3!} D_x^+ [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] - \frac{\tau^2 h_2}{48} \partial_{ttt} u(x_m, \tilde{\eta}_{m_n}) \end{aligned}$$

$$\begin{aligned}
& -\frac{\tau^2 h_2^2}{144} \partial_{xttt} u(\tilde{\zeta}_{m_n}, \tilde{\eta}_{n_m}) - \frac{h_2^3}{12} \partial_{xxxx} u(\hat{\zeta}_{m_n}, t_{n+\frac{1}{2}}) \\
& + \frac{h_2^3}{4!} \partial_{xxxx} u(\zeta_{m_n}, t_{n+\frac{1}{2}}) + \frac{\tau^2}{8} \partial_{xtt} u(\vartheta_{m_n}, \eta_{n_m}),
\end{aligned} \tag{2.28}$$

where $\vartheta_{m_n}, \zeta_{m_n}, \tilde{\zeta}_{m_n}, \hat{\zeta}_{m_n} \in (x_m, x_{m+1}), \eta_{n_m}, \tilde{\eta}_{n_m} \in (t_n, t_{n+1})$. Subtracting (2.27) from (2.28) and using (2.11), we obtain

$$\begin{aligned}
& D_x^+ U_m^{n+\frac{1}{2}} - D_x^- U_m^{n+\frac{1}{2}} - \frac{h_1 + h_2}{2} [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] \\
& - \frac{1}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) [D_t^+ U_m^n - f(x_m, t_{n+\frac{1}{2}})] \\
& = K D_t^+ u(x_m, t_n) + \tilde{r}_m^n, \quad n = 0, 1, \dots, N-1,
\end{aligned} \tag{2.29}$$

where

$$\begin{aligned}
\tilde{r}_m^n & := \frac{\tau^2}{8} \partial_{xtt} [u(\vartheta_{m_n}, \eta_{n_m}) - u(\theta_{m_n}, \eta_{n_m})] - \frac{\tau^2}{144} \partial_{xttt} [h_2^2 u(\tilde{\zeta}_{m_n}, \tilde{\eta}_{n_m}) - h_1^2 u(\tilde{\sigma}_{m_n}, \tilde{\eta}_{n_m})] \\
& - \frac{1}{12} [h_2^3 \partial_{xxxx} u(\hat{\zeta}_{m_n}, t_{n+\frac{1}{2}}) + h_1^3 \partial_{xxxx} u(\hat{\sigma}_{m_n}, t_{n+\frac{1}{2}})] - \frac{K}{24} \tau^2 \partial_{ttt} u(x_m, \tilde{\eta}_{n_m}) \\
& + \frac{1}{4!} [h_2^3 \partial_{xxxx} u(\zeta_{m_n}, t_{n+\frac{1}{2}}) + h_1^3 \partial_{xxxx} u(\sigma_{m_n}, t_{n+\frac{1}{2}})] \\
& - \frac{\tau^2}{48} (h_1 + h_2) \partial_{ttt} u(x_m, \tilde{\eta}_{n_m}).
\end{aligned} \tag{2.30}$$

Under assumption (2.26), we obtain the following estimate of \tilde{r}_m^n :

$$|\tilde{r}_m^n| \leq C(\tau^2 + h_1^3 + h_2^3). \tag{2.31}$$

Dividing both sides of (2.29) by $(h_1 + h_2)/2$ and noting the definition of the operator D_x^2 , we obtain

$$\begin{aligned}
& \left[1 + K\delta_{m,m} + \frac{\delta_{m,m}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) \right] D_t^+ U_m^n - D_x^2 U_m^{n+\frac{1}{2}} \\
& = \left[1 + \frac{\delta_{m,m}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) \right] f(x_m, t_{n+\frac{1}{2}}) + \tilde{R}_m^n, \quad 0 \leq n < N,
\end{aligned} \tag{2.32}$$

where

$$\tilde{R}_m^n := -\frac{2\tilde{r}_m^n}{h_1 + h_2}. \tag{2.33}$$

Then we obtain from (2.31) and (2.33) the following estimate of \tilde{R}_m^n :

$$|\tilde{R}_m^n| \leq C(h_1 + h_2)^{-1} (\tau^2 + h_1^3 + h_2^3). \tag{2.34}$$

Omitting the small term \tilde{R}_m^n in (2.32), we derive another approximation to the heat equation at $x = x_m$

$$\begin{aligned}
& \left[1 + K\delta_{m,m} + \frac{\delta_{m,m}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) \right] D_t^+ u_m^n - D_x^2 u_m^{n+\frac{1}{2}} \\
& = \left[1 + \frac{\delta_{m,m}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) \right] f(x_m, t_{n+\frac{1}{2}}), \quad n = 0, 1, 2, \dots, N-1.
\end{aligned} \tag{2.35}$$

Based on the above preparations, setting $u_j^0 = u_0(x_j)$ for $j \in \mathcal{T}_h^0$, we propose another Crank-Nicolson finite difference (CNFD-2) scheme for the problem (1.1)-(1.3)

$$\begin{aligned} & \left[1 + K\delta_{m,j} + \frac{\delta_{m,j}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) \right] D_t^+ u_j^n - D_x^2 u_j^{n+\frac{1}{2}} \\ = & \left[1 + \frac{\delta_{m,j}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) \right] f(x_j, t_{n+\frac{1}{2}}), \quad j \in \mathcal{T}_h, \quad n = 0, 1, \dots, N-1, \end{aligned} \quad (2.36a)$$

$$u_0^n = 0, \quad u_j^n = 0, \quad n = 0, 1, \dots, N, \quad (2.36b)$$

$$u_j^0 = u_0(x_j), \quad j \in \mathcal{T}_h^0. \quad (2.36c)$$

Remark 2.1. From the derivation of the two CNFD schemes, we can see that the main and only difference between the CNFD-1 scheme and the CNFD-2 scheme is the different approximation to the IIM condition. It should be pointed out that the stencil of these two schemes could ensure that ξ is a grid point.

3. Numerical Analysis

In this section, we consider the unique solvability of the two CNFD schemes and build the optimal error bounds of the numerical solutions.

3.1. Preparatory lemmas

In this subsection, we introduce some lemmas which will be used repeatedly in our subsequent numerical analysis.

Lemma 3.1. *For any grid function $u^n \in Z_h^0$ for $n = 0, 1, 2, \dots, N$, there are*

$$(D_x^2 u^n, v^n) = -\langle D_x^+ u^n, D_x^+ v^n \rangle, \quad (3.1)$$

$$(D_x^2 u^{n+\frac{1}{2}}, D_t^+ u^n) = -\frac{1}{2\tau} (|u^{n+1}|_1^2 - |u^n|_1^2). \quad (3.2)$$

Proof. With summation-by-parts formula, we have

$$\begin{aligned} (D_x^2 u^n, v^n) &= h_1 \sum_{j=1}^{m-1} D_x^2 u_j^n v_j^n + h_2 \sum_{j=m+1}^{J-1} D_x^2 u_j^n v_j^n + \frac{h_1 + h_2}{2} D_x^2 u_m^n v_m^n \\ &= h_1 \sum_{j=1}^{m-1} \frac{1}{h_1} (D_x^+ u_j^n - D_x^+ u_{j-1}^n) v_j^n + h_2 \sum_{j=m+1}^{J-1} \frac{1}{h_2} (D_x^+ u_j^n - D_x^+ u_{j-1}^n) v_j^n \\ &\quad + D_x^+ u_m^n v_m^n - D_x^- u_m^n v_m^n \\ &= -h_1 \sum_{j=0}^{m-1} D_x^+ u_j^n D_x^+ v_j^n - h_2 \sum_{j=m}^{J-1} D_x^+ u_j^n D_x^+ v_j^n = -\langle D_x^+ u^n, D_x^+ v^n \rangle. \end{aligned}$$

