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NUMERICAL SOLUTION OF THE TIME FRACTIONAL ORDER DIFFUSION EQUATION WITH MIXED BOUNDARY CONDITIONS USING MIMETIC FINITE DIFFERENCE

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Abstract This paper is devoted to the numerical treatment of time fractional diffusion equation with mixed boundary conditions. A new scheme based on the combination of the implicit finite difference method for Caputo derivative in time and the mimetic finite difference in space is derived for solving this problem. The numerical results are provided to demonstrate the effectiveness of the proposed method as compared with other finite difference methods.

Keywords Fractional derivative of Caputo, discrete divergence, Mimetic finite difference, fractional diffusion equation.

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1. Introduction

Fractional partial differential equations (FPDEs) plays an important role in various fields of science and engineering, which has received increasing attention during the past 20 years. The various applications of fractional PDEs verified experimentally started to accelerate, see [3, 7, 9, 13, 15, 17].

Mainardi [12] proposed the fractional version of the time diffusion equation, which is obtained from the classical diffusion equation by replacing the first-order time derivative with a fractional derivative of order $\alpha \in (0, 1)$. Later Gorenflo et al. [8] showed that this equation is derived by considering continuous time random walk problems, which are in general non-Markovian processes. In the last years, a number of numerical methods have been developed to solve the time fractional diffusion equation with Dirichlet boundary conditions. Liu et al. [10] used a first-order finite difference scheme in both time and space directions and derived the stability estimates for this equation. Yuste [18] presented a difference scheme based on the weighted average methods for ordinary (non-fractional) diffusion equations. In [11], a finite difference/spectral method based on a finite difference scheme in time and Legendre spectral methods in space is designed.

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There is considerable literature on the development and applications of numerical methods for the time fractional diffusion equation with Dirichlet/Neumann boundary conditions. However, to the best of author's knowledge, we did not find any paper dealing with the time-fractional diffusion equation with mixed boundary conditions. We believe that it is very important to develop a numerical method to solve this kind of equation with mixed boundary conditions. Therefore in this paper, we propose a new numerical method to solve the time fractional diffusion equation with mixed boundary conditions. This new numerical method is a combination of the implicit finite difference method to approximate the time fractional derivative and the mimetic finite difference method to approximate the spatial variable. More precisely, we are going to study the following fractional problem

$$c\varrho\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \lambda\frac{\partial^2 u(x,t)}{\partial x^2} + g(x,t)\ , \quad (x,t) \in D = [0,L]\times[0,T], \tag{1.1}$$

where $\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}$ is the Caputo fractional derivative of order $\alpha \in (0,1)$ defined as

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial u(x,s)}{\partial s}(t-s)^{-\alpha}ds, \qquad 0 \le t \le T. \tag{1.2}$$

Consider the initial condition associated with equation (1.1),

$$u(x,0) = f(x)\ , \qquad x \in [0,L], \tag{1.3}$$

and the Neumann-Robin type boundary condition

$$\begin{cases} -\lambda\frac{\partial u(0,t)}{\partial x} = q(t) & ,\ t \in [0,T] \\ -\lambda\frac{\partial u(L,t)}{\partial x} = h(t)\Big(u(L,t) - u^\infty\Big), \end{cases} \tag{1.4}$$

where: c is the specific heat capacity, λ : is the thermal conductivity coefficient, ϱ is the density, h is the heat transfer coefficient, u^∞ is the environmental temperature and q be the heat flux.

2. Preliminary Results

The basic idea of the numerical scheme for the time fractional diffusion equation is combining the implicit finite differences method to discretize the temporal variable [11] and the mimetic finite difference scheme to discretize the spatial variable [4]. The values of the functions u and g in the mesh points are denoted by $u_i^n = u(x_i, t_n)$ and $g_i = g(x_i)$, respectively.

2.1. Discretization in time: an implicit finite difference scheme

We follow the ideas of [11] to discretize the Caputo fractional partial derivative with respect to the time. Let us discretize the time interval as $t_k := k\Delta t,\ k = 0, 1, 2, \cdots, K$, where $\Delta t := \frac{T}{K}$ is the time step. Then from the quadrature formula as in [3], for all $0 \le k \le K-1$, we have

$$\begin{aligned}\frac{\partial^\alpha u(x,t_{k+1})}{\partial t^\alpha} &= \frac{1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\int_{t_j}^{t_{j+1}}\frac{\partial u(x,s)}{\partial s}\frac{ds}{(t_{k+1}-s)^\alpha}\\ &= \frac{1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\frac{u(x,t_{j+1})-u(x,t_j)}{\Delta t}\int_{t_j}^{t_{j+1}}\frac{ds}{(t_{k+1}-s)^\alpha} + r_{\Delta t}^{k+1},\end{aligned}$$

where

$$r_{\Delta t}^{k+1} \le c_u\left[\frac{1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\int_{t_j}^{t_{j+1}}\frac{t_{j+1}+t_j-2s}{(t_{k+1}-s)}ds + O\left(\Delta t^2\right)\right], \tag{2.1}$$

is the truncation error given in [11] and c_u is a constant which depends only of u. For the reader's convenience, we are going to give the brief description of the proof of (2.1).

$$\begin{aligned}&\frac{1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\int_{t_j}^{t_{j+1}}\frac{t_{j+1}+t_j-2s}{(t_{k+1}-s)^\alpha}ds\\ =&\frac{1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\left[\underbrace{\int_{t_j}^{t_{j+1}}\frac{(t_{j+1}+t_j)}{(t_{k+1}-s)^\alpha}ds}_{*}\underbrace{-2\int_{t_j}^{t_{j+1}}\frac{s}{(t_{k+1}-s)^\alpha}ds}_{**}\right].\end{aligned} \tag{2.2}$$

Handling each term one by one, we have

$$(*) = \int_{t_j}^{t_{j+1}}\frac{(t_{j+1}+t_j)}{(t_{k+1}-s)^\alpha}ds = \frac{(t_{j+1}+t_j)}{(1-\alpha)}\left[(t_{k+1}-t_j)^{1-\alpha}-(t_{k+1}-t_{j+1})^{1-\alpha}\right]. \tag{2.3}$$

