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Numerical Heat Transfer, Part B: Fundamentals
An International Journal of Computation and Methodology

ISSN: 1040-7790 (Print) 1521-0626 (Online) Journal homepage: https://www.tandfonline.com/loi/unhb20

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To cite this article: G. Sudha Priya , P. Prakash , J. J. Nieto & Z. Kayar (2013) Higher-Order Numerical Scheme for the Fractional Heat Equation with Dirichlet and Neumann Boundary Conditions, Numerical Heat Transfer, Part B: Fundamentals, 63:6, 540-559, DOI: 10.1080/10407790.2013.778719

To link to this article: https://doi.org/10.1080/10407790.2013.778719

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Published online: 02 May 2013.

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Numerical Heat Transfer, Part B, 63: 540–559, 2013
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ISSN: 1040-7790 print/1521-0626 online
DOI: 10.1080/10407790.2013.778719

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HIGHER-ORDER NUMERICAL SCHEME FOR THE FRACTIONAL HEAT EQUATION WITH DIRICHLET AND NEUMANN BOUNDARY CONDITIONS

G. Sudha Priya[1], P. Prakash[1], J. J. Nieto[2,3], and Z. Kayar[2,4]

[1]*Department of Mathematics, Periyar University, Salem, Tamil Nadu, India*
[2]*Departamento de Análisis Matemático, Facultad de Mathemáticas, Universidad de Santiago de Compostela, Santiago de Compostela, Spain*
[3]*Department of Mathematics, King Abdulaziz University, Jeddah, Saudi Arabia*
[4]*Department of Mathematics, Middle East Technical University, Ankara, Turkey*

In this article, we consider a higher-order numerical scheme for the fractional heat equation with Dirichlet and Neumann boundary conditions. By using a fourth-order compact finite-difference scheme for the spatial variable, we transform the fractional heat equation into a system of ordinary fractional differential equations which can be expressed in integral form. Further, the integral equation is transformed into a difference equation by a modified trapezoidal rule. Numerical results are provided to verify the accuracy and efficiency of the proposed algorithm.

1. INTRODUCTION

In recent years, considerable interest in fractional differential equations has been stimulated due to their numerous applications in many fields of science and engineering. Important phenomena in physics, viscoelasticity, fluid mechanics, and control theory are well described by differential equations of fractional order. Chang et al. [1] discussed the existence and uniqueness of almost-periodic and pseudo-almost-periodic mild solutions to a class of partial differential equations via fractional operators. Various applications of fractional calculus, such as control theory, are found in [2]. These applications in interdisciplinary sciences show the importance and necessity of fractional calculus. Silva and Gosselin [3] considered the convective and diffusive terms of the two-dimensional energy equations. More recently, the idea has

Received 11 December 2012; accepted 5 February 2013.

The work of the first author is supported by the University Grants Commission—Research Fellowships in Science for Meritorious Students [No. F.4-1/2006(BSR)/11-105/2008(BSR)]. Research co-financed by EC fund FEDER.

Address correspondence to J. J. Nieto, Departamento de Análisis Matemático, Facultad de Matemáticas, Universidad de Santiago de Compostela, Santiago de Compostela 15782, Spain. E-mail: juanjose.nieto.roig@usc.es

emerged that the space and/or time fractional partial differential equation, obtained from the standard partial differential equation that replaces the space-derivative and/or time derivative by a fractional derivative, may more accurately describe some physical problems than the corresponding standard partial differential equation. Consequently, considerable attention has been given to the solutions of the fractional diffusion equation. From a physical point of view, this fractional heat/diffusion equation is obtained from a fractional Fick's law replacing the classical Fick's law, which describes transpose processes with a long memory [4]. Oldham and Spanier [5] considered a fractional diffusion equation that contains a first-order derivative in space and a half-order derivative in time, and they also discussed the relationship between their fractional diffusion equation and a regular diffusion equation. Poldlubny [6] discussed Nigmatullin's fractional diffusion equation and Schneider-Wyss fractional diffusion equations in which the solutions are obtained with help of the Laplace and Fourier transforms combined with the Mittag-Leffler function. Metzler and Klafter [7] used the method of images and Fourier-transform techniques to solve a fractional diffusion equation for absorbing and reflecting boundary conditions, and they also presented a separation-of-variables method for a fractional diffusion equation with a potential. Recently, Agrawal [8] presented a general solution for a fractional diffusion-wave equation defined in a bounded space domain by the finite sine and Laplace transform technique. However, the availability of numerical methods for solving fractional diffusion equation would be most desirable, especially for those cases where no analytical solution is available. Langlands and Henry [9] investigated the accuracy and stability of an implicit numerical scheme for solving a fractional diffusion equation with zero flux boundary condition. Liu et al. [10–12] has used the finite-difference method for various fractional diffusion equations based on Grunwald-Letnikov/shifted Grunwald-Letnikov definitions of fractional derivatives. Sun et al. [13–15] concentrated on $L1$ discretization, which is derived by Oldham and Spanier [5] for promoting the temporal accuracy. The numerical schemes proposed in [13–15] have convergence of order $O(\tau^{2-\gamma}+h^4)$, where γ, τ, and h are the order of the time derivative, time step, and spatial size, respectively. However, higher-order numerical schemes for heat equation are still limited.

In this article we consider the fourth-order compact scheme in space and modified trapezoidal rule that have been obtained for the fractional heat equation with Dirichlet and Neumann boundary conditions to increase the order of convergence from $O(\tau^{2-\gamma}+h^4)$ to $O(\tau^2+h^4)$.

The remainder of the article is organized as follows: in Section 2 and Section 3, we present the higher-order-accurate numerical method and its matrix form for the fractional heat equation with Dirichlet and Neumann boundary conditions, respectively. The solvability of the linear system of equations is also discussed in Section 3. Some numerical results are provided in Section 4 which show that this method is computationally efficient. Some concluding remarks are provided in Section 5.

2. FRACTIONAL HEAT EQUATION WITH DIRICHLET BOUNDARY CONDITION

Throughout the article, we use the "empty sum" convention $\sum_{l=k}^{n} u^l = 0$ for $n < k$. We introduce a uniform grid of points $(x_j,\ t_k)$, with $x_j = jh$, $j = 0,$

1, 2,. . ., m, and $t_k = k\tau$, $k = 0, 1, 2,\ldots, n$ where m and n are positive integers, $h = L/m$ is the mesh-width in x, and $\tau = T/n$ is the time step where $L > 0$ and $T > 0$. Let $\Omega_h = \{x_j | 0 \le j \le m\}$ and $\Omega_\tau = \{t_k | 0 \le k \le n\}$.

Consider the fractional heat equation

$$\frac{\partial u(x,t)}{\partial t} = {}_0D_t^{1-\gamma}\left[K_\gamma \frac{\partial^2 u(x,t)}{\partial x^2}\right] + f(x,t) \qquad 0 < x < L, 0 < t \le T \tag{1}$$

with initial condition

$$u(x,0) = w(x) \qquad 0 \le x \le L \tag{2}$$

and boundary condition

$$u(0,t) = \phi(t) \qquad u(L,t) = \xi(t) \qquad 0 \le t \le T \tag{3}$$

where K_γ is the generalized diffusion constant, $0 < \gamma < 1$, ${}_0D_t^{1-\gamma}u(x,t)$ denotes the Riemann-Liouville fractional derivative of order $1-\gamma$ of the function $u(x, t)$ defined by [5, 6, 16, 17],

$${}_0D_t^{1-\gamma}u(x,t) = \frac{1}{\Gamma(\gamma)}\frac{\partial}{\partial t}\int_0^t \frac{u(x,\tau)}{(t-\tau)^{1-\gamma}}\, d\tau$$

and $f(x, t)$, $w(x)$, $\phi(t)$, and $\xi(t)$ are known smooth functions satisfying $\phi(0) = w(0)$ and $\xi(0) = w(L)$. Then Eq. (1) can be written in the equivalent form

$${}_0D_t^{\gamma}[u(x,t) - u(x,0)] = K_\gamma \frac{\partial^2 u(x,t)}{\partial x^2} + g(x,t) \tag{4}$$

where $g(x,t) = {}_0D_t^{\gamma-1}f(x,t)$, ${}_0D_t^{\gamma-1}f(x,t)$ denotes the Riemann-Liouville fractional integral operator of order $1-\gamma$ of the function $f(x, t)$ defined by [5, 6, 16, 17],

$${}_0D_t^{\gamma-1}f(x,t) = \frac{1}{\Gamma(1-\gamma)}\int_0^t \frac{f(x,\tau)}{(t-\tau)^{\gamma}}\, d\tau$$