This proves the Eq. (3.1) in the lemma. For the Eq. (3.2), a straightforward calculation proves that

$$\begin{aligned} (D_x^2 u^{n+\frac{1}{2}}, D_t^+ u^n) &= \frac{1}{2\tau} (D_x^2 u^n + D_x^2 u^{n+1}, u^{n+1} - u^n) \\ &= \frac{1}{2\tau} [(D_x^2 u^{n+1}, u^{n+1}) - (D_x^2 u^n, u^n) + (D_x^2 u^n, u^{n+1}) - (D_x^2 u^{n+1}, u^n)] \end{aligned}$$

$$\begin{aligned}
&= -\frac{1}{2\tau} [\langle D_x^+ u^{n+1}, D_x^+ u^{n+1} \rangle - \langle D_x^+ u^n, D_x^+ u^n \rangle + \langle D_x^+ u^n, D_x^+ u^{n+1} \rangle - \langle D_x^+ u^{n+1}, D_x^+ u^n \rangle] \\
&= -\frac{1}{2\tau} (|u^{n+1}|_1^2 - |u^n|_1^2),
\end{aligned}$$

where (3.1) was used. This completes the proof. \square

Lemma 3.2. *For any grid function $w \in Z_h^0$, there is the following embedding inequality:*

$$\|w\|_\infty \leq \frac{\sqrt{b-a}}{2} |w|_1.$$

Proof. For any $j \in \mathcal{T}_h$, we have

$$\begin{aligned}
w_j &= \sum_{s=1}^j (w_s - w_{s-1}) = \sum_{s=1}^j \tilde{h}_s D_x^- w_s, \\
w_j &= - \sum_{s=j+1}^J (w_s - w_{s-1}) = - \sum_{s=j+1}^J \tilde{h}_s D_x^- w_s,
\end{aligned}$$

where

$$\tilde{h}_s = \begin{cases} h_1, & j = 0, 1, 2, \dots, m, \\ h_2, & j = m+1, m+2, \dots, J. \end{cases}$$

Squaring both sides of the above two equations and applying Cauchy's inequality, we have

$$|w_j|^2 \leq \left(\sum_{s=0}^{j-1} \tilde{h}_s \right) \sum_{s=0}^{j-1} \tilde{h}_s |D_x^+ w_s|^2 = (x_j - a) \sum_{s=0}^{j-1} \tilde{h}_s |D_x^+ w_s|^2, \quad (3.3)$$

$$|w_j|^2 \leq \left(\sum_{s=j}^{J-1} \tilde{h}_s \right) \sum_{s=j}^{J-1} \tilde{h}_s |D_x^+ w_s|^2 = (b - x_j) \sum_{s=j}^{J-1} \tilde{h}_s |D_x^+ w_s|^2. \quad (3.4)$$

Operating $(b - x_j) \times (3.3) + (x_j - a) \times (3.4)$ yields

$$(b - a)|w_j|^2 \leq (x_j - a)(b - x_j) \sum_{s=0}^{J-1} \tilde{h}_s |D_x^+ w_j|^2 \leq \frac{(b - a)^2}{4} |w|_1^2, \quad j \in \mathcal{T}_h, \quad (3.5)$$

which yields

$$\|w\|_\infty \leq \frac{\sqrt{b-a}}{2} |w|_1. \quad (3.6)$$

This completes the proof. \square

3.2. Unique solvability

In this subsection, we discuss the solvability of the above two CNFD schemes.

Theorem 3.1. *The finite difference scheme (2.24a)-(2.24c) is uniquely solvable.*

Proof. According to (2.24c), we can see that u^0 exists, then by using mathematical induction, we assume that u^n is known and try to prove that the solution u^{n+1} of the CNFD-1 scheme exists. In fact, for a given u^n , the CNFD-1 scheme (2.24a)-(2.24c) just is a nonhomogeneous system of linear algebraic equations with respect to the unknown u^{n+1} . To analyze the unique solvability of the system of linear algebraic equations (2.24a)-(2.24c), we just only prove that the corresponding homogeneous system

$$\frac{1}{\tau}(1 + K\delta_{m,j})u_j^{n+1} - \frac{1}{2}D_x^2 u_j^{n+1} = 0, \quad j \in \mathcal{T}_h, \quad n = 0, 1, \dots, N-1, \quad (3.7a)$$

$$u_0^{n+1} = 0, \quad u_j^{n+1} = 0, \quad n = 0, 1, \dots, N-1 \quad (3.7b)$$

has a unique zero solution. Computing the inner production of (3.7a) with τu^{n+1} gives

$$\|u^{n+1}\|^2 + K|u_m^{n+1}|^2 + \frac{\tau}{2}|u^{n+1}|_1^2 = 0, \quad (3.8)$$

where Lemma 3.1 was used. Noting $K > 0$, we obtain from (3.8) that

$$u_j^{n+1} = 0, \quad j \in \mathcal{T}_h^0. \quad (3.9)$$

This completes the proof. \square

Theorem 3.2. *The finite difference scheme (2.36a)-(2.36c) is uniquely solvable.*

Proof. Firstly, we can see from (2.36c) that u^0 exists, then by using mathematical induction, we assume that u^n is known and try to prove that the solution u^{n+1} of the CNFD-2 scheme exists. To do this, we just only prove that the homogeneous system of linear algebraic equations

$$\begin{aligned} & \frac{1}{\tau} \left(1 + K\delta_{m,j} + \frac{\delta_{m,j}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) \right) u_j^{n+1} \\ & - \frac{1}{2} D_x^2 u_j^{n+1} = 0, \quad j \in \mathcal{T}_h, \quad n = 0, 1, \dots, N-1, \end{aligned} \quad (3.10a)$$

$$u_0^{n+1} = 0, \quad u_j^{n+1} = 0, \quad n = 0, 1, \dots, N-1 \quad (3.10b)$$

has a unique zero solution. Computing the inner production of (3.10a) with τu^{n+1} yields

$$\begin{aligned} & \|u^{n+1}\|^2 + \frac{h_1 + h_2}{2} K \delta_{m,m} |u_m^{n+1}|^2 + \frac{h_1 + h_2}{2} \frac{\delta_{m,m}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) u_m^{n+1} u_m^{n+1} \\ & + \frac{\tau}{2} |u^{n+1}|_1^2 = 0, \quad n = 0, 1, \dots, N-1, \end{aligned} \quad (3.11)$$

where Lemma 3.1 was used. For the third term on the right-hand side of (3.11), we use Cauchy's inequality to obtain the following estimate:

$$\begin{aligned} & \frac{h_1 + h_2}{2} \frac{\delta_{m,m}}{6} (h_2^2 D_x^+ - h_1^2 D_x^-) u_m^{n+1} u_m^{n+1} \\ & = \frac{1}{6} [h_2 (u_{m+1}^{n+1} - u_m^{n+1}) - h_1 (u_m^{n+1} - u_{m-1}^{n+1})] u_m^{n+1} \\ & \geq -\frac{h_2}{12} (|u_{m+1}^{n+1}|^2 + |u_m^{n+1}|^2) - \frac{h_1 + h_2}{6} |u_m^{n+1}|^2 - \frac{h_1}{12} (|u_{m-1}^{n+1}|^2 + |u_m^{n+1}|^2) \\ & = -\frac{h_1}{12} |u_{m-1}^{n+1}|^2 - \frac{h_2}{12} |u_{m+1}^{n+1}|^2 - \frac{h_1 + h_2}{4} |u_m^{n+1}|^2, \quad n = 0, 1, \dots, N-1. \end{aligned} \quad (3.12)$$