Now we consider $(**)$, from the definition of $t_k = k\Delta t$ and using integration by parts, we obtain

$$\begin{aligned}(**) &= -2\int_{t_j}^{t_{j+1}}\frac{s}{(t_{k+1}-s)^\alpha}ds\\ &= -2\left[-\left(\frac{1}{1-\alpha}\right)(s)\left(t_{k+1}-s\right)^{1-\alpha}\Big|_{t_j}^{t_{j+1}} + \frac{1}{1-\alpha}\int_{t_j}^{t_{j+1}}(t_{k+1}-s)^{1-\alpha}ds\right]\\ &= -2\Bigg[-\left(\frac{1}{1-\alpha}\right)\left((t_{j+1})(t_{k+1}-t_{j+1})^{1-\alpha}-(t_j)(t_{k+1}-t_j)^{1-\alpha}\right)\\ &\quad -\left(\frac{1}{1-\alpha}\right)\left(\frac{1}{2-\alpha}\right)\\ &\quad (t_{k+1}-s)^{2-\alpha}\Bigg]\left((\Delta t)^{2-\alpha}(k-j)^{2-\alpha}-(\Delta t)^{2-\alpha}(k+1-j)^{2-\alpha}\right)\\ &= \left(\frac{2}{1-\alpha}\right)(j+1)\,(\Delta t)^{2-\alpha}(k-j)^{1-\alpha} - \left(\frac{2}{1-\alpha}\right)\left(j\,(\Delta t)^{2-\alpha}\right)(k+1-j)^{1-\alpha}\\ &\quad + 2\left(\frac{1}{1-\alpha}\right)\left(\frac{1}{2-\alpha}\right)(\Delta t)^{2-\alpha}(k-j)^{2-\alpha}\end{aligned}$$

$$-2\left(\frac{1}{1-\alpha}\right)\left(\frac{1}{2-\alpha}\right)(\Delta t)^{2-\alpha}(k+1-j)^{2-\alpha}. \tag{2.4}$$

Therefore, equation (2.2) becomes

$$\begin{aligned}
&\frac{1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\Bigg\{\left(\frac{1}{1-\alpha}\right)((j+1)\Delta t+(j)\Delta t)\Big[((k+1)\Delta t-(j)\Delta t)^{1-\alpha}\\
&-((k+1)\Delta t-(j+1)\Delta t)^{1-\alpha}\Big]+\left(\frac{2}{1-\alpha}\right)(j+1)(\Delta t)^{2-\alpha}(k-j)^{1-\alpha}\\
&-\left(\frac{2}{1-\alpha}\right)(j)(\Delta t)^{2-\alpha}(k+1-j)^{1-\alpha}+\left(\frac{2}{1-\alpha}\right)\left(\frac{1}{2-\alpha}\right)\\
&(\Delta t)^{2-\alpha}(k-j)^{2-\alpha}-\left(\frac{2}{1-\alpha}\right)\left(\frac{1}{2-\alpha}\right)(\Delta t)^{2-\alpha}(k+1-j)^{2-\alpha}\Bigg\}\\
=&\frac{-1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\left(\frac{1}{1-\alpha}\right)(2j+1)(\Delta t)^{2-\alpha}\left((k-j)^{1-\alpha}-(k+1-j)^{1-\alpha}\right)\\
&+\frac{1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\left(\frac{2}{1-\alpha}\right)(\Delta t)^{2-\alpha}\left[(j+1)(k+1)^{1-\alpha}-j(k+1-j)^{1-\alpha}\right]\\
&+\frac{1}{\Gamma(1-\alpha)}\sum_{j=0}^{k}\frac{2}{(1-\alpha)(2-\alpha)}(\Delta t)^{2-\alpha}\left[(k-j)^{2-\alpha}-(k+1-j)^{2-\alpha}\right].
\end{aligned} \tag{2.5}$$

Now for each term in the summation, we have

a)
$$\begin{aligned}
&\sum_{j=0}^{k}(2j+1)\left[(k-j)^{1-\alpha}-(k+1-j)^{1-\alpha}\right]\\
=&k^{1-\alpha}-(k+1)^{1-\alpha}+3(k-1)^{1-\alpha}-3(k)^{1-\alpha}\\
&+5(k-2)^{1-\alpha}-5(k-1)^{1-\alpha}+7(k-3)^{1-\alpha}-7(k-2)^{1-\alpha}\\
&+9(k-4)^{1-\alpha}-9(k-3)^{1-\alpha}+\cdots-(2k+1)(1)^{1-\alpha}\\
=&-2(k)^{1-\alpha}-(k-1)^{1-\alpha}-2(k-1)^{1-\alpha}(k-2)^{1-\alpha}\\
&-2(k-3)^{1-\alpha}-\cdots-2(1)^{1-\alpha}.
\end{aligned}$$

b)
$$\begin{aligned}
&2\sum_{j=0}^{k}\left[(j+1)(k-j)^{1-\alpha}-(j)(k+1-j)^{1-\alpha}\right]\\
=&2\Big[(k)^{1-\alpha}+2(k-1)^{1-\alpha}-(k)^{1-\alpha}+3(k-2)^{1-\alpha}-2(k-1)^{1-\alpha}\\
&+4(k-3)^{1-\alpha}-3(k-2)^{1-\alpha}+5(k-4)^{1-\alpha}-4(k-3)^{1-\alpha}\\
&+6(k-5)^{1-\alpha}-5(k-4)^{1-\alpha}+\cdots-k(1)^{1-\alpha}\Big]\\
=&2(0)=0.
\end{aligned}$$

c)
$$2\sum_{j=0}^{k}\left[(k-j)^{2-\alpha}-(k+1-j)^{2-\alpha}\right]$$

$$
\begin{aligned}
=&2\Big[(k)^{2-\alpha}-(k+1)^{2-\alpha}+(k-1)^{2-\alpha}-(k)^{2-\alpha}+(k-2)^{2-\alpha}-(k-1)^{2-\alpha}\\
&+(k-3)^{2-\alpha}-(k-2)^{2-\alpha}+(k-4)^{2-\alpha}-(k-3)^{2-\alpha}+\cdots-(1)^{2-\alpha}\Big]\\
=&2\Big[(k)^{2-\alpha}-(k+1)^{2-\alpha}+(k-1)^{2-\alpha}-(k)^{2-\alpha}+(k-2)^{2-\alpha}-(k-1)^{2-\alpha}\\
&+(k-3)^{2-\alpha}-(k-2)^{2-\alpha}+(k-4)^{2-\alpha}-(k-3)^{2-\alpha}+\cdots-(1)^{2-\alpha}\Big]\\
=&2\,(k+1)^{2-\alpha}.
\end{aligned}
$$