Using the relationship between the Caputo fractional derivative and the Riemann-Liouville fractional derivative [6, 14], Eq. (4) can be written as

$${}_0^C D_t^{\gamma} u(x,t) = K_\gamma \frac{\partial^2 u(x,t)}{\partial x^2} + g(x,t) \tag{5}$$

where ${}_0^C D_t^{\gamma} u(x,t)$ denotes the Caputo fractional derivative of order γ of the function $u(x, t)$ defined by [6, 14],

$$ {}_0^C D_t^\gamma u(x,t) = \frac{1}{\Gamma(1-\gamma)} \int_0^t \frac{\partial u(x,\tau)}{\partial \tau} \frac{d\tau}{(t-\tau)^\gamma} $$

2.1. The Solution Vector

The exact solution u of the initial and boundary-value problem (2), (3), and (5) at the point $(x_j, t_k) \in \Omega_h \times \Omega_\tau$ is denoted by u_j^k, and the corresponding solution vector is denoted by $u^k = (u_1^k, \cdots, u_{m-1}^k)^T$. The exact solution of an approximating ordinary fractional differential equation and difference equation at the same point will be denoted by $U_j(t_k)$ and U_j^k, and the corresponding solution vectors are denoted by $U(t_k) = (U_1(t_k), \ldots, U_{m-1}(t_k))^T$ and $U^k = (U_1^k, \cdots, U_{m-1}^k)^T$, respectively.

2.2. Discretization in Space: Semi-discrete Scheme

We use the fourth-order compact difference scheme for the second derivative:

$$ \frac{\partial^2 u(x,t)}{\partial x^2}\Big|_{x=x_j} = \frac{1}{h^2} \frac{\delta_x^2}{1 + (\frac{\delta_x^2}{12})} u(x_j,t) + O(h^4) $$

where $\delta_x^2 u(x_j,t) = u(x_{j-1},t) - 2u(x_j,t) + u(x_{j+1},t)$. Thus, we may approximate the initial and boundary-value problem (2),(3), and (5) by the following semi-discrete scheme:

$$ \begin{aligned} {}_0^C D_t^\gamma U_j(t) &= \frac{K_\gamma}{h^2} \frac{\delta_x^2}{1 + (\frac{\delta_x^2}{12})} U_j(t) + g(x_j,t) \qquad 1 \le j \le m-1, \quad 0 < t \le T \\ U_0(t) &= \phi(t) \qquad U_m(t) = \xi(t) \qquad 0 \le t \le T \\ U_j(0) &= w(x_j) \qquad 0 \le j \le m \end{aligned} \tag{6} $$

2.3. Fully Discrete Scheme

The equivalent form of (6) is given by

$$ \begin{aligned} U_j(t) &= U_j(0) + J^\gamma \left[\frac{K_\gamma}{h^2} \frac{\delta_x^2}{1 + (\frac{\delta_x^2}{12})} U_j(t) + g(x_j,t) \right] \qquad 1 \le j \le m-1, \quad 0 < t \le T \\ U_0(t) &= \phi(t) \qquad U_m(t) = \xi(t) \qquad 0 \le t \le T \\ U_j(0) &= w(x_j) \qquad 0 \le j \le m, \end{aligned} \tag{7} $$

where J^γ denotes the Riemann-Liouville fractional integral of order γ defined by [6, 18],

$$J^{\gamma} f(t) = \frac{1}{\Gamma(\gamma)} \int_0^t (t-\tau)^{\gamma-1} f(\tau)\, d\tau$$

By using the modified trapezoidal rule [18] for the Riemann fractional integral, Eq. (7) is approximated by, for $1 \le k \le n$,

$$\begin{aligned} U_j^k &= U_j^0 + \frac{\tau^{\gamma}}{\Gamma(2+\gamma)} \left(\frac{K_{\gamma}}{h^2} \sum_{i=0}^{k} a_{k,i} \frac{\delta_x^2}{1+(\frac{\delta_x^2}{12})} U_j^i + \sum_{i=0}^{k} a_{k,i} g_j^i \right) \\ U_0^k &= \phi(t_k) \qquad U_m^k = \xi(t_k) \\ U_j^0 &= w(x_j) \qquad 0 \le j \le m, \end{aligned}$$

where

$$a_{k,i} = \begin{cases} (k-1)^{\gamma+1} - (k-\gamma-1)k^{\gamma} & i = 0 \\ (k-i+1)^{\gamma+1} - 2(k-i)^{\gamma+1} + (k-i-1)^{\gamma+1} & 1 \le i \le k-1 \\ 1 & i = k \end{cases} \tag{8}$$

and $g_j^k = g(x_j, t_k)$. Introducing the scaling parameter $\mu = \frac{K_{\gamma}\tau^{\gamma}}{\Gamma(\gamma+2)h^2}$ and arranging the terms, we have

$$\begin{aligned} &(1-12\mu) U_{j-1}^k + (10+24\mu) U_j^k + (1-12\mu) U_{j+1}^k \\ &\quad = (1+12\mu a_{k,0}) U_{j-1}^0 \\ &\qquad + (10-24\mu a_{k,0}) U_j^0 + (1+12\mu a_{k,0}) U_{j+1}^0 \\ &\qquad + 12\mu \sum_{i=1}^{k-1} a_{k,i} (U_{j-1}^i - 2U_j^i + U_{j+1}^i) \\ &\qquad + \frac{\tau^{\gamma}}{\Gamma(\gamma+2)} \sum_{i=0}^{k} a_{k,i} (g_{j-1}^i + 10 g_j^i + g_{j+1}^i), \quad 1 \le j \le m-1 \\ &\quad U_0^k = \phi(t_k) \qquad U_m^k = \xi(t_k), \\ &\quad U_j^0 = w(x_j) \qquad 0 \le j \le m. \end{aligned} \tag{9}$$

Let us rewrite this system of equations (9) in the following matrix form:

$$A U^k = B_k U^0 + 12\mu \sum_{i=1}^{k-1} a_{k,i} C U^i + G^k \qquad 1 \le k \le n \tag{10}$$

where the tridiagonal matrices in (10) are given by

$$A=\begin{pmatrix} 10+24\mu & 1-12\mu & & & \\ 1-12\mu & 10+24\mu & 1-12\mu & & \\ & \ddots & \ddots & \ddots & \\ & & 1-12\mu & 10+24\mu & 1-12\mu \\ & & & 1-12\mu & 10+24\mu \end{pmatrix}_{(m-1)\times(m-1)},$$

$$C=\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}_{(m-1)\times(m-1)},$$

for $1\le k\le n$,

$$B_k=\begin{pmatrix} 10_24\mu a_{k,0} & 1+12\mu a_{k,0} & & & \\ 1+12\mu a_{k,0} & 10-24\mu a_{k,0} & 1+12\mu a_{k,0} & & \\ & \ddots & \ddots & \ddots & \\ & & 1+12\mu a_{k,0} & 10-24\mu a_{k,0} & 1+12\mu a_{k,0} \\ & & & 1+12\mu a_{k,0} & 10-24\mu a_{k,0} \end{pmatrix}_{(m-1)\times(m-1)},$$