Instituting (3.12) to (3.11) gives

$$\|u^{n+1}\|^2 - \frac{h_1}{12}|u_{m-1}^{n+1}|^2 - \frac{h_2}{12}|u_{m+1}^{n+1}|^2 - \frac{h_1+h_2}{4}|u_m^{n+1}|^2 + K|u_m^{n+1}|^2 + \frac{\tau}{2}|u^{n+1}|_1^2 \leq 0. \quad (3.13)$$

For the first four terms on the left-hand side of (3.13), by direct calculation, we have the following estimate:

$$\|u^{n+1}\|^2 - \frac{h_1}{12}|u_{m-1}^{n+1}|^2 - \frac{h_2}{12}|u_{m+1}^{n+1}|^2 - \frac{h_1+h_2}{4}|u_m^{n+1}|^2 \geq \frac{1}{2}\|u^{n+1}\|^2. \quad (3.14)$$

Instituting (3.14) into (3.13) gives

$$\frac{1}{2}\|u^{n+1}\|^2 + K|u_m^{n+1}|^2 + \frac{\tau}{2}|u^{n+1}|_1^2 \leq 0. \quad (3.15)$$

Noting $K > 0$, then we immediately obtain from (3.15) that

$$u_j^{n+1} = 0, \quad j \in \mathcal{T}_h^0. \quad (3.16)$$

This completes the proof. \square

3.3. Error estimates

In this subsection, we establish the optimal point-wise error estimates of the proposed CNFD-1 scheme and CNFD-2 scheme without imposing any constraints on the grid ratios.

3.3.1. Error bound of the CNFD-1 scheme

For convenience, we reformulate (2.15) and (2.19) together with initial and boundary conditions into the following concise form:

$$(1 + K\delta_{m,j})D_t^+ U_j^n - D_x^2 U_j^{n+\frac{1}{2}} - f(x_j, t_{n+\frac{1}{2}}) = R_j^n, \quad j \in \mathcal{T}_h, \quad 0 \leq n < N, \quad (3.17a)$$

$$U_0^n = 0, \quad U_J^n = 0, \quad n = 0, 1, \dots, N, \quad (3.17b)$$

$$U_j^0 = u_0(x_j), \quad j \in \mathcal{T}_h^0, \quad (3.17c)$$

where $R^n \in Z_h^0$ is the called local truncation error of the CNFD-1 scheme. Define the ‘‘error’’ function $e^n \in Z_h^0$ as

$$e_j^n = U_j^n - u_j^n, \quad j \in \mathcal{T}_h^0, \quad 0 \leq n \leq N,$$

then by subtracting (2.24) from (3.17), we have the following ‘‘error’’ equation:

$$(1 + K\delta_{m,j})D_t^+ e_j^n - D_x^2 e_j^{n+\frac{1}{2}} = R_j^n, \quad j \in \mathcal{T}_h, \quad n = 0, 1, \dots, N-1, \quad (3.18a)$$

$$e_0^n = 0, \quad e_J^n = 0, \quad n = 0, 1, \dots, N, \quad (3.18b)$$

$$e_j^0 = 0, \quad j \in \mathcal{T}_h^0. \quad (3.18c)$$

For the error bound of the numerical solution of the CNFD-1 scheme, we have the following result.

Theorem 3.3. *Under assumption (2.8), there exists $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, when $0 < h \leq h_0, 0 < \tau \leq \tau_0$, the CNFD-1 scheme (2.24) satisfies the following optimal error estimates:*

$$|e^n|_1 \leq C(\tau^2 + h_1^2 + h_2^2), \quad \|e^n\|_\infty \leq C(\tau^2 + h_1^2 + h_2^2), \quad n = 1, 2, \dots, N. \quad (3.19)$$

Proof. Computing the inner product of (3.18a) with $D_t^+ e^n$ gives

$$\|D_t^+ e^n\|^2 + \frac{1}{2\tau} (|e^{n+1}|_1^2 - |e^n|_1^2) + K |D_t^+ e_m^n|^2 = (R^n, D_t^+ e^n), \quad n = 0, 1, \dots, N-1. \quad (3.20)$$

For the item on the right-hand side of (3.20), we apply Cauchy's inequality and the estimate of the local truncation error given in (2.14), (2.17) and (2.22) to obtain that

$$\begin{aligned} (R^n, D_t^+ e^n) &\leq \frac{h_1}{4} \sum_{j=1}^{m-1} |R_j^n|^2 + h_1 \sum_{j=1}^{m-1} |D_t^+ e_j^n|^2 + \frac{h_2}{4} \sum_{j=m+1}^{J-1} |R_j^n|^2 \\ &\quad + h_2 \sum_{j=m+1}^{J-1} |D_t^+ e_j^n|^2 + \frac{1}{4K} |r_m^n|^2 + K |D_t^+ e_m^n|^2 \\ &\leq \|D_t^+ e^n\|^2 + K |D_t^+ e_m^n|^2 + C(\tau^2 + h_1^2 + h_2^2)^2. \end{aligned} \quad (3.21)$$

Instituting (3.21) into (3.20) yields

$$|e^{n+1}|_1^2 - |e^n|_1^2 \leq C\tau(\tau^2 + h_1^2 + h_2^2)^2, \quad n = 0, 1, \dots, N-1. \quad (3.22)$$

Summing up the Eq. (3.22) over n gives

$$|e^{n+1}|_1^2 \leq |e^0|_1^2 + C(n+1)\tau(\tau^2 + h_1^2 + h_2^2)^2, \quad n = 0, 1, \dots, N-1. \quad (3.23)$$

This together with $e^0 = 0$ and $n\tau = t_n \leq T, n = 1, 2, \dots, N$ give

$$|e^n|_1 \leq C(\tau^2 + h_1^2 + h_2^2), \quad n = 1, 2, \dots, N. \quad (3.24)$$

Furthermore, we use Lemma 3.2 to obtain that

$$\|e^n\|_\infty \leq C(\tau^2 + h_1^2 + h_2^2), \quad n = 1, 2, \dots, N. \quad (3.25)$$

This completes the proof. \square

3.3.2. Error bound of the CNFD-2 scheme

To analyze the CNFD-2 scheme (2.36), we reformulate (2.32) and (2.19) together with initial and boundary conditions into the following concise form:

$$\begin{aligned} &\left[1 + K\delta_{m,j} + \frac{\delta_{m,j}}{6}(h_2^2 D_x^+ - h_1^2 D_x^-)\right] D_t^+ U_j^n - D_x^2 U_j^{n+\frac{1}{2}} \\ &\quad - \left[1 + \frac{\delta_{m,j}}{6}(h_2^2 D_x^+ - h_1^2 D_x^-)\right] f(x_j, t_{n+\frac{1}{2}}) = \tilde{R}_j^n, \quad j \in \mathcal{T}_h, \quad 0 \leq n < N, \end{aligned} \quad (3.26a)$$

$$U_0^n = 0, \quad U_J^n = 0, \quad n = 0, 1, \dots, N, \quad (3.26b)$$

$$U_j^0 = u_0(x_j), \quad j \in \mathcal{T}_h^0. \quad (3.26c)$$

Define the ‘‘error’’ functions $\tilde{e}^n \in Z_h^0$ of the CNFD-2 scheme as

$$\tilde{e}_j^n = U_j^n - u_j^n, \quad j \in \mathcal{T}_h^0, \quad 0 \leq n \leq N,$$

then by subtracting (2.36) from (3.26), we have the following “error” equation:

$$\begin{aligned} & \left[1 + K\delta_{m,j} + \frac{\delta_{m,j}}{6}(h_2^2 D_x^+ - h_1^2 D_x^-) \right] D_t^+ \tilde{e}_j^n \\ & - D_x^2 \tilde{e}_j^{n+\frac{1}{2}} = \tilde{R}_j^n, \quad j \in \mathcal{T}_h, \quad n = 0, 1, \dots, N-1, \end{aligned} \quad (3.27a)$$

$$\tilde{e}_0^n = 0, \quad \tilde{e}_j^n = 0, \quad n = 0, 1, \dots, N, \quad (3.27b)$$

$$\tilde{e}_j^0 = 0, \quad j \in \mathcal{T}_h^0. \quad (3.27c)$$

For the error estimate of the CNFD-2 scheme, we have the following result.