Further, by substituting the values of (a), (b) and (c) in (2.5), we obtain

$$
\begin{aligned}
&\frac{-1}{\Gamma(2-\alpha)}(\Delta t)^{2-\alpha}\Big[-2\,(k)^{1-\alpha}-(k+1)^{1-\alpha}-2\,(k-1)^{1-\alpha}-2\,(k-2)^{1-\alpha}\\
&-2\,(k-3)^{1-\alpha}-\cdots-2\,(1)^{1-\alpha}\Big]+0+\frac{1}{\Gamma(3-\alpha)}(\Delta t)^{2-\alpha}(-2)\,(k+1)^{2-\alpha}\\
=&\frac{(\Delta t)^{2-\alpha}}{\Gamma(2-\alpha)}\Big[(k+1)^{1-\alpha}+2\Big((k)^{1-\alpha}+(k-1)^{1-\alpha}+(k-2)^{1-\alpha}+\cdots+(1)^{1-\alpha}\Big)\\
&-\frac{2}{(2-\alpha)}(k+1)^{2-\alpha}\Big].
\end{aligned}
\tag{2.6}
$$

Let

$$
\begin{aligned}
S(k)=&(k+1)^{1-\alpha}+2\Big((k)^{1-\alpha}+(k-1)^{1-\alpha}+(k-2)^{1-\alpha}+\cdots+(1)^{1-\alpha}\Big)\\
&-\frac{2}{2-\alpha}(k-1)^{1-\alpha}.
\end{aligned}
$$

Now we are going to show that $|S(k)|$ is bounded for all $\alpha\in[0,1]$, and $\forall\ k\geq 1$, in the following lemma. Just for the reader's convenience, we give the details of the proof here.

Lemma 2.1 ([11]). *For all $\alpha\in[0,1]$ and for all $k\geq 1$, there is a positive constant $C\geq 0$, independent of α and k, such that $|S(k)|\leq C$.*

Proof. For $\alpha=0$ we have

$$
\begin{aligned}
S(k)&=(k+1)+2\,[k+(k-1)+(k-2)+(k-3)+\cdots+1]-(k+1)^2\\
&=(k+1)\,[1-(k+1)]+2\Big[\underbrace{1+2+\cdots+(k-3)+(k-2)+(k-1)+k}\Big]\\
&=(k+1)\,(1-k-1)+2\frac{k\,(k+1)}{2}=0.
\end{aligned}
\tag{2.7}
$$

Now for $\alpha\in(0,1]$, we claim that

$$
\begin{aligned}
S(k)=&(k+1)^{1-\alpha}+2\left[(k)^{1-\alpha}+(k-1)^{1-\alpha}+(k-2)^{1-\alpha}+\cdots+(1)^{1-\alpha}\right]\\
&-\left(\frac{2}{2-\alpha}\right)(k+1)^{2-\alpha}=\sum_{i=0}^{k}a_i,
\end{aligned}
\tag{2.8}
$$

where,

$$a_i = (i+1)^{1-\alpha} + (i)^{1-\alpha} - \frac{2}{2-\alpha}\left[(i+1)^{2-\alpha} - (i)^{2-\alpha}\right].$$

Thus we have,

$$\begin{aligned}\sum_{i=0}^{k} a_i &= a_0 + a_1 + a_2 + a_3 + \cdots + a_k \\ &= 2\bigg[(1)^{1-\alpha} + (2)^{1-\alpha} + (3)^{1-\alpha} + (4)^{1-\alpha} + \cdots + (k-2)^{1-\alpha} + (k-1)^{1-\alpha} \\ &\quad + (k)^{1-\alpha}\bigg] + (k+1)^{1-\alpha} - \frac{2}{2-\alpha}(k+1)^{2-\alpha} \\ &= S(k).\end{aligned}$$

According to (2.8), we will show that $\sum_{i=1}^{\infty} a_i$ is convergent. Therefore, it is enough to prove that $|a_i| \le \frac{1}{i^{1+\alpha}}$, for i large enough. Note that for $i \ge 2$, we have

$$\begin{aligned}|a_i| &= (i+1)^{1-\alpha} + (i)^{1-\alpha} - \frac{2}{2-\alpha}\left[(i+1)^{2-\alpha} - (i)^{2-\alpha}\right], \\ |a_i| &= (i)^{1-\alpha}\left|\left(1+\frac{1}{i}\right)^{1-\alpha} + 1 - \frac{2i}{2-\alpha}\left(\left(1+\frac{1}{i}\right)^{2-\alpha} - 1\right)\right|.\end{aligned} \tag{2.9}$$

Let

$$\Theta_1 = \left(1+\frac{1}{i}\right)^{1-\alpha} \qquad \text{and} \qquad \Theta_2 = \left(1+\frac{1}{i}\right)^{2-\alpha} - 1.$$

So, by Newton's binomial theorem

$$\begin{aligned}\Theta_1 =& 1 + (1-\alpha).\frac{1}{i} + \frac{(1-\alpha)(-\alpha)}{2!}\left(\frac{1}{i^2}\right) + \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(\frac{1}{i^3}\right) \\ &+ \frac{(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)}{4!}\left(\frac{1}{i^4}\right) + \cdots\end{aligned} \tag{2.10}$$

and

$$\begin{aligned}\Theta_2 =& 1 + \frac{(2-\alpha)}{1!}.\frac{1}{i} + \frac{(2-\alpha)(1-\alpha)}{2!}\frac{1}{i^2} + \frac{(2-\alpha)(1-\alpha)(-\alpha)}{3!}\frac{1}{i^3} \\ &+ \frac{(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)}{4!}\frac{1}{i^4} + \cdots.\end{aligned} \tag{2.11}$$

Combining (2.9), (2.10), (2.11) and taking $i = k$, we get

$$|a_k| = (k)^{1-\alpha}\left|\frac{1}{3!}(1-\alpha)(-\alpha).\frac{1}{k^2} + \frac{2}{4!}(1-\alpha)(-\alpha)(-\alpha-1) - \frac{1}{k^3} + \cdots\right|.$$