and finally the column vectors in $R^{(m-1)}$ are given by

$$G^k=\begin{pmatrix} \frac{\tau^\gamma}{\Gamma(2+\gamma)}\sum_{i=0}^{k} a_{k,i}(g_0^i+10g_1^i+g_2^i)-(1-12\mu)\phi(t_k)+(1+12\mu a_{k,0})\phi(t_0)+12\mu\sum_{i=0}^{k-1}a_{k,i}\phi(t_i) \\ \frac{\tau^\gamma}{\Gamma(2+\gamma)}\sum_{i=0}^{k} a_{k,i}(g_1^i+10g_2^i+g_3^i) \\ \vdots \\ \frac{\tau^\gamma}{\Gamma(2+\gamma)}\sum_{i=0}^{k} a_{k,i}(g_{m-3}^i+10g_{m-2}^i+g_{m-1}^i) \\ \frac{\tau^\gamma}{\Gamma(2+\gamma)}\sum_{i=0}^{k} a_{k,i}(g_{m-2}^i+10g_{m-1}^i+g_m^i)-(1-12\mu)\xi(t_k)+(1+12\mu a_{k,0})\xi(t_0)+12\mu\sum_{i=0}^{k-1}a_{k,i}\xi(t_i) \end{pmatrix}_{(m-1)\times 1}.$$

3. FRACTIONAL HEAT EQUATION WITH NEUMANN BOUNDARY CONDITION

Consider the following fractional heat equation:

$$\frac{\partial u(x,t)}{\partial t}={}_0D_t^{1-\gamma}\left[K_\gamma\frac{\partial^2 u(x,t)}{\partial x^2}\right]+f(x,t)\qquad 0\le x\le L,\quad 0<t\le T \tag{11}$$

with initial condition

$$u(x,0) = w(x) \qquad 0 \le x \le L \tag{12}$$

and boundary condition

$$u_x(0,t) = \phi(t) \qquad u_x(L,t) = \xi(t) \qquad 0 < t \le T \tag{13}$$

where $w(x)$, $\phi(t)$, and $\xi(t)$ are known smooth functions. As discussed in Section 2, (11) can be put in the following equivalent form:

$$ {}_0^C D_t^\gamma u(x,t) = K_\gamma \frac{\partial^2 u(x,t)}{\partial x^2} + g(x,t) \qquad 0 \le x \le L, \quad 0 < t \le T \tag{14}$$

3.1. The Solution Vector

The exact solution $\tilde{u}$ of initial and boundary-value problem (12), (13), and (14) at the point $(x_j, t_k) \in \Omega_h \times \Omega_\tau$ is denoted by $\tilde{u}_j^k$, and the corresponding solution vector is denoted by $\tilde{u}^k = (\tilde{u}_0^k, \tilde{u}_1^k, \cdots, \tilde{u}_m^k)^T$. The exact solution of an approximating ordinary fractional differential equation and difference equation at the same point will be denoted by $\tilde{U}_j(t_k)$, and $\tilde{U}_j^k$, and the corresponding solution vectors are denoted by $\tilde{U}(t_k) = (\tilde{U}_0(t_k), \tilde{U}_1(t_k), \cdots, \tilde{U}_m(t_k))^T$ and $\tilde{U}^k = (\tilde{U}_0^k, \tilde{U}_1^k, \cdots, \tilde{U}_m^k)^T$, respectively.

3.2. Discretization in Space: Semi-discrete Scheme

We use the fourth-order compact difference schemes for the first and second derivatives:

$$\begin{aligned} \frac{\partial \tilde{u}(x,t)}{\partial x}|_{x=x_j} &= \frac{\delta_x}{2h\left(1 + \frac{\delta_x^2}{6}\right)} \tilde{u}(x_j,t) + O(h^4) \\ \frac{\partial^2 \tilde{u}(x,t)}{\partial x^2}|_{x=x_j} &= \frac{\delta_x^2}{h^2\left(1 + \frac{\delta_x^2}{12}\right)} \tilde{u}(x_j,t) + O(h^4) \end{aligned} \tag{15}$$

where $\delta_x \tilde{u}(x_j,t) = \tilde{u}(x_{j+1},t) - \tilde{u}(x_{j-1},t)$, $\delta_x^2 \tilde{u}(x_j,t) = \tilde{u}(x_{j-1},t) - 2\tilde{u}(x_j,t) + \tilde{u}(x_{j+1},t)$. It follows from (13) and (14) that

$$\begin{aligned} \tilde{u}_x(0,t) &= \phi(t) \\ K_\gamma \tilde{u}_{xxx}(0,t) &= g_x C D_t^\gamma \phi(t) - g_x(0,t) \end{aligned} \tag{16}$$

Also from (15) and (16) it follows that

$$\tilde{u}(x_{-1},t) = \tilde{u}(x_1,t) - 2h\left\{\frac{\phi(t) + h^2}{6K_\gamma}[{}_0^C D_t^\gamma \phi(t) - (g_x)(x_0,t)]\right\} + O(h^5) \tag{17}$$

A similar method to that used to obtain Eq. (17) is applied to derive Eq. (18) at the point $(x_m, t) = (L, t)$. Therefore, the Caputo derivative of $\xi(t)$ should be taken,

$$\tilde{u}(x_{m+1}, t) = \tilde{u}(x_{m-1}, t) + 2h\left\{\xi(t) + \frac{h^2}{6K_\gamma}\left[{}_0^C D_t^\gamma \xi(t) - (g_x)(x_m, t)\right]\right\} + O(h^5) \tag{18}$$

where $x_{-1} = -h$ and $x_{m+1} = L + h$ are fictitious points. Thus, we may approximate the initial boundary value problem (12)–(14) by the following semi-discrete scheme:

For $0 < t \le T$,

$$\begin{aligned} &{}_0^C D_t^\gamma \tilde{U}_j(t) = \frac{K_\gamma}{h^2}\frac{\delta_x^2}{1 + (\frac{\delta_x^2}{12})}\tilde{U}_j(t) + g(x_j, t) \qquad 0 \le j \le m \\ &\tilde{U}_{-1}(t) = \tilde{U}_1(t) - 2h\chi_1(t) \qquad \tilde{U}_{m+1}(t) = \tilde{U}_{m-1}(t) + 2h\chi_2(t) \\ &\tilde{U}_j(0) = w(x_j) \qquad 0 \le j \le m, \end{aligned} \tag{19}$$

where

$$\chi_1(t) = \phi(t) + \frac{h^2}{6K_\gamma}\left[{}_0^C D_t^\gamma \phi(t) - (g_x)(x_0, t)\right]$$

$$\chi_2(t) = \xi(t) + \frac{h^2}{6K_\gamma}\left[{}_0^C D_t^\gamma \xi(t) - (g_x)(x_m, t)\right]$$

3.3. Fully Discrete Scheme

The equivalent form of (19) for $0 < t \le T$ is

$$\begin{aligned} &\tilde{U}_j(t) = \tilde{U}_j(0) + J^\gamma\left[\frac{K_\gamma}{h^2}\frac{\delta_x^2}{1 + (\frac{\delta_x^2}{12})}\tilde{U}_j(t) + g(x_j, t)\right] \qquad 0 \le j \le m \\ &\tilde{U}_{-1}(t) = \tilde{U}_1(t) - 2h\chi_1(t) \qquad \tilde{U}_{m+1}(t) = \tilde{U}_{m-1}(t) + 2h\chi_2(t) \\ &\tilde{U}_j(0) = w(x_j) \qquad 0 \le j \le m \end{aligned} \tag{20}$$