Theorem 3.4. *Under assumption (2.26), there exists $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, when $0 < h \leq h_0, 0 < \tau \leq \tau_0$, the CNFD-2 scheme (2.36) satisfies the following optimal error estimates:*

$$|\tilde{e}^n|_1 \leq C(\tau^2 + h_1^2 + h_2^2), \quad \|\tilde{e}^n\|_\infty \leq C(\tau^2 + h_1^2 + h_2^2), \quad n = 1, 2, \dots, N. \quad (3.28)$$

Proof. Computing the inner product of (3.27a) with $D_t^+ \tilde{e}^n$ gives

$$\begin{aligned} & \|D_t^+ \tilde{e}^n\|^2 + \frac{1}{6}[h_2(D_t^+ \tilde{e}_{m+1}^n - D_t^+ \tilde{e}_m^n) - h_1(D_t^+ \tilde{e}_m^n - D_t^+ \tilde{e}_{m-1}^n)]D_t^+ \tilde{e}_m^n \\ & + \frac{1}{2\tau}(|\tilde{e}^{n+1}|_1^2 - |\tilde{e}^n|_1^2) + K|D_t^+ \tilde{e}_m^n|^2 = (\tilde{R}^n, D_t^+ \tilde{e}^n), \quad n = 0, 1, \dots, N-1. \end{aligned} \quad (3.29)$$

For the item on the right-hand side of (3.29), by using Cauchy’s inequality and the estimate of the local truncation error given in (2.22), (2.31) and (2.34), we obtain

$$\begin{aligned} (\tilde{R}^n, D_t^+ \tilde{e}^n) & \leq \frac{h_1}{2} \sum_{j=1}^{m-1} |\tilde{R}_j^n|^2 + \frac{h_1}{2} \sum_{j=1}^{m-1} |D_t^+ \tilde{e}_j^n|^2 + \frac{h_2}{2} \sum_{j=m+1}^{J-1} |\tilde{R}_j^n|^2 \\ & + \frac{h_2}{2} \sum_{j=m+1}^{J-1} |D_t^+ \tilde{e}_j^n|^2 + \frac{1}{4K} |\tilde{r}_m^n|^2 + K|D_t^+ \tilde{e}_m^n|^2 \\ & \leq \frac{1}{2} \|D_t^+ \tilde{e}^n\|^2 + K|D_t^+ \tilde{e}_m^n|^2 + C(\tau^2 + h_1^2 + h_2^2)^2. \end{aligned} \quad (3.30)$$

For the item on the left-hand side of (3.29), we again apply Cauchy’s inequality to obtain that

$$\begin{aligned} & \frac{1}{6}[h_2(D_t^+ \tilde{e}_{m+1}^n - D_t^+ \tilde{e}_m^n) - h_1(D_t^+ \tilde{e}_m^n - D_t^+ \tilde{e}_{m-1}^n)]D_t^+ \tilde{e}_m^n \\ & \geq -\frac{h_1}{12}|D_t^+ \tilde{e}_{m-1}^n|^2 - \frac{h_2}{12}|D_t^+ \tilde{e}_{m+1}^n|^2 - \frac{h_1 + h_2}{4}|D_t^+ \tilde{e}_m^n|^2. \end{aligned} \quad (3.31)$$

Instituting (3.30) and (3.31) into (3.29) and noting

$$\|D_t^+ \tilde{e}^n\|^2 - \frac{h_1}{12}|D_t^+ \tilde{e}_{m-1}^n|^2 - \frac{h_2}{12}|D_t^+ \tilde{e}_{m+1}^n|^2 - \frac{h_1 + h_2}{4}|D_t^+ \tilde{e}_m^n|^2 \geq \frac{1}{2} \|D_t^+ \tilde{e}^n\|^2, \quad (3.32)$$

we have

$$|\tilde{e}^{n+1}|_1^2 - |\tilde{e}^n|_1^2 \leq C\tau(\tau^2 + h_1^2 + h_2^2)^2, \quad n = 0, 1, \dots, N-1. \quad (3.33)$$

Summing up the Eq. (3.33) over n gives

$$|\tilde{e}^{n+1}|_1^2 \leq |\tilde{e}^0|_1^2 + C(n+1)\tau(\tau^2 + h_1^2 + h_2^2)^2, \quad n = 0, 1, \dots, N-1. \quad (3.34)$$

This together with $\tilde{e}^0 = 0$ and $n\tau = t_n \leq T, n = 1, 2, \dots, N$ give

$$|\tilde{e}^n|_1 \leq C(\tau^2 + h_1^2 + h_2^2), \quad n = 1, 2, \dots, N. \quad (3.35)$$

Furthermore, we use Lemma 3.2 to obtain that

$$\|\tilde{e}^n\|_\infty \leq C(\tau^2 + h_1^2 + h_2^2), \quad n = 1, 2, \dots, N. \quad (3.36)$$

This completes the proof. \square

Remark 3.1. Regarding the comparison between our two CNFD schemes and the box scheme proposed by Sun and Zhu [20], each has its advantages and disadvantages. The box scheme was designed by using the method of order reduction which allows the grid stencil to be non-uniform and makes sure the local truncation error at each grid point is second-order accurate in space. Furthermore, the authors used the standard energy method to prove that the convergence rate of the box scheme is second-order both in space and in time. However, even on a uniform grid stencil and nonsingular points, it is difficult to improve the accuracy of this box scheme. Although our CNFD schemes are not suitable for non-uniform grid stencils, they offer the following advantages:

1. They are more concise in both derivation and form compared to the box scheme.
2. Different mesh sizes can be adopted in different subintervals separated by the singular points, ensuring that these singular points are exactly grid nodes.
3. We perform a meticulous analysis of the local truncation error for the scheme at each grid node and prove that the two CNFD schemes are second-order accurate in both space and time without any requirement on the grid ratio.
4. At the nonsingular grid node, one can use the compact finite difference method to discretize the heat equation and apply high-order Taylor's expansion to approximate the IIM conditions at the singular points to design a high-order accurate numerical scheme.

This high-order accurate scheme is fairly conventional, so it is not presented in this paper for brevity.