Therefore

$$|a_k| \le \frac{(1-\alpha)(\alpha)}{3!}\frac{1}{k^{1+\alpha}}\left(1 + \frac{1}{k} + \frac{1}{k^2} + \cdots\right) \le \frac{2(1-\alpha)(\alpha)}{3!}\frac{1}{k^{1+\alpha}} \le \frac{1}{k^{1+\alpha}}. \tag{2.12}$$

Hence, we conclude that $|S(k)|$ is bounded. □

From Lemma 2.1 and since $\frac{1}{\Gamma(2-\alpha)} \leq 2$, for all $\alpha \in [0,1]$, we have

$$\left| \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \int_{t_j}^{t_{j+1}} \frac{t_{j+1}+t_j-2s}{(t_{k+1}-s)^{\alpha}} ds \right| \leq 2\Delta t^{2-\alpha}. \tag{2.13}$$

Now by using (2.13), we get

$$\begin{aligned}
\frac{\partial^\alpha u(x,t_{k+1})}{\partial t^\alpha} &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \int_{t_j}^{t_{j+1}} \frac{\partial u(x;s)}{\partial t}(t_{k+1}-s)^{-\alpha} ds \\
=& \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \left[\frac{u_i^{j+1}-u_i^j}{\Delta t} + O(\Delta t) \right] \int_{t_j}^{t_j+1} ((k+1)(\Delta t)-s)^{-\alpha} ds \\
=& \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \left[\frac{u_i^{j+1}-u_i^j}{\Delta t} + O(\Delta t) \right] \left(\frac{-1}{1-\alpha} \right) \\
&\times \left[\Big((k+1)(\Delta t)-(j+1)\Delta t\Big)^{1-\alpha} - \Big((k+1)\Delta t - j\Delta t\Big)^{1-\alpha} \right] \\
=& \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \left[\frac{u_i^{j+1}-u_i^j}{\Delta t} + O(\Delta t) \right] \left(\frac{-1}{1-\alpha} \right) \\
&\times \left[(k-j)^{1-\alpha}(\Delta t)^{1-\alpha} - (k+1-j)^{1-\alpha}(\Delta t)^{1-\alpha} \right] \\
=& \frac{1}{\Gamma(1-\alpha)} \left(\frac{1}{1-\alpha} \right) \left(\frac{1}{\Delta t^\alpha} \right) \sum_{j=0}^{k} \left\{ \left(u_i^{j+1} - u_i^j \right) \left[(k-j+1)^{1-\alpha} - (k-j)^{1-\alpha} \right] \right\} \\
&+ \left(\frac{1}{\Gamma(1-\alpha)} \right) \left(\frac{1}{1-\alpha} \right) \sum_{j=0}^{k} \left[(k-j+1)^{1-\alpha} - (k-j)^{1-\alpha} \right] + O(\Delta t^{2-\alpha}).
\end{aligned} \tag{2.14}$$

Thus the approximation of the fractional derivative is given by

$$\frac{\partial^\alpha u_i^\alpha}{\partial t^\alpha} = O(\alpha, \Delta t) \sum_{j=0}^{k} \omega(\alpha, j)(u_i^{k-j+1} - u_i^{k-j}), \tag{2.15}$$

where

$$O(\alpha, \Delta t) = \frac{1}{\Gamma(1-\alpha)(1-\alpha)\Delta t^\alpha}.$$

Taking

$$\omega_j^{(\alpha)} = (j+1)^{1-\alpha} - (j)^{1-\alpha}, \quad \forall\ j = 0, 1, 2 \cdots, k,$$

we get

$$\begin{aligned}
\frac{\partial^\alpha u(x,t_{k+1})}{\partial t^\alpha} &= O\left(\alpha, \Delta t\right) \sum_{j=0}^{k} (u_i^{j+1} - u_i^j) \left[(j+1)^{1-\alpha} - (j)^{1-\alpha} \right] \\
&\quad + \frac{1}{(1-\alpha)\Gamma(1-\alpha)} \sum_{j=0}^{k} \left[(j+1)^{1-\alpha} - (j)^{1-\alpha} \right] \sigma(\Delta t^{2-\alpha}).
\end{aligned} \tag{2.16}$$

Therefore, the expression for fractional derivative becomes,

$$\frac{\partial^{\alpha} u(x,t_{k+1})}{\partial t^{\alpha}} = O\left(\alpha, \Delta t\right) \sum_{j=0}^{k} (u_i^{j+1} - u_i^{j}) \left[(j+1)^{1-\alpha} - (j)^{1-\alpha} \right] + \sigma(\Delta t).$$

Remark 2.1. The expression (2.15) provides the values of the time fractional derivative at $t = 0$, which is not required by the implicit finite difference scheme.

2.2. Discretization in space using the mimetic finite difference scheme

Now we are going to use a discrete version of the divergence theorem to determine the discrete gradient. The divergence theorem states that

$$\int_{\Omega} \nabla.\overrightarrow{v} f \; dV + \int_{\Omega} \overrightarrow{v} \nabla f \; dV = \int_{\partial\Omega} f \overrightarrow{v} \overrightarrow{n} \; dS, \tag{2.17}$$

where Ω is a domain and $\partial\Omega$ is the boundary of the domain, $\overrightarrow{n}$ is the exterior normal, f is a scalar function defined over the boundary $\partial\Omega$.

Let f, g be the scalar fields and $\overrightarrow{v}$, $\overrightarrow{w}$ be the vector fields, the appropriate inner product of the continuum are given by

$$\langle f, g \rangle = \int_{\Omega} fg \; dV, \qquad \langle \overrightarrow{v}, \overrightarrow{w} \rangle = \int_{\Omega} \overrightarrow{v} \overrightarrow{w} \; dV. \tag{2.18}$$

Thus the equation (2.17) can be written as

$$\langle \nabla.\overrightarrow{v}, f \rangle + \langle \overrightarrow{v}, \nabla f \rangle = \int_{\partial\Omega} f \overrightarrow{v} \overrightarrow{n} \; dS. \tag{2.19}$$

The divergence theorem in one dimension becomes an integration by parts, thus we have

$$\int_0^1 \frac{dv}{dx} f \; dx + \int_0^1 v \frac{df}{dx} \; dx = v(1)f(1) - v(0)f(0). \tag{2.20}$$

A discrete form of the conservation law needs to be constructed in order to satisfy the local conservation in each cell interval so that the law of global conservation is fulfilled throughout the investigated interval.