By using the modified trapezoidal rule for the Riemann-Liouville fractional integral, (20) is approximated by, for $1 \le k \le n$,

$$\tilde{U}_j^k = \tilde{U}_j^0 + \frac{\tau^\gamma}{\Gamma(2+\gamma)}\left(\frac{K_\gamma}{h^2}\sum_{i=0}^{k} a_{k,i}\frac{\delta_x^2}{1 + (\frac{\delta_x^2}{12})}\tilde{U}_j^i + \sum_{i=0}^{k} a_{k,i} g_j^i\right) \qquad 0 \le j \le m \tag{21}$$

$$\tilde{U}_{-1}^k = \tilde{U}_1^k - 2h\chi_1(t_k) \tag{22}$$

$$\tilde{U}_{m+1}^k = \tilde{U}_{m-1}^k + 2h\chi_2(t_k) \tag{23}$$

$$\tilde{U}_j^0 = w(x_j) \qquad 0 \le j \le m$$

where $a_{k,\,i}$ is defined as (8) and $g_j^k = g(x_j, t_k)$. Substituting (22) and (23) in (21) when $j=0$ and $j=m$, respectively, and arranging the terms, we have, for $1 \le k \le n$,

$$\begin{aligned}(10+24\mu)\tilde{U}_0^k + 2(1-12\mu)\tilde{U}_1^k &= (10-24\mu a_{k,0})\tilde{U}_0^0 \\ &+ 2(1+12\mu a_{k,0})\tilde{U}_1^0 + 12\mu\sum_{i=1}^{k-1} a_{k,i}(2\tilde{U}_1^i - 2\tilde{U}_0^i) + \frac{\tau^\gamma}{\Gamma(\gamma+2)}\sum_{i=0}^{k} a_{k,i}(g_{-1}^i + 10g_0^i + g_1^i) \\ &+ 2h(1-12\mu)\chi_1(t_k) - 2h(1+12\mu a_{k,0})\chi_1(t_0) - 24\mu h\sum_{i=1}^{k-1} a_{k,i}\chi_1(t_i)\end{aligned}$$

$$\begin{aligned}(1-12\mu)\tilde{U}_{j-1}^k + (10+24\mu)\tilde{U}_j^k + (1-12\mu)\tilde{U}_{j+1}^k &= (1+12\mu a_{k,0})\tilde{U}_{j-1}^0 \\ &+ (10-24\mu a_{k,0})\tilde{U}_j^0 + (1+12\mu a_{k,0})\tilde{U}_{j+1}^0 + 12\mu\sum_{i=1}^{k-1} a_{k,i}(\tilde{U}_{j-1}^i - 2\tilde{U}_j^i + \tilde{U}_{j+1}^i) \\ &+ \frac{\tau^\gamma}{\Gamma(\gamma+2)}\sum_{i=0}^{k} a_{k,i}(g_{j-1}^i + 10g_j^i + g_{j+1}^i) \qquad 1 \le j \le m-1\end{aligned} \tag{24}$$

$$\begin{aligned}2(1-12\mu)\tilde{U}_{m-1}^k + (10+24\mu)\tilde{U}_m^k &= 2(1+12\mu a_{k,0})\tilde{U}_{m-1}^0 \\ &+ (10-24\mu a_{k,0})\tilde{U}_m^0 + 12\mu\sum_{i=1}^{k-1} a_{k,i}(2\tilde{U}_{m-1}^i - 2\tilde{U}_m^i) + \frac{\tau^\gamma}{\Gamma(\gamma+2)}\sum_{i=0}^{k} a_{k,i}(g_{m-1}^i + 10g_m^i \\ &+ g_{m+1}^i) - 2h(1-12\mu)\chi_2(t_k) + 2h(1+12\mu a_{k,0})\chi_2(t_0) + 24\mu h\sum_{i=1}^{k-1} a_{k,i}\chi_2(t_i) \\ \tilde{U}_j^0 &= w(x_j) \qquad 0 \le j \le m\end{aligned}$$

We need the values of g_{-1}^i and g_{m+1}^i, and these may be obtained from the Taylor series expansion. Using the Taylor series expansion of g_1^k and g_{-1}^i about the point (x_0, t_i), then $g_{-1}^i + 10g_0^i + g_1^i$ can be written as $12g_0^i + h^2(g_{xx})_0^i + O(h^4)$. Similarly, $g_{m-1}^i + 10g_m^i + g_{m+1}^i$ can be written as $12g_m^i + h^2(g_{xx})_m^i + O(h^4)$ by using the Taylor series expansion of g_{m-1}^i and g_{m+1}^i about the point (x_m, t_i).

Remark. Since $g(x, t)$ is known function, the exact value of $g(x, t)$ at the points $(x_{-1}, t_i) = (-h, t_i)$ and $(x_{m+1}, t_i) = (L+h, t_i)$ may be used.

Let us rewrite this system of equations (24) in the following matrix form:

$$\tilde{A}\tilde{U}^k = \tilde{B}_k\tilde{U}^0 + 12\mu\sum_{i=1}^{k-1} a_{k,i}\tilde{C}\tilde{U}^i + \tilde{G}^k \qquad 1 \le k \le n \tag{25}$$

where the tridiagonal matrices in (25) are given by

$$\tilde{A} = \begin{pmatrix} 10_{+}24\mu & 2(1-12\mu) & & & & \\ 1-12\mu & 10+24\mu & 1-12\mu & & & \\ & \ddots & \ddots & \ddots & & \\ & & 1-12\mu & 10+24\mu & 1-12\mu & \\ & & & 2(1-12\mu) & 10+24\mu & \end{pmatrix}_{(m+1)\times(m+1)},$$

$$\tilde{C} = \begin{pmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2 \end{pmatrix}_{(m+1)\times(m+1)},$$

for $1 \le k \le n$,

$$\tilde{B}_k = \begin{pmatrix} 10-24\mu a_{k,0} & 2(1+12\mu a_{k,0}) & & & \\ 1+12\mu a_{k,0} & 10-24\mu a_{k,0} & 1+12\mu a_{k,0} & & \\ & \ddots & \ddots & \ddots & \\ & & 1+12\mu a_{k,0} & 10-24\mu a_{k,0} & 1+12\mu a_{k,0} \\ & & & 2(1+12\mu a_{k,0}) & 10-24\mu a_{k,0} \end{pmatrix}_{(m+1)\times(m+1)},$$

and finally the column vectors in $R^{(m+1)}$ are given by

$$\tilde{G}^k = \begin{pmatrix} \frac{\tau^\gamma}{\Gamma(2+\gamma)} \sum_{i=0}^{k} a_{k,i}(12g_0^i + h^2(g_{xx})_0^i) + 2h(1-12\mu)\chi_1(t_k) - 2h(1+12\mu a_{k,0})\chi_1(t_0) - 24h\mu \sum_{i=0}^{k-1} a_{k,i}\chi_1(t_i) \\ \frac{\tau^\gamma}{\Gamma(2+\gamma)} \sum_{i=0}^{k} a_{k,i}(g_0^i + 10g_1^i + g_2^i) \\ \vdots \\ \frac{\tau^\gamma}{\Gamma(2+\gamma)} \sum_{i=0}^{k} a_{k,i}(g_{m-2}^i + 10g_{m-1}^i + g_m^i) \\ \frac{\tau^\gamma}{\Gamma(2+\gamma)} \sum_{i=0}^{k} a_{k,i}(12g_m^i + h^2(g_{xx})_m^i) - 2h(1-12\mu)\chi_2(t_k) + 2h(1+12\mu a_{k,0})\chi_2(t_0) + 24h\mu \sum_{i=0}^{k-1} a_{k,i}\chi_2(t_i) \end{pmatrix}_{(m+1)\times 1}.$$