4. Extension to Multiple-concentrated-capacity Case

In this section, we extend the two CNFD schemes to solve the heat equation with capacity coefficient containing multiple Dirac delta functions, i.e. we consider the following problem:

$$\left[1 + \sum_{s=1}^{n_0} K_s \delta(x - \xi_s) \right] \partial_t u(x, t) - \partial_{xx} u(x, t) = f(x, t), \quad (x, t) \in (a, b) \times (0, T], \quad (4.1a)$$

$$u(a, t) = 0, \quad u(b, t) = 0, \quad t \in (0, T], \quad (4.1b)$$

$$u(x, 0) = u_0(x), \quad x \in [a, b], \quad (4.1c)$$

where $\xi_s \in (a, b), s = 1, 2, \dots, n_0$ and $\xi_j \neq \xi_k$ if $j \neq k$. Similarly, we can obtain the following IIM conditions:

$$\partial_x u(\xi_s + 0, t) - \partial_x u(\xi_s - 0, t) = K_s \partial_t u(\xi_s, t), \quad t \in (0, T], \quad s = 1, 2, \dots, n_0, \quad (4.2)$$

where K_s ($s = 1, 2, \dots, n_0$) are positive constants. Then we can utilize the IIM conditions (4.2) to reformulate the heat system (4.1) into the following initial-boundary value problem of the heat equation:

$$\partial_t u(x, t) - \partial_{xx} u(x, t) = f(x, t), \quad x \in (a, b) \setminus \{\xi_1, \xi_2, \dots, \xi_{n_0}\}, \quad t \in (0, T], \quad (4.3a)$$

$$\partial_x u(\xi_s + 0, t) - \partial_x u(\xi_s - 0, t) = K \partial_t u(\xi_s, t), \quad s = 1, 2, \dots, n_0, \quad t \in (0, T], \quad (4.3b)$$

$$u(\xi_s + 0, t) = u(\xi_s - 0, t), \quad s = 1, 2, \dots, n_0, \quad t \in (0, T], \quad (4.3c)$$

$$u(a, t) = 0, \quad u(b, t) = 0, \quad t \in (0, T], \quad (4.3d)$$

$$u(x, 0) = u_0(x), \quad x \in [a, b]. \quad (4.3e)$$

Choosing a positive integer N , we still denote the step size by $\tau := T/N$ and denote time steps as $t_n := n\tau$ for $n = 0, 1, 2, \dots, N$ on the interval $[0, T]$. Choosing $n_0 + 1$ positive integers m_1, m_2, \dots, m_{n_0} and J satisfying $1 < m_1 < m_2 < \dots < m_{n_0} < J$, we define mesh sizes

$$h_1 := \frac{\xi_1 - a}{m_1}, \quad h_2 := \frac{\xi_2 - \xi_1}{m_2 - m_1}, \quad \dots, \quad h_{n_0+1} := \frac{b - \xi_{n_0}}{J - m_{n_0}}$$

on the $n_0 + 1$ subintervals $[a, \xi_1], [\xi_1, \xi_2], \dots, [\xi_{n_0}, b]$, and we denote grid points as

$$x_j := a + \sum_{s=0}^j \tilde{h}_s, \quad j = 0, 1, 2, \dots, J$$

with

$$\tilde{h}_j := \begin{cases} h_1, & j = 0, 1, 2, \dots, m_1, \\ h_2, & j = m_1 + 1, \dots, m_2, \\ \vdots & \vdots \\ h_{n_0+1}, & j = m_{n_0} + 1, \dots, J. \end{cases} \quad (4.4)$$

It is clear that $x_{m_s} = \xi_s$ for $s = 1, 2, \dots, n_0$. We still denote

$$\Omega_h := \{x_j \mid j = 0, 1, \dots, J\}, \quad \Omega_\tau := \{t_n \mid n = 0, 1, \dots, N\},$$

then the computational domain $[a, b] \times [0, T]$ is partitioned by $\Omega_{h,\tau} := \Omega_h \times \Omega_\tau$. In addition, introduce the grid function space

$$Z_h^0 := \{u := (u_0, u_1, \dots, u_J)^\top \mid u_0 = u_J = 0\} \subseteq \mathbb{C}^{J+1},$$

and the index sets

$$\begin{aligned} \mathcal{T}_h &:= \{j \mid j = 1, 2, \dots, J-1\}, \\ \mathcal{T}_h^0 &:= \{j \mid j = 0, 1, 2, \dots, J\}, \\ \mathcal{T}_h^m &:= \{j \mid j = 1, 2, \dots, J-1\} \setminus \{m_1, m_2, \dots, m_{n_0}\}. \end{aligned}$$

In this section, we still use u_j^n and U_j^n to denote the approximation and exact value of u at the point $(x_j, t_n) \in \Omega_{h,\tau}$, respectively. And we use $U^n \in Z_h^0$ and $u^n \in Z_h^0$ to denote the exact solution vector and the numerical solution vector, respectively.

We introduce finite difference discretization operators for $u^n \in Z_h^0$ as follows:

$$D_x^- u_j^n := \begin{cases} \frac{u_j^n - u_{j-1}^n}{\tilde{h}_j}, & j = 1, 2, \dots, J, \\ 0, & j = 0, \end{cases} \quad (4.5)$$

$$D_x^+ u_j^n := \begin{cases} D_x^- u_{j+1}^n, & j = 0, 1, \dots, J-1, \\ 0, & j = J, \end{cases} \quad (4.6)$$

$$D_x^2 u_j^n := \begin{cases} \frac{2(D_x^+ u_j^n - D_x^- u_j^n)}{\tilde{h}_j + \tilde{h}_{j+1}}, & j = 1, 2, \dots, J-1, \\ 0, & j = 0, J. \end{cases} \quad (4.7)$$

The discrete inner product, standard l^2 -norm, l^∞ -norm and H^1 -seminorm for $v^n, u^n \in Z_h^0$ are given as

$$(v^n, u^n) := \frac{1}{2} \sum_{j=0}^{J-1} \tilde{h}_j (v_j^n u_j^n + v_{j+1}^n u_{j+1}^n), \quad \|u^n\| := \sqrt{(u^n, u^n)}, \quad (4.8)$$

$$\langle D_x^+ v^n, D_x^+ u^n \rangle := \sum_{j=0}^{J-1} \tilde{h}_j D_x^+ v_j^n D_x^+ u_j^n, \quad |v^n|_1 := \sqrt{\langle D_x^+ v^n, D_x^+ v^n \rangle}, \quad (4.9)$$

$$\|u^n\|_\infty := \max_{0 \leq j \leq J} |u_j^n|, \quad |u^n|_1 := \sqrt{\sum_{j=0}^{J-1} \tilde{h}_j |D_x^+ u_j^n|^2}. \quad (4.10)$$

Based on the above preliminary work, we give the following CNFD-1 scheme for the initial-boundary value problem (4.1):

$$\left(1 + \sum_{s=1}^{n_0} K_s \delta_{s,j}\right) D_t^+ u_j^n - D_x^2 u_j^{n+\frac{1}{2}} = f(x_j, t_{n+\frac{1}{2}}), \quad j \in \mathcal{T}_h, \quad n = 0, 1, \dots, N-1, \quad (4.11a)$$

$$u_0^n = 0, \quad u_J^n = 0, \quad n = 0, 1, \dots, N, \quad (4.11b)$$

$$u_j^0 = u_0(x_j), \quad j \in \mathcal{T}_h^0, \quad (4.11c)$$

where

$$\delta_{s,j} = \begin{cases} 0, & j \neq m_s, \\ \frac{2}{\tilde{h}_j + \tilde{h}_{j+1}}, & j = m_s, \end{cases} \quad s = 1, 2, \dots, n_0. \quad (4.12)$$

Assume that

$$u(\xi_s, \cdot) \in C^3([0, T]), \quad u \in C^{0,3}(\bar{Q}_s) \cap C^{2,2}(\bar{Q}_s) \cap C^{4,0}(\bar{Q}_s), \quad s = 1, 2, \dots, n_0, \quad (4.13)$$

where

$$Q_s = (x_{m_s}, \xi_{m_{s+1}}) \times (0, T], \quad s = 0, 1, 2, \dots, J$$

with $m_0 = 0$ and $m_{n_0+1} = J$, then by using similar proof as that of Theorem 3.3, we can establish the optimal error estimate of the CNFD-1 scheme (4.11a)-(4.11c) for solving the problem (4.1) as follows.