Definition 2.1. Let $\overrightarrow{v} : R \to R^{N+1}$, be a discrete vector function defined on the nodes of the one-dimensional mesh, such that $v(t) = (v_0(t), v_1(t), \cdots, v_N(t))$, $\forall\, t \in R$. $D_v \in R^N$ represents the approximation in the centers of the cells $\nabla \overrightarrow{v}$, the divergence in the centers of the cell are defined as:

$$D_v \subset R^{N+1} \to R^N$$
$$(D_v)_{i+\frac{1}{2}} = \frac{(v_{i+1} - v_i)}{h} \qquad \text{for } i = 0, 1, 2, \cdots, n-1.$$

The approximation of the divergence in the centers of the cells coincide with the central difference scheme, which is expressed as the matrix $D_{(N)\times(N+1)}$

$$D = \frac{1}{h}\begin{pmatrix} -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \cdots & 0 \\ 0 & 0 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}_{(N)\times(N+1)} .$$

Definition 2.2. Let $f = (f_0,\ f_{1/2},\ f_{3/2}, \cdots,\ f_{N-1/2},\ f_N)^T \in R^{N+2}$ be a discrete function defined in the center of the cell and in the domain border of a one-dimensional mesh. Further, let $Gf \in R^{N+1}$ represents the approximations at the nodes ∇f. The gradient $Gf \subset R^{N+2} \to R^{N+1}$ defined in a one-dimensional mesh at the boundary points, has the form

$$(Gf)_0 = \frac{-\frac{8}{3}f_0 + 3f_{\frac{1}{2}} - \frac{1}{3}f_{\frac{3}{2}}}{h},$$
$$(Gf)_N = \frac{\frac{8}{3}f_N - 3f_{N-\frac{1}{2}} + \frac{1}{3}f_{N-\frac{3}{2}}}{h}.$$

The gradient Gf at the interior points coincides with the central difference scheme, that is

$$(Gf)_i = \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{h} \quad \text{for } i = 1, 2, \cdots n-1,$$

matrix $G_{(N+1)\times(N+2)}$ is expressed as,

$$G = \frac{1}{h}\begin{pmatrix} \frac{-8}{3} & 3 & \frac{-1}{3} & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ 0 & -1 & 1 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ 0 & 0 & -1 & 1 & \cdots & \cdots & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & -1 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & 0 & -1 & 1 & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & \frac{1}{3} & -3 & \frac{8}{3} \end{pmatrix}_{(N+1)\times(N+2)} .$$

Remark 2.2. Now we have the matrix operators, the conditions of the discrete operators gradient (G) and divergence (D) will be reformulated, where (D) indicates the approach for the divergence operator applied to the vector function in the cell centers and (G) denotes the approximation for the gradient operator applied to the scalar function in the nodes of the cells and the border.

In figure (1), the cell with uniform spacing and length $h = \frac{1}{N}$, over the interval $[0, 1]$ is considered. The investigated interval is divided into n sub-intervals, each node has coordinate $x_i = (i \times h)$, for $0 \leq i \leq N$.

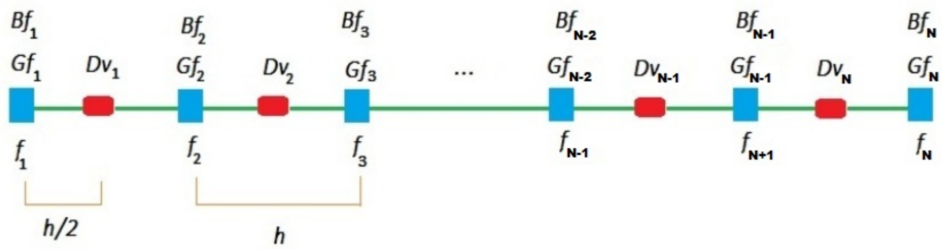


Figure 1. One-dimensional Uniform Staggered Mesh

Each cell has a central point, which means that interval $[x_i, x_{i+1}]$ includes the center with coordinates $x_{i+1/2}$.

The discrete form of the gradient operator (G) inside the domain and in the border are given by (see [4,5])

$$(Gu)_i = \frac{u_{1+\frac{1}{2}} - u_{1+\frac{1}{2}}}{h} \quad 1 \leq i \leq N, \tag{2.21}$$

$$(Gu)_0 = \frac{-8}{3h} u_0 + \frac{3}{h} u_{\frac{1}{2}} - \frac{1}{3h} u_{\frac{3}{2}}, \tag{2.22}$$

$$(Gu)_N = \frac{8}{3h} u_N - 3u_{N-\frac{1}{2}} + \frac{1}{3h} u_{N-\frac{3}{2}}. \tag{2.23}$$

The mimetic discretization of the divergence (D) in the centers of each cell is given by

$$(D_v)_{i+\frac{1}{2}} = \frac{v_{i+1} - v_i}{h} \quad 0 \leq i \leq N. \tag{2.24}$$

Definition 2.3. Let $v : R \to R^{N+1}$, be a discrete vector function defined on the nodes of the one-dimensional mesh such that $v(t) = (v_0(t), v_1(t), v_2(t), \ldots, v_N(t))$, $\forall\ t \in R$. Further, let $D_v \in R^N$, represents the discrete approximation of the divergence (D) in the centers of the cells, the divergence $(\widehat{D})$ is defined as :

$$\widehat{D}_v : R^{N+1} \to R^{N+2},$$
$$\left(\widehat{D}_v\right)_{i+\frac{1}{2}} = \frac{(v_{i+1} - v_i)}{h}, \quad \forall\ \text{i} = 0, 1, \ldots, n-1;$$
$$(D_v)_0 = (D_v)_N = 0.$$

The Matrix operator $\widehat{D}$ is expressed as :

$$\widehat{D} = \frac{1}{h} \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \cdots & 0 \\ 0 & 0 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}_{(N+2)\times(N+1)}.$$