Theorem 1. [18] Suppose that the interval [0, T] is subdivided into n subintervals [t_k, t_{k+1}] of equal width $\tau = T/n$ by using the nodes $t_k = k\tau$, for $k = 0, 1, \ldots, n$. The modified trapezoidal rule,

$$T_a(f, \tau, \gamma) = \frac{\tau^\gamma}{\Gamma(2+\gamma)} \sum_{k=0}^{n} a_{n,k} f(t_k)$$

is an approximation to the fractional integral

$$(J^\gamma f(t))(T) = T(f, \tau, \gamma) - E_{T_a}(f, \tau, \gamma) \qquad T > 0, \quad \gamma > 0$$

where $a_{n,\,k}$ is defined as in (8). Furthermore,

a. if $f(t) \in C^2[0, T]$, there is a constant C'_γ depending only on γ so that the error term $E_{T_a}(f, \tau, \gamma)$ has the form

$$|E_{T_a}(f, \tau, \gamma)| \leq C'_\gamma \|f''\|_\infty T^\gamma \tau^2 = O(\tau^2)$$

b. if $f(t) = t^p$ for some $p \in (0, 2)$ and $Q := \min(2, p+1)$, there is a constant $C'_{\gamma,p}$ depending on γ and p so that the error term $E_{T_a}(f, \tau, \gamma)$ has the form

$$|E_{T_a}(f, \tau, \gamma)| \leq C'_{\gamma,p} T^{\gamma+p-Q} \tau^Q = O(\tau^Q)$$

Theorem 2. The difference equations (9) and (24) have a unique solution.

Proof. For any $\mu = K_\gamma \tau^\gamma / \Gamma(2+\gamma) h^2 > 0$, the coefficient matrices A and $\tilde{A}$ for the difference equations are strictly diagonally dominant. Consequently, the matrices A and $\tilde{A}$ are nonsingular, thus are invertible. This completes the proof of the theorem.

4. NUMERICAL EXPERIMENTS

Example 1 Fractional heat equation with Dirichlet boundary condition [19]

$$\begin{aligned}
&\frac{\partial u(x,t)}{\partial t} = {}_0 D_t^{1-\gamma}\left[\frac{\partial^2 u(x,t)}{\partial x^2}\right] + \left(2t + \frac{8\pi^2}{\Gamma[2+\gamma]} t^{1+\gamma}\right)\sin(2\pi x) \quad 0 < x < 1, \;\; 0 < t \leq 1 \\
&u(x,0) = 0 \quad 0 \leq x \leq 1 \\
&u(0,t) = 0 \quad u(1,t) = 0 \quad 0 \leq t \leq 1
\end{aligned} \tag{26}$$

The exact solution of (26) is

$$u(x, t) = t^2 \sin(2\pi x)$$

The error is defined as

$$\overline{E}_\infty(h, \tau) = \max_{0 \leq j \leq m} |u(x_j, t_n) - U_j^n|$$

Denote

$$\text{Order} = \frac{\overline{E}_\infty(h, \tau)}{\overline{E}_\infty(h/2, \tau/2)}$$

In Table 1 we have compared the errors as well as their convergence order for the difference scheme ($L1C$) in [14] and compact modified trapezoidal rule (CT) (9) in the case when h and τ decrease simultaneously. The exact solution and the convergence of the numerical solution of CT scheme defined by (9) of Example 1 for $\gamma = 0.5$ are given in Figures 1 and 2, respectively.

Table 1. Maximum errors and convergence orders of $L1C$ and CT (9) schemes when $\gamma = 0.5$

$\gamma = 0.5$	$\overline{E}_\infty(h,\tau)$(L1C)	Order (L1C)	$\overline{E}_\infty(h,\tau)$(CT)	Order (CT)
$h=\tau=1/100$	0.0000115382	1.49771	3.00526×10^{-7}	2.24466
$h=\tau=1/200$	7.73015×10^{-6}	1.49498	6.34119×10^{-8}	2.06813
$h=\tau=1/400$	1.4496×10^{-6}	*	1.51218×10^{-8}	*

Example 2. Fractional heat equation with Dirichlet boundary condition [14]

$$\begin{aligned}
&\frac{\partial u(x,t)}{\partial t} = {}_0D_t^{1-\gamma}\left[\frac{\partial^2 u(x,t)}{\partial x^2}\right] + e^x\left[(1+\gamma)t^\gamma - \frac{\Gamma[2+\gamma]}{\Gamma[1+2\gamma]}t^{2\gamma}\right] \quad 0<x<1 \quad 0<t\le 1\\
&u(x,0) = 0 \qquad 0\le x\le 1\\
&u(0,t) = t^{\gamma+1} \qquad u(1,t) = et^{\gamma+1} \qquad 0\le t\le 1.
\end{aligned} \tag{27}$$

The exact solution of (27) is

$$u(x,t) = e^x t^{\gamma+1}$$

We show that the numerical results of the CT scheme defined by (9) are apparently more accurate than those of [14] with the same mesh. In Tables 2 and 3 we have

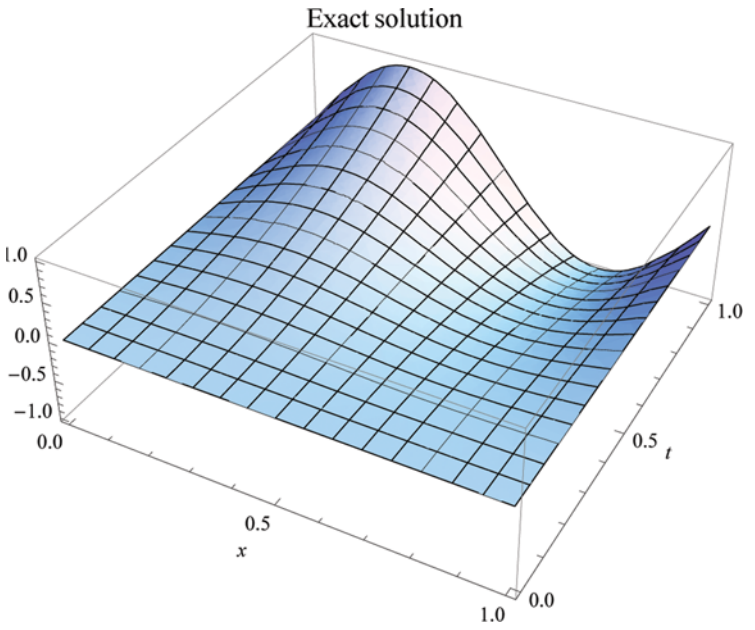


Figure 1. Exact solution for Example 1 at $\gamma = 0.5$ (color figure available online).