Theorem 4.1. *Under the assumptions (4.13), there exists $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, when $0 < h \leq h_0, 0 < \tau \leq \tau_0$, the finite difference scheme (4.11a)-(4.11c) satisfies the following error estimates:*

$$|e^n|_1 \leq C(\tau^2 + \tilde{h}^2), \quad \|e^n\|_\infty \leq C(\tau^2 + \tilde{h}^2), \quad n = 0, 1, 2, \dots, N, \quad (4.14)$$

where $\tilde{h} = \max_{1 \leq s \leq n_0+1} \tilde{h}_s$.

Similarly, we can extend the CNFD-2 scheme to the multiple-concentrated-capacity case and establish the optimal error estimate without any constraint on the grid ratio.

We give the following CNFD-2 scheme for the initial-boundary value problem (4.1):

$$\begin{aligned} & \left[1 + \sum_{s=1}^{n_0} K_s \delta_{s,j} + \sum_{s=1}^{n_0} \frac{\delta_{s,j}}{6} (\tilde{h}_{s+1}^2 D_x^+ - \tilde{h}_s^2 D_x^-) \right] D_t^+ u_j^n - D_x^2 u_j^{n+\frac{1}{2}} \\ &= \left[1 + \sum_{s=1}^{n_0} \frac{\delta_{s,j}}{6} (\tilde{h}_{s+1}^2 D_x^+ - \tilde{h}_s^2 D_x^-) \right] f(x_j, t_{n+\frac{1}{2}}), \\ & \quad j \in \mathcal{T}_h, \quad s = 1, 2, \dots, n_0, \quad n = 0, 1, \dots, N-1, \end{aligned} \quad (4.15a)$$

$$u_0^n = 0, \quad u_j^n = 0, \quad n = 0, 1, \dots, N, \quad (4.15b)$$

$$u_j^0 = u_0(x_j), \quad j \in \mathcal{T}_h^0. \quad (4.15c)$$

Assume that

$$u(\xi_s, \cdot) \in C^3([0, T]), \quad u \in C^{1,3}(\bar{Q}_s) \cap C^{2,2}(\bar{Q}_s) \cap C^{4,0}(\bar{Q}_s), \quad s = 1, 2, \dots, n_0, \quad (4.16)$$

where

$$Q_s = (x_{m_s}, \xi_{m_{s+1}}) \times (0, T], \quad s = 0, 1, 2, \dots, J$$

with $m_0 = 0$ and $m_{n_0+1} = J$.

By using similar proof as that of Theorem 3.4, we can establish the optimal error estimate of the CNFD-2 scheme (4.15a)-(4.15c) for solving the problem (4.1) as follows.

Theorem 4.2. *Under the assumptions (4.16), there exists $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, when $0 < h \leq h_0, 0 < \tau \leq \tau_0$, the finite difference scheme (4.15a)-(4.15c) satisfies the following error estimates:*

$$|e^n|_1 \leq C(\tau^2 + h^2), \quad \|e^n\|_\infty \leq C(\tau^2 + h^2), \quad n = 0, 1, 2, \dots, N, \quad (4.17)$$

where $h = \max_{1 \leq s \leq n_0+1} h_s$.

5. Numerical Experiments

In this section, several numerical results are carried out to test our theoretical analysis and simulate the dynamics of the heat equation with concentrated capacity.

5.1. Spatial/temporal resolution

In this subsection, we try to test the spatial and temporal error bounds of the proposed CNFD schemes.

Example 5.1. We use the two CNFD schemes to solve the following initial-boundary value problem:

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f, \quad x \in (0, \xi) \cup (\xi, 1), \quad t \in (0, 5], \quad (5.1a)$$

$$u(\xi + 0, t) - u(\xi - 0, t) = 0, \quad t \in (0, 5], \quad (5.1b)$$

$$\frac{\partial u}{\partial x}(\xi + 0, t) - \frac{\partial u}{\partial x}(\xi - 0, t) = K \frac{\partial u}{\partial t}(\xi, t), \quad t \in (0, 5], \quad (5.1c)$$

$$u(0, t) = 0, \quad u(1, t) = 0, \quad t \in (0, 5], \quad (5.1d)$$

$$u(x, 0) = u_0(x), \quad x \in [0, 1], \quad (5.1e)$$

where $\xi = 2/3$, $K = 2$ and

$$u_0(x) = 2x^2(1-x) \left(\left| x - \frac{2}{3} \right| + 1 \right), \quad x \in [0, 1],$$

$$f(x, t) = -\cos(t)\phi(x) - (2 - \sin(t))\phi'', \quad x \in [0, 1], \quad t \in (0, 5],$$

$$\phi(x) = x^2(1-x) \left(\left| x - \frac{2}{3} \right| + 1 \right), \quad x \in [0, 1].$$

We test and study the temporal and spatial errors of the two CNFD schemes on uniform meshes, and compare them with the schemes given in [8, 20]. For simplicity, we use BE scheme and box scheme to denote the finite difference scheme given in [8] and the finite difference scheme in [20], respectively. The numerical “exact” solution is computed by the CNFD-2 scheme with a very fine mesh size $h_e = 1/9000$ and time step $\tau_e = 0.0005$. Then, we measure the spatial discretization errors on uniform meshes. We fix the time step $\tau = 0.0005$ sufficiently small, such that the discretization errors from time direction are negligible, and solve the four finite difference schemes under different numbers of spatial grids J . Table 5.1 lists the spatial errors $\|e^n\|_\infty$ at $T = 5$ with different mesh sizes for different numerical methods. The l^∞ -error of the numerical solutions at the terminal time $T = 5$ and their corresponding convergence rates in time, along with the spatial mesh refinement and their corresponding convergence rates are presented in Table 5.1. The spatial convergence rate observed for the four schemes is approximately 2, consistent with the expected value. Specifically, from Table 5.1, the spatial error of the CNFD-1 scheme is slightly better than that of the box scheme, while the spatial error of the CNFD-2 scheme is much smaller than that of the box scheme. It is obvious that

Table 5.1: Spatial errors $\|e^n\|_\infty$ of different numerical methods at $T = 5$ on uniform meshes.

$e_{\infty, h, \tau}$	$h_0 = 1/15$	$h_0/2$	$h_0/4$	$h_0/8$	$h_0/20$	$h_0/40$
CNFD-1 scheme	4.78E-3	1.20E-3	2.99E-4	7.47E-5	1.19E-5	2.98E-6
Order	—	2.00	2.00	2.00	2.00	2.00
CNFD-2 scheme	1.97E-3	4.93E-4	1.23E-4	3.08E-5	4.92E-6	1.23E-6
Order	—	2.00	2.00	2.00	2.00	2.00
BE scheme	4.78E-3	1.20E-3	2.99E-4	7.47E-5	1.19E-5	2.98E-6
Order	—	2.00	2.00	2.00	2.00	2.00
Box scheme	6.09E-3	1.52E-3	3.81E-4	9.52E-5	1.52E-5	3.79E-6
Order	—	2.00	2.00	2.00	2.00	2.01

Table 5.2: Temporal errors $\|e^n\|_\infty$ of different numerical methods at $T = 5$ on uniform meshes.