2.3. Discrete divergence theorem (Castillo-Grone approach [4, 5])

The equation (2.19) can be represented in the form of a weighted inner product of discrete vector and scalar functions on a stepped grid as,

$$\langle \widehat{D}v, f\rangle_Q + \langle v, Gf\rangle_P = \langle Bv, f\rangle_I \tag{2.25}$$

where D, G and B are the discrete versions of their corresponding continuums: divergence ($\nabla.$), gradient (∇) and the border operator ($\frac{\partial}{\partial \overrightarrow{n}}$). The $\langle\ ,\ \rangle$ represents the generalization of the inner product with weights Q, P and I. Using the identity (2.25), a relation is obtained for the border operator

$$B = Q\widehat{D} + G^t P, \tag{2.26}$$

where $[Q], [P]$ and $[I]$ are positive definite matrices of order $(N+2)\times(N+2)$, $(N+1)\times(N+1)$ and $(N+2)\times(N+2)$ respectively, which are used to determine the form of $\widehat{D}$ and G. Thus the matrix B is given as,

$$B = \begin{pmatrix} -1 & 0 & 0\cdots 0 & 0 & 0 \\ \frac{1}{8} & -\frac{1}{8} & 0\cdots 0 & 0 & 0 \\ -\frac{1}{8} & \frac{1}{8} & 0\cdots 0 & 0 & 0 \\ 0 & 0 & 0\cdots 0 & 0 & 0 \\ \vdots & \vdots & \vdots\ \ddots\ \vdots & \vdots & \vdots \\ 0 & 0 & 0\cdots 0 & 0 & 0 \\ 0 & 0 & 0\cdots 0 & -\frac{1}{8} & \frac{1}{8} \\ 0 & 0 & 0\cdots 0 & \frac{1}{8} & -\frac{1}{8} \\ 0 & 0 & 0\cdots 0 & 0 & 1 \end{pmatrix}_{(N+2)\times(N+2)}.$$

The mimetic operators gradient (G), divergence ($\widehat{D}$) are of second order, both inside of the domain as well as at the border, in an uniform staggered mesh of a one-dimensional domain.

Thus, (2.17) can be written as

$$\langle \nabla.\overrightarrow{v}, f\rangle + \langle \overrightarrow{v}, \nabla f\rangle = \int_{\partial\Omega} f\overrightarrow{v}\overrightarrow{n}\, dS. \tag{2.27}$$

3. Numerical Scheme

3.1. Incorporation of discrete temporal and spatial scheme for fractional order diffusion equation

From (1.1), we have

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{a\partial^2 u(x,t)}{\partial x^2} + \overline{g}(x,t), \tag{3.1}$$

where $a = \frac{\lambda}{c\varrho}$ is the thermal diffusion coefficient and $\overline{g}(x,t) = \frac{g(x,t)}{c\varrho}$. Using implicit finite difference relation for fractional order time derivative and mimetic discretization for the spatial variable, we obtain

$$O(\alpha,k)\sum_{j=0}^{k}\omega(\alpha,j)\left(u_i^{k-j+1}-u_i^{k-j}\right)=a[D][G]u_i^k+\overline{g}_i^k,$$

Now, $\forall\ k \geq 1$ and $i = 0$, we have

$$\begin{aligned}&O(\alpha,k)\,\omega(\alpha,0)\left(u_0^{k+1}-u_0^k\right)+O(\alpha,k)\sum_{j=0}^{k}\omega(\alpha,j)\left(u_0^{k-j+1}-u_0^{k-j}\right)\\ =&a[D][G]u_0^{k+1}+\overline{g}_0^{k+1},\\ &O(\alpha,k)\left(u_0^{k+1}-u_0^k\right)+O(\alpha,k)\sum_{j=1}^{k}\omega(\alpha,j)\left(u_0^{k-j+1}-u_0^{k-j}\right)=a[D][G]u_0^k+\overline{g}_0^k.\end{aligned} \tag{3.2}$$

Using the approximations for Neumann and Robin boundary conditions (1.4), we get

$$\frac{-\lambda\partial u(0,t)}{\partial x}=q(t)\approx-\lambda[B][G]u_i^{k+1}=q_k \qquad t\in[0,T], \tag{3.3}$$

$$\frac{-\lambda\partial u(L,t)}{\partial x}=h(t)u(L,t)-h(t)u^{\infty},$$

$$h(t)\,u(L,t)+\lambda\frac{\partial u}{\partial x}(L,t)=h(t)\,u^{\infty}\approx h(t)\,u^{k+1}+\beta[B][G]u^{k+1}=h(t)\,u^{\infty} \tag{3.4}$$

substituting (3.3) in (3.2), equation becomes

$$O(\alpha,k)\left(u_0^{k+1}-u_0^k\right)+O(\alpha,k)\sum_{j=1}^{k}\omega(\alpha,j)\left(u_0^{k-j+1}-u_0^{k-j}\right)=a[D][G]u_0^{k+1}+\overline{g}_0^k,$$

$$\beta[B][G]u_0^{k+1}=q_k, \qquad \beta=-\lambda,$$

$$\begin{aligned}&O(\alpha,k)\left(u_0^{k+1}-u_0^k\right)+O(\alpha,k)\sum_{j=1}^{k}\omega(\alpha,j)\left(u_0^{k-j+1}-u_0^{k-j}\right)\\ =&\left(a[D][G]-\beta[B][G]\right)u_0^{k+1}+\overline{g}_0^{k+1}+q^{k+1},\\ &\left(O(\alpha,k)-a[D][G]+\beta[B][G]\right)u_0^{k+1}\\ =&O(\alpha,k)\,u_0^k-O(\alpha,k)\sum_{j=1}^{k}\omega(\alpha,j)\left(u_0^{k-j+1}-u_0^{k-j}\right)+\overline{g}_0^{k+1}+q^{k+1}.\end{aligned} \tag{3.5}$$

Further, $\forall\ k \geq 1$ and $i = 1, 2, \ldots, N-1$, we have

$$\begin{aligned}&O(\alpha,k)\left(u_i^{k+1}-u_i^k\right)+O(\alpha,k)\sum_{j=1}^{k}\omega(\alpha,j)\left(u_i^{k-j+1}-u_i^{k-j}\right)\\ =&a[D][G]u_i^{k+1}+\overline{g}_i^{k+1},\end{aligned}$$

$$\begin{aligned}&\left(O\left(\alpha,k\right)-a[D][G]\right)u_i^{k+1}\\=&O\left(\alpha,k\right)u_i^k-O\left(\alpha,k\right)\sum_{j=1}^{k}\omega\left(\alpha,j\right)\left(u_i^{k-j+1}-u_i^{k-j}\right)+\overline{g}_i^{k+1}.\end{aligned}\tag{3.6}$$