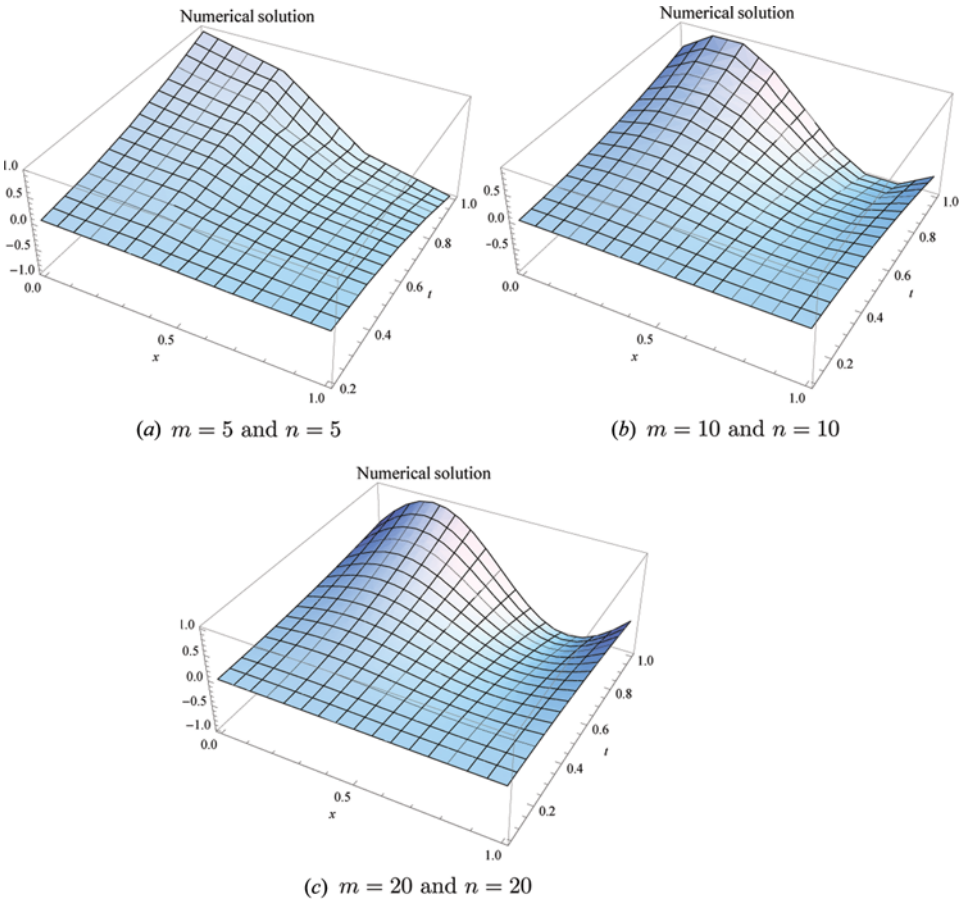


Figure 2. Numerical solution of the CT scheme defined by (9) for Example 1 at $\gamma = 0.5$ (color figure available online).

compared with the values $\gamma = 0.25$ and $\gamma = 0.75$, respectively. The comparisons between the absolute errors of the $L1C$ scheme and the CT scheme defined by (9) at selected points and $\gamma = 0.5$ are given in Figures 3 and 4, respectively.

Table 2. Some results of (9) compared with $L1C$ when $\gamma = 0.25$

$\gamma = 0.25$	$\overline{E}_\infty(h,\tau)$(L1C)	$\overline{E}_\infty(h,\tau)$(CT)
$h = 1/4$, $\tau = 1/4$	0.00072822	3.05274×10^{-6}
$h = 1/8$, $\tau = 1/64$	6.0359×10^{-6}	1.91141×10^{-7}
$h = 1/16$, $\tau = 1/1{,}024$	3.846×10^{-8}	1.2037×10^{-8}
$h = 1/8$, $\tau = 1/8$	0.00022328	1.91142×10^{-7}
$h = 1/16$, $\tau = 1/128$	1.8709×10^{-6}	1.2037×10^{-8}
$h = 1/32$, $\tau = 1/2{,}048$	1.4338×10^{-8}	7.52629×10^{-10}

Table 3. Some results of (9) compared with $L1C$ when $\gamma = 0.75$

$\gamma = 0.75$	$\overline{E}_\infty(h,\tau)$(L1C)	$\overline{E}_\infty(h,\tau)$(CT)
$h = 1/4,\ \tau = 1/4$	0.0173	2.90372×10^{-6}
$h = 1/8,\ \tau = 1/64$	0.00053739	1.81805×10^{-7}
$h = 1/16,\ \tau = 1/1{,}024$	0.000016874	1.14604×10^{-8}
$h = 1/8,\ \tau = 1/8$	0.0072	1.81807×10^{-7}
$h = 1/16,\ \tau = 1/128$	0.00022716	1.14604×10^{-8}
$h = 1/32,\ \tau = 1/2{,}048$	7.1085×10^{-6}	7.16363×10^{-10}

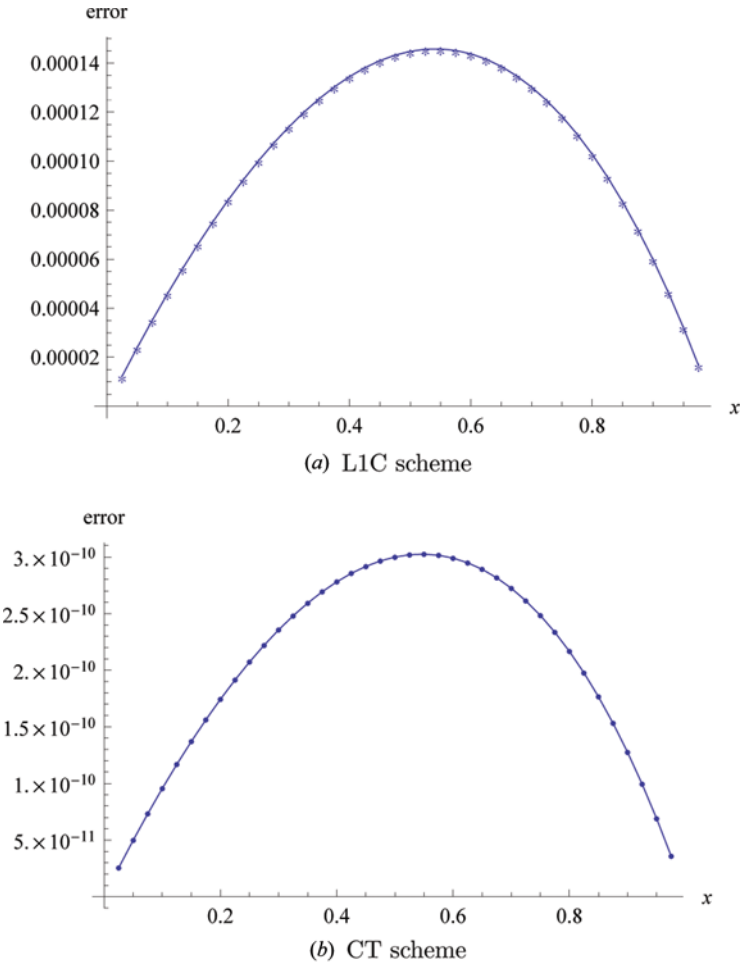


Figure 3. Absolute errors for Example 2 at $\gamma = 0.5$, $m = 40$, and $n = 40$ (color figure available online).

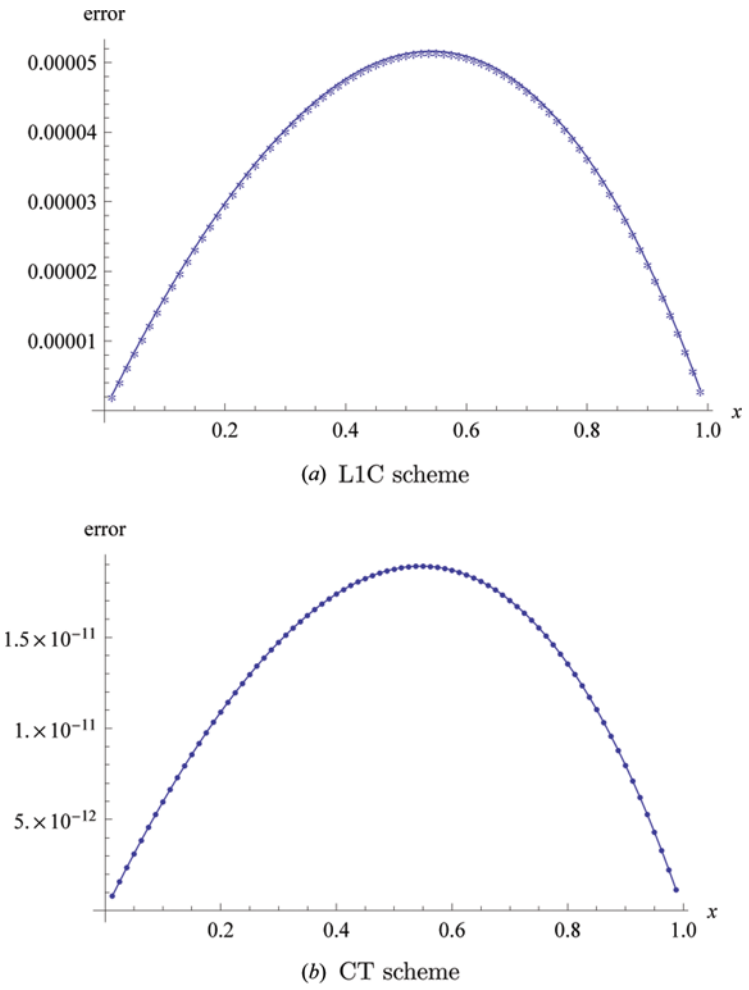


Figure 4. Absolute errors for Example 2 at $\gamma = 0.5$, $m = 80$, and $n = 80$ (color figure available online).