$e_{\infty,h,\tau}$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$
CNFD-1 scheme	4.87E-5	1.29E-5	3.31E-6	8.37E-7	2.10E-7	5.17E-8
Order	—	1.92	1.96	1.98	2.00	2.02
CNFD-2 scheme	4.87E-5	1.29E-5	3.31E-6	8.37E-7	2.10E-7	5.17E-8
Order	—	1.92	1.96	1.98	2.00	2.02
BE scheme	3.55E-3	1.80E-3	8.98E-4	4.42E-4	2.12E-4	9.69E-5
Order	—	0.98	1.00	1.02	1.06	1.13
Box scheme	2.43E-4	6.05E-5	1.51E-5	3.77E-6	9.38E-7	2.31E-7
Order	—	2.00	2.00	2.00	2.01	2.02

the convergence speed of the CNFD-1 scheme and the CNFD-2 scheme are significantly better than that of the box scheme. Furthermore, the spatial errors of the CNFD-1 scheme and BE scheme are nearly identical, aligning with theoretical expectations.

Next we test the temporal errors at $T = 5$ on uniform meshes, listed in Table 5.2 under different $\tau_0 = 0.1$ with a very small number of spatial grids $J = 9000$ such that the discretization errors in space are negligible. To compute the temporal errors, we set the solution obtained by the numerical “exact” solution. The l^∞ -error of the numerical solutions at the terminal time $T = 5$, obtained with different time step sizes and their corresponding convergence rates in time are reported in Table 5.2. It is observed that the temporal convergence rates of BE scheme converge to 1, while the rates of other schemes converge to 2, where the expected temporal convergence rates are clearly observed. From Table 5.2, it is evident that the temporal errors of the CNFD-1 scheme and the CNFD-2 scheme are nearly identical, yet they are smaller than those of the box scheme. This underscores the superior convergence speed of both CNFD-1 and CNFD-2 schemes over the box scheme and BE schemes.

Through the analysis of Tables 5.1 and 5.2, we compared the CNFD-1 scheme, the CNFD-2 scheme, BE scheme and the box scheme, we know that the CNFD-1 scheme, the CNFD-2 scheme and the box scheme are second-order accurate both in spatial and temporal directions, and the CNFD-2 scheme has a smaller error than the other schemes. But the BE scheme is second-order accurate in spatial direction and only first-order accurate in temporal direction.

5.2. Evolution of the solution and its spatial first-order derivative

In this subsection, we investigate the influence of the IIM condition on the heat equation over time $t \in [0, 5]$. We first study in Fig. 5.1 the solution of the heat equation with a single concentrated capacity over time, here we choose $\xi = 2/3$, $K = 2$ and fix $m = 3000$, $J = 4000$ and $N = 1000$.

Then, we study in Fig. 5.2 the solution of the heat equation with two concentrated capacities over time, here we take $K_1 = 2$, $K_2 = 2$, $\xi_1 = 7/12$, $\xi_2 = 2/3$ and fix $m_1 = 3000$, $m_2 = 600$, $J = 5100$ and $N = 1000$.

Lastly, we study in Fig. 5.3 that the spatial first-order derivative of the solution of the heat equation with concentrated capacity over time $t \in [0, 5]$, here we choose $\xi = 2/3$, $K = 2$ and fix $m = 3000$, $J = 4000$ and $N = 1000$.

We can observe from the above three figures that the solution is continuous but its spatial first-order derivative is discontinuous at the point $x = \xi$, as is consistent with the continuity

property of the solution of the original problem. Furthermore, it can be observed from the three figures that the solution of the heat system is piecewise smooth, which verifies the regularity assumption of the solution of the heat system.

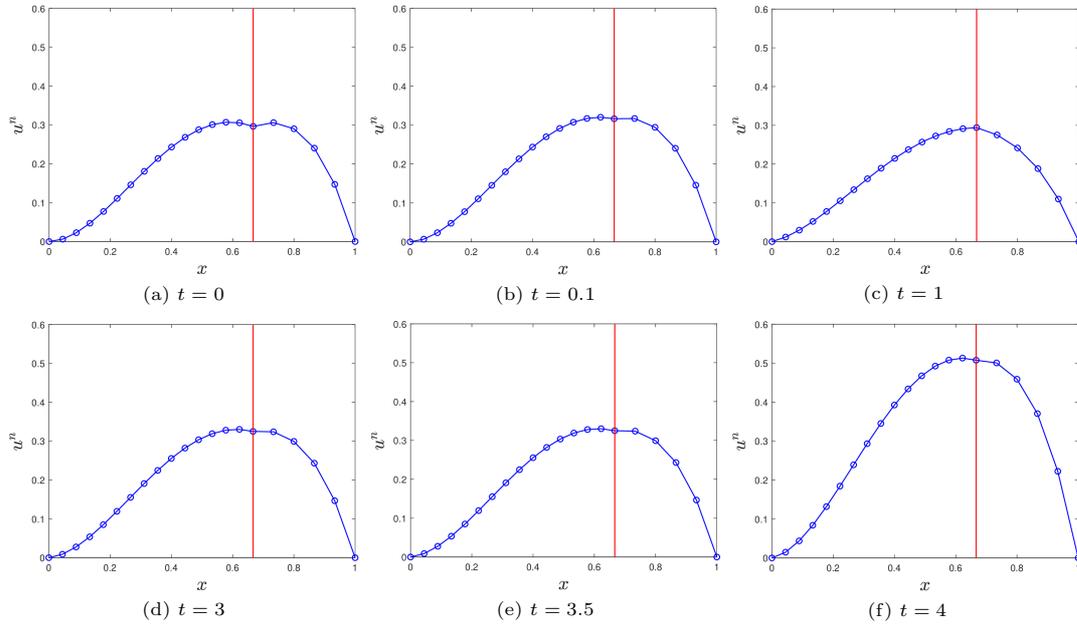


Fig. 5.1. Snapshots of the numerical solution of CNFD-1 scheme at time $t = 0, 0.1, 1, 3, 3.5, 4$.

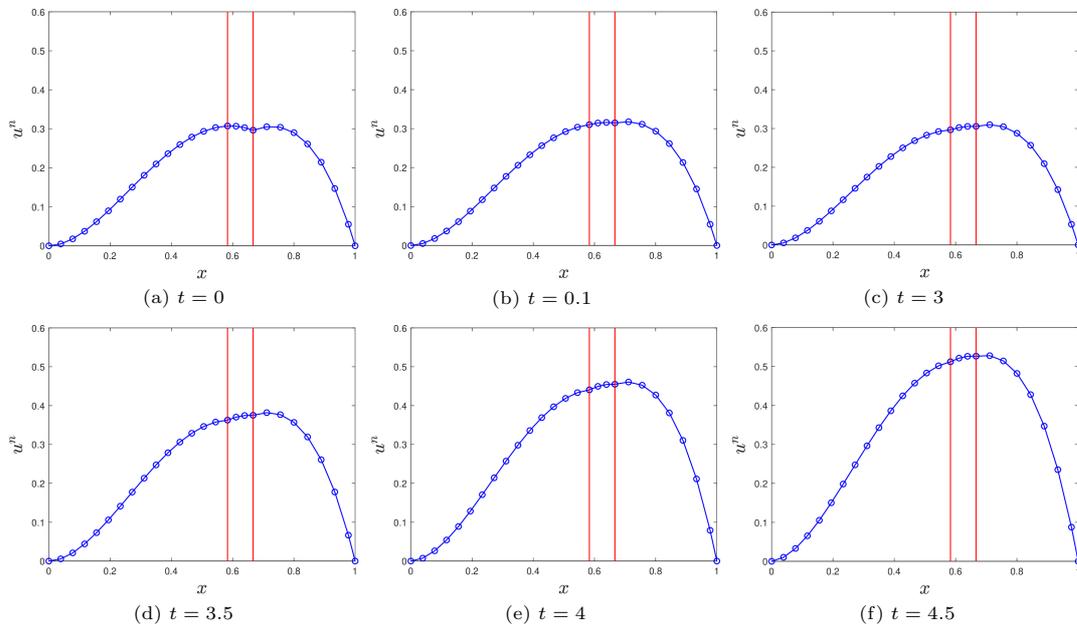


Fig. 5.2. Snapshots of the numerical solution of CNFD-1 scheme with two concentrated capacities at time $t = 0, 0.1, 3, 3.5, 4, 4.5$.