And, $\forall\ k\geq 1$ and $i=N$, we have

$$\begin{aligned}&O\left(\alpha,k\right)\left(u_N^{k+1}-u_N^k\right)+O\left(\alpha,k\right)\sum_{j=1}^{k}\omega\left(\alpha,j\right)\left(u_N^{k-j+1}-u_N^{k-j}\right)\\=&a[D][G]\left(u_N^{k+1}\right)+\overline{g}_N^{k+1},\\&h\left(t\right)u_N^{k+1}+\beta[B][G]u_N^{k+1}=h\left(t\right)u^{\infty},\quad \beta=\lambda.\end{aligned}$$

Thus, we obtain

$$\begin{aligned}&O\left(\alpha,k\right)u_N^{k+1}-O\left(\alpha,k\right)u_N^k+O\left(\alpha,k\right)\sum_{j=1}^{k}\omega\left(\alpha,j\right)\left(u_N^{k-j+1}-u_N^{k-j}\right)\\=&\left(a[D][G]-h\left(t\right)-\beta[B][G]\right)u_N^{k+1}+h\left(t\right)u^{\infty}+\overline{g}_N^{k+1},\\&\left(O\left(\alpha,k\right)-a[D][G]+h\left(t\right)+\beta[B][G]\right)u_N^{k+1}\\=&O\left(\alpha,k\right)u_N^k-O\left(\alpha,k\right)\sum_{j=1}^{k}\omega\left(\alpha,j\right)\left(u_N^{k-j+1}-u_N^{k-j}\right)+h\left(t\right)u^{\infty}+\overline{g}_N^{k+1}.\end{aligned}\tag{3.7}$$

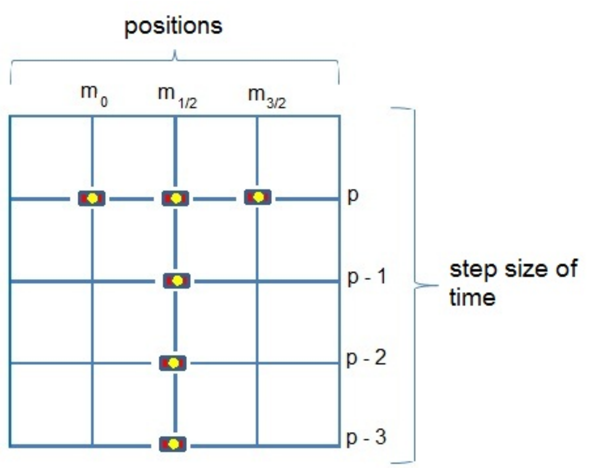


Figure 2. Mesh for the Fractional Order Derivative

4. Numerical Results

In this section, numerical tests are considered to show the numerical performance of the proposed formulation. From (1.1) and (3.1), the fractional partial differential equation in time with $\alpha=0.5$ is given as

$$\frac{\partial^{0.5}u(x,t)}{\partial t^{0.5}}=\frac{\partial^2u(x,t)}{\partial x^2}+e^xt^{0.5}\left(-t+\frac{\sqrt{t}\Gamma(2+\alpha)}{\Gamma(\frac{3}{2}+\alpha)}\right),\tag{4.1}$$

with domain

$$D = \{(x,t) : x,t \in [0,1]\}, \tag{4.2}$$

the initial condition

$$u\,(x,0) = 0, \tag{4.3}$$

and Neumann and Robin type boundary conditions

$$\left.\begin{aligned} -\frac{\partial u}{\partial x}(0,t) &= -t^{1+0.5}, \\ u(1,t) + \frac{\partial u}{\partial x}(1,t) &= 0. \end{aligned}\right\} \tag{4.4}$$

The exact solution is represented by the function: $u(x,t) = e^x t^{1+0.5}$.
The mimetic scheme used for the spatial discretization is expressed as

$$\begin{aligned} &\frac{\partial^2 u(x,t)}{\partial x^2} \approx D.(KG)u(x,t) \ \ . \ \ g(x,t) = g_i(x,t), \\ &h(t) \approx A, \ \ \frac{\partial u}{\partial x} \approx B.G, \ \ q(t) \approx q_i(t). \end{aligned}$$

This can be written mimetically as

$$MI = \left[\widehat{A} + BG + \widehat{D}.(G)\right] u(x,t),$$

where $\widehat{A}$ is a diagonal matrix of order $(N+2) \times (N+2)$ that has non-null entries. The elements corresponding to the boundary conditions are

$$\widehat{A}(1,1) = 0 \qquad \widehat{A}(N+2, N+2) = -1.$$

The purpose of this example is to study the influence of the time-step length Δt on the numerical solution obtained with Mimetic finite difference scheme. We evaluate the error between the exact and approximate solution with the maximum norm. The following Table shows the error in the maximum norm for the implicit finite difference (I.F.D) and the mimetic finite difference method (M.F.D) at time $t = 1$ and $t = 0.75$. It can be seen from the Table 1 that the error decreases when the time step is reduced. Though the approximation error is optimal when the grid size reduces, there is a significant difference in error distribution between Mimetic and Implicit discretization. For a 5x5 partitioned mesh, an error of order 0.7595488400681551 is obtained. Further refinement of the mesh with 8x8 elements, error 0.298728797488391 is obtained. These errors are higher in the case of I.F.D method, see Table 1 compare to M.F.D scheme. This behavior is expected as M.F.D method is of second order in time, while the Implicit scheme is of first order only, which supports the proposed numerical scheme for fractional order PDEs.

Further, the distribution of error obtained with the M.F.D scheme for different time steps and different time instances are depicted in the following figures. As expected, the distribution of error reduces when the time step is reduced, see Figures 3 (a), 4 (a), and 5 (a) at time $t = 1$. In addition, we can observe that distribution of error reduced by half with each successive refinement. Similar is the case of distribution error at time $t = 0.75$, see Figures 6 (a), 7 (a), and 8 (a). This behavior supports the Mimetic finite difference over Implicit finite difference method.