Example 3. Fractional heat equation with Neumann boundary condition [15]

$$\begin{aligned}\frac{\partial u(x,t)}{\partial t} &= {}_0D_t^{1-\gamma}\left[\frac{\partial^2 u(x,t)}{\partial x^2}\right] + e^x\left[(2+\gamma)x^2(1-x)^2 t^{1+\gamma}\right. \\ &\quad \left. - \frac{\Gamma(3+\gamma)}{\Gamma(2\gamma+2)} t^{2\gamma+1}(2 - 8x + x^2 + 6x^3 + x^4)\right] \\ &\quad 0 \le x \le 1 \qquad 0 < t \le 1 \\ &\quad u(x,0) = 0 \\ &\quad u_x(0,t) = 0 \qquad u_x(1,t) = 0\end{aligned} \tag{28}$$

Table 4. Maximum errors and convergence orders of Box and CT (24) schemes with different γ

γ	(h, τ)	$E_\infty(h, \tau)$ (BoxL1)	Order1 (BoxL1)	$E_\infty(h, \tau)$ (CT)	Order 1 (CT)
$\gamma = 0.3$	(1/20, 1/200)	0.00006157	1.3179	0.0000298287	1.94813
	(1/40, 1/400)	0.0000247	1.4527	7.73015×10^{-6}	1.95926
	(1/80, 1/800)	9.022×10^{-6}	*	1.98788×10^{-6}	*
$\gamma = 0.5$	(1/20, 1/200)	0.0003877	1.3816	0.0000426633	1.98006
	(1/40, 1/400)	0.0001488	1.4215	0.0000108143	1.98609
	(1/80, 1/800)	0.00005554	*	2.72976×10^{-6}	*
$\gamma = 0.7$	(1/20, 1/200)	0.001184	1.2495	0.0000541512	1.99399
	(1/40, 1/400)	0.0004978	1.2694	0.0000135943	1.99632
	(1/80, 1/800)	0.00002037	*	3.40726×10^{-6}	*

Table 5. When $h = 1/1{,}000$, the maximum errors of Box and CT (24) schemes with $\gamma = 0.3$

τ	$E_\infty(h, \tau)$ (BoxL1)	Order3 (BoxL1)	$E_\infty(h, \tau)$ (CT)	Order3 (CT)
$\frac{1}{2}$	0.00477651	1.49137	0.00240873	1.87643
$\frac{1}{4}$	0.00169888	1.55881	0.000656035	1.90646
$\frac{1}{8}$	0.000576654	*	0.000174995	*

Table 6. When $h = 1/1{,}000$, the maximum errors of Box and CT (24) schemes with $\gamma = 0.5$

τ	$E_\infty(h, \tau)$ (BoxL1)	Order3 (BoxL1)	$E_\infty(h, \tau)$ (CT)	Order3 (CT)
$\frac{1}{2}$	0.0111597	1.34019	0.00382813	1.93026
$\frac{1}{4}$	0.00440774	1.39065	0.00100443	1.95345
$\frac{1}{8}$	0.00168109	*	0.000259343	*

Table 7. When $h = 1/1{,}000$, the maximum errors of Box and CT (24) schemes with $\gamma = 0.7$

τ	$E_\infty(h, \tau)$ (BoxL1)	Order3 (BoxL1)	$E_\infty(h, \tau)$ (CT)	Order3 (CT)
$\frac{1}{2}$	0.0215705	1.2211	0.00515961	1.96387
$\frac{1}{4}$	0.00925279	1.23886	0.00132262	1.98036
$\frac{1}{8}$	0.00392049	*	0.000335187	*

Table 8. When $\tau = 1/1{,}000$, the maximum errors of Box and CT (24) schemes with $\gamma = 0.3$

h	$E_\infty(h, \tau)$ (BoxL1)	Order2 (BoxL1)	$E_\infty(h, \tau)$ (CT)	Order2 (CT)
$\frac{1}{2}$	0.835762	1.80605	0.369597	3.75345
$\frac{1}{4}$	0.239005	1.98365	0.0274049	3.88014
$\frac{1}{8}$	0.060432	*	0.00186118	*

Table 9. When $\tau = 1/1{,}000$, the maximum errors of Box and CT (24) schemes with $\gamma = 0.5$

h	$E_\infty(h, \tau)$ (BoxL1)	Order2 (BoxL1)	$E_\infty(h, \tau)$ (CT)	Order2 (CT)
$\frac{1}{2}$	0.653235	1.77513	0.307866	3.76369
$\frac{1}{4}$	0.190854	1.9854	0.0226662	3.88555
$\frac{1}{8}$	0.0481988	*	0.0015336	*

Table 10. When $\tau = 1/1{,}000$, the maximum errors of Box and CT (24) schemes with $\gamma = 0.7$

h	$E_\infty(h, \tau)$ (BoxL1)	Order2 (BoxL1)	$E_\infty(h, \tau)$ (CT)	Order2 (CT)
$\frac{1}{2}$	0.498576	1.73541	0.255221	3.77734
$\frac{1}{4}$	0.149734	1.9892	0.0186133	3.89319
$\frac{1}{8}$	0.0377148	*	0.00125272	*

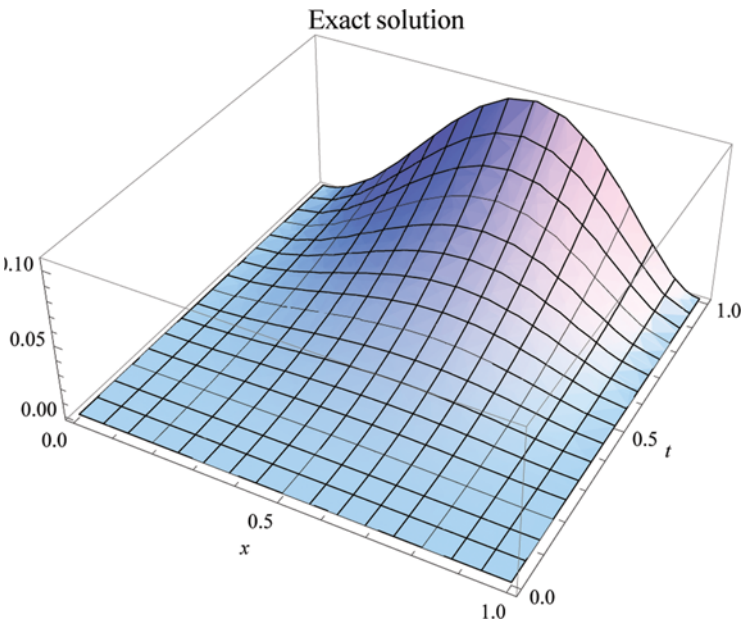


Figure 5. Exact solution for Example 3 at $\gamma = 0.5$ (color figure available online).