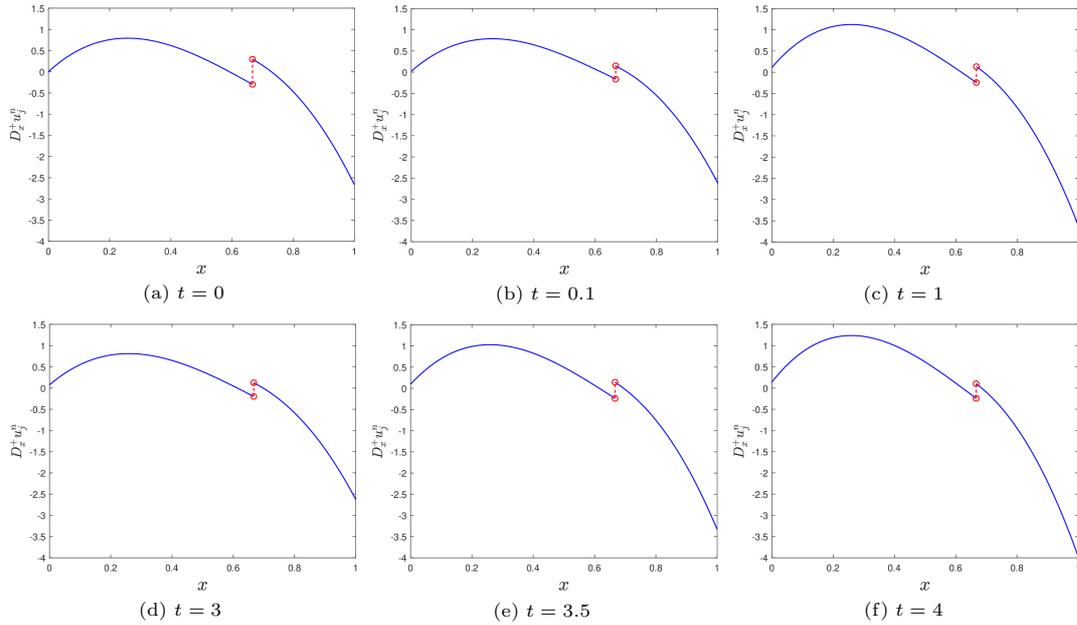


Fig. 5.3. Snapshots of $D_x^+ U$ of CNFD-1 scheme at time $t = 0, 0.1, 1, 3, 3.5, 4$.

6. Conclusion

In this paper, we proposed and analyzed two CNFD schemes for solving the heat equation with concentrated capacity. By introducing embedding inequalities and H^1 technique, we rigorously established the optimal point-wise error estimates of the numerical solutions, which showed that the two proposed numerical schemes are second-order accurate in both spatial and temporal directions. Numerical experiments were carried out to confirm the theoretical results, and furthermore the errors of the two CNFD schemes are showed to be smaller than the finite difference schemes proposed in literature. To propose efficient and accurate finite difference schemes for solving the two-dimensional heat equation with concentrated capacity [18] and establish the unconditional error estimates will be given in our near future work.

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References

- [1] D.G. Aronson, The theory of difference schemes. An introduction (S.K. Godunov and V.S. Ryabenki), *SIAM Rev.*, **11** (1969), 92–93.
- [2] M. Baerns, H. Hofmann, and A. Renken, *Chemical Reaction Technology. Textbook of Industrial Chemistry*, 1987.
- [3] D. Bojović and B.S. Jovanović, Convergence of finite difference method for the parabolic problem with concentrated capacity and variable operator, *J. Comput. Appl. Math.*, **189** (2006), 286–303.
- [4] I.A. Braianov, Convergence of a Crank-Nicolson difference scheme for heat equations with interface in the heat flow and concentrated heat capacity, in: *Lecture Notes in Computer Science*, Springer, **1196** (1997), 58–65.

- [5] I.A. Braianov and L.G. Vulkov, Grid approximation for the solution of the singularly perturbed heat equation with concentrated capacity, *J. Math. Anal. Appl.*, **237** (1999), 672–697.
- [6] I.A. Braianov and L.G. Vulkov, Uniform difference schemes for a heat equation with concentrated heat capacity, *Zh. Vychisl. Math. Math. Phys.*, **39** (1999), 254–267.
- [7] J. Escher, Quasilinear parabolic systems with dynamical boundary conditions, *Comm. Partial Differential Equations*, **18** (1993), 1309–1364.
- [8] B.S. Jovanović and L.G. Vulkov, On the convergence of finite difference schemes for the heat equation with concentrated capacity, *Numer. Math.*, **89** (2001), 715–734.
- [9] B.S. Jovanović and L.G. Vulkov, On the convergence of difference schemes for parabolic problems with concentrated data, *Int. J. Numer. Anal. Mod.*, **5** (2008), 386–406.
- [10] B.S. Jovanović and L.G. Vulkov, Finite difference approximations for some interface problems with variable coefficients, *Appl. Numer. Math.*, **59** (2009), 349–372.
- [11] Z.L. Li, An overview of the immersed interface method and its applications, *Taiwanese J. Math.*, **7** (2003), 1–49.
- [12] A.V. Lykov, Heat and mass transfer, *Int. J. Heat Mass Transf.*, **16** (1973), 1062–1063.
- [13] G.N. Polozhiy and G. Weiss, Equations of mathematical physics, *Phys. Today*, **21** (1968), 93–93.
- [14] G.I. Shishkin, A difference scheme for a singularly perturbed parabolic equation with discontinuous coefficients and concentrated factors, *USSR Comput. Math. Math. Phys.*, **29** (1989), 9–19.
- [15] G.I. Shishkin, Grid approximations of the solution and diffusion flux for singularly perturbed equations with Neumann boundary conditions, *Numer. Anal. Appl.*, **1196** (1997), 58–65.
- [16] G.I. Shishkin, Singularly perturbed boundary value problems with concentrated sources and discontinuous initial conditions, *Comput. Math. Math. Phys.*, **37** (1997), 417–434.
- [17] B.V. Sredojevic and D.R. Bojović, Finite difference approximation for parabolic interface problem with time-dependent coefficients, *Publ. Inst. Math.*, **99** (2016), 67–76.
- [18] B.V. Sredojevic and D.R. Bojović, Finite difference approximation for the 2D heat equation with concentrated capacity, *Filomat*, **32** (2018), 6979–6987.
- [19] Z.Z. Sun, A new class of difference schemes for linear parabolic equations in 1-D, *Math. Numer. Sin.*, **16** (1994), 115–130.
- [20] Z.Z. Sun and Y.L. Zhu, A second order accurate difference scheme for the heat equation with concentrated capacity, *Numer. Math.*, **97** (2004), 379–395.
- [21] R.D. Vold and M. J. Vold, *Colloid and Interface Chemistry*, Reading, Mass.: Addison-Wesley, 1983.