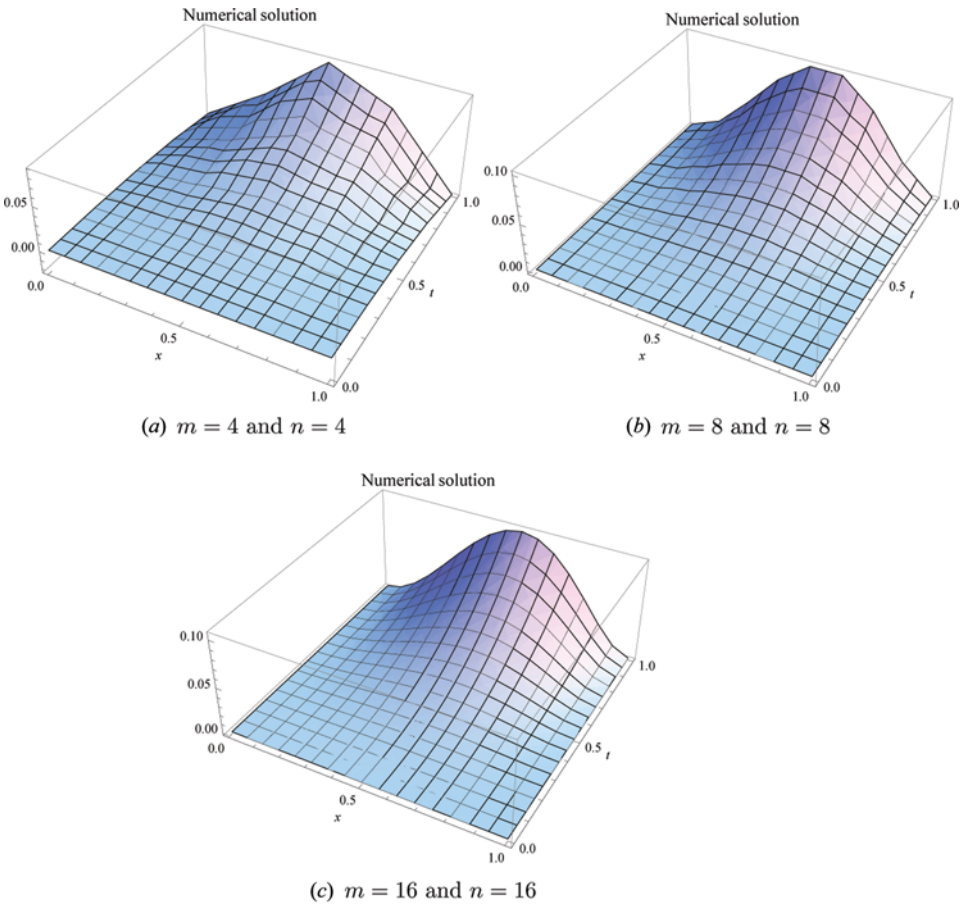


Figure 6. Numerical solution of the CT scheme defined by (24) for Example 3 at $\gamma = 0.5$ (color figure available online).

The exact solution of (28) is

$$u(x,t) = e^x x^2 (1-x)^2 t^{2+\gamma}$$

The error is defined as

$$E_\infty(h,\tau) = \max_{\substack{0 \le j \le m \\ 1 \le k \le n}} |u(x_j,t_k) - U_j^k|$$

Denote

$$\text{Order 1} = \frac{E_\infty(h,\tau)}{E_\infty(h/2,\tau/2)} \qquad \text{order 2} = \frac{E_\infty(h,\tau)}{E_\infty(h/2,\tau)} \qquad \text{order 3} = \frac{E_\infty(h,\tau)}{E_\infty(h,\tau/2)}$$

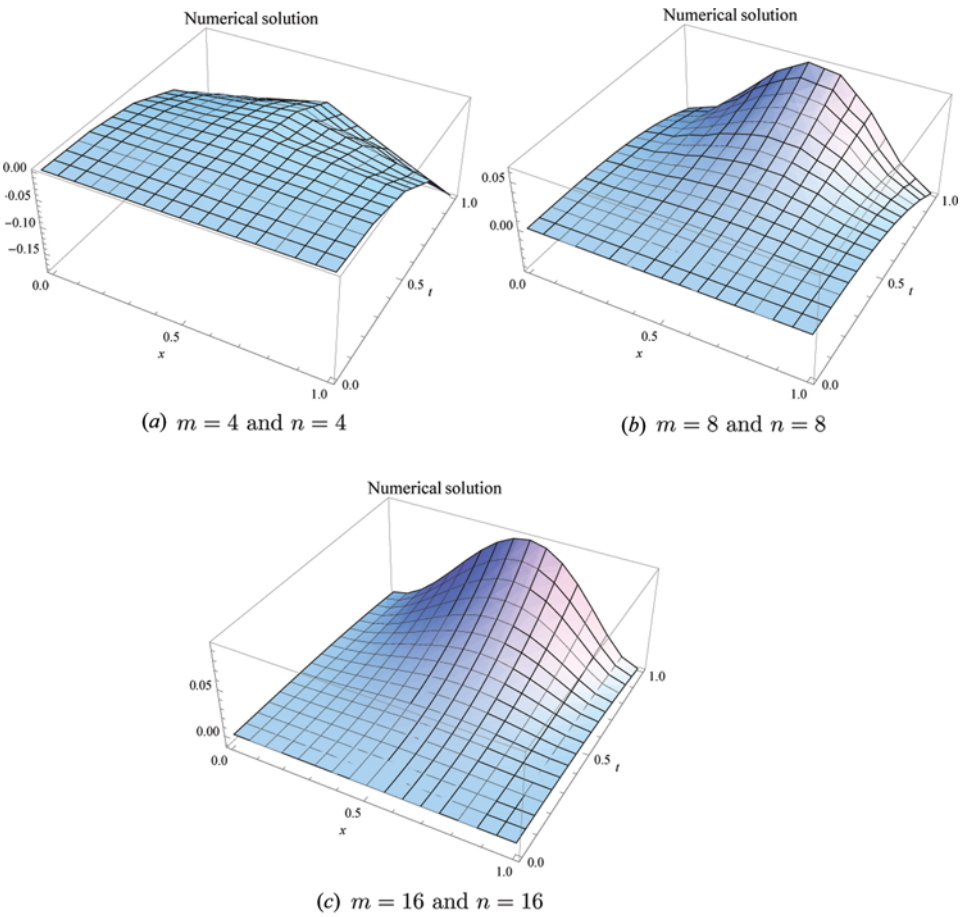


Figure 7. Numerical solution of the Box scheme for Example 3 at $\gamma = 0.5$ (color figure available online).

In Table 4 we have compared the maximum errors as well as their convergence order for the difference scheme (Box scheme) in [15] and the compact modified trapezoidal rule (24) in the case when h and τ decrease simultaneously with different γ. In Tables 5, 6, and 7 we have compared the maximum errors as well as their convergence order for these difference schemes with $\gamma = 0.3$, $\gamma = 0.5$, and $\gamma = 0.7$, respectively, when h is sufficiently small. In Tables, 8, 9, and 10 we have compared the maximum errors as well as their convergence order for these difference schemes with $\gamma = 0.3$, $\gamma = 0.5$, and $\gamma = 0.7$, respectively, when τ is sufficiently small. The exact solution and convergence of the numerical solution of the Box scheme and CT scheme defined by (24) for $\gamma = 0.5$ are given in Figures 5, 6, and 7, respectively.

5. CONCLUSION

In this article, a combination of compact finite-difference scheme in space and modified trapezoidal rule in time is proposed for the fractional sub-diffusion

equation with Dirichlet and Neumann boundary conditions. Numerical examples are presented to verify the effectiveness of the new scheme. Numerical solutions of the fractional heat equation with Dirichlet and Neumann boundary conditions are compared with $L1C$ scheme [14] and Box scheme [15], respectively. As can be realized from Tables 5–10, the numerical scheme has convergence of order $O(\tau^2 + h^4)$. This shows that the method is more accurate.

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