Table 1. Variation of the approximation error for I.F.D and M.F.D scheme with different time grid refinement level

Grid($\Delta x \times \Delta t$)	$E(\Delta x, \Delta t)$			
	I.F.D		M.F.D	
	$t = 1$	$t = 0.75$	$t = 1$	$t = 0.75$
$\frac{1}{100} \times \frac{1}{100}$	0.01080850	0.00414288	0.00423427	0.00190269
$\frac{1}{100} \times \frac{1}{200}$	0.00384188	0.00146142	0.00224898	$9.34982209e^{-04}$
$\frac{1}{100} \times \frac{1}{300}$	0.00205081	$7.73882266e^{-04}$	0.00141923	$5.76161563e^{-04}$

Furthermore, the next Figures show the Approximate and exact solutions for different time steps. This shows that the approximation error between the exact solution and the discrete one improves with the further refinement of the mesh, see Figures 3 (b), 4 (b), 5 (b) at time $t = 1$, and Figures 3 (b), 4 (b), 5 (b) at time $t = 0.75$. This comparative study is performed in order to see the effects of Mimetic finite difference method.

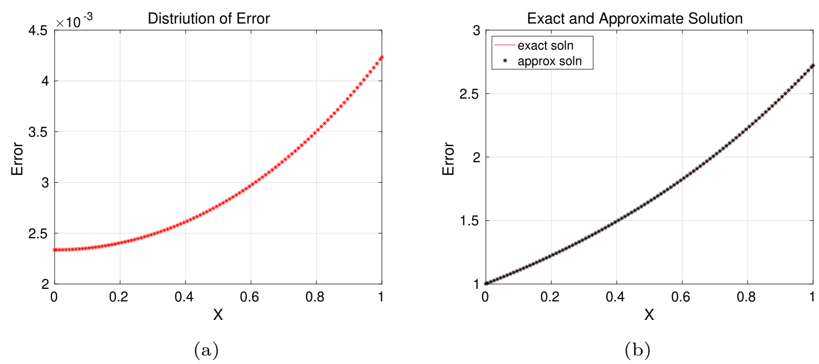


Figure 3. Approximation error obtained with M.F.D method with grid size $1/100 \times 1/100$, at time $t = 1$ (a) Distribution of error, (b) comparison of exact and approximate solution.

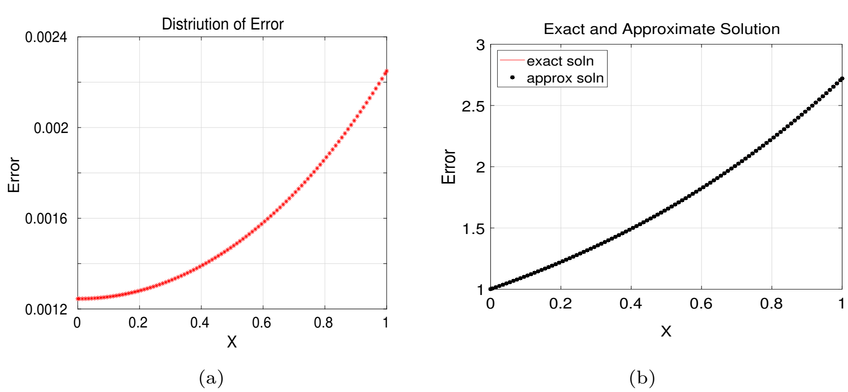
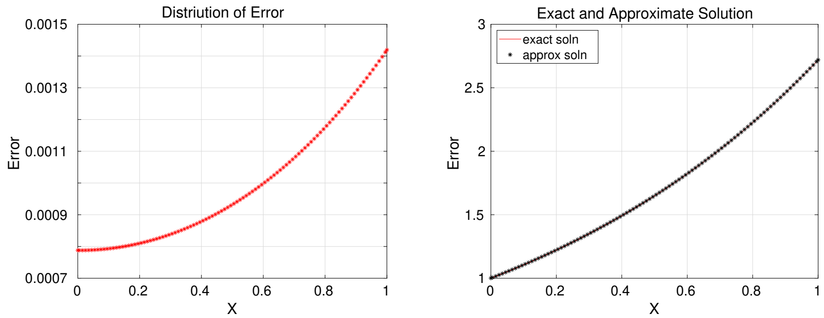
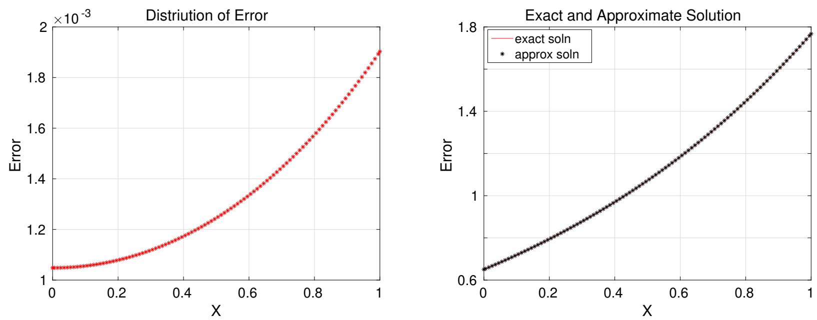


Figure 4. Approximation error obtained with M.F.D method with grid size $1/100 \times 1/200$, at time $t = 1$ (a) Distribution of error, (b) comparison of exact and approximate solution.



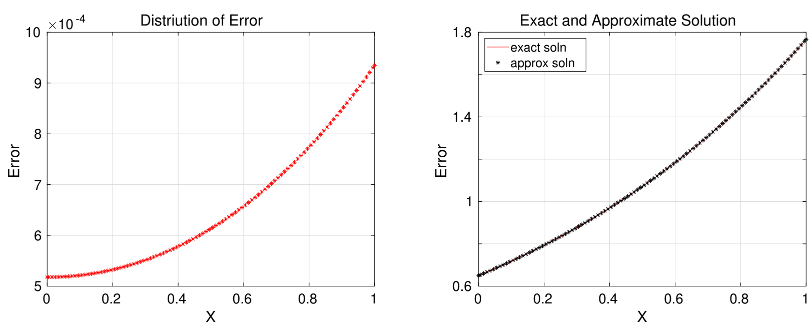
(a) (b)

Figure 5. Approximation error obtained with M.F.D method with grid size $1/100\times1/300,$ at time $t=1$ (a) Distribution of error, (b) comparison of exact and approximate solution.



(a) (b)

Figure 6. Approximation error obtained with M.F.D method with grid size $1/100\times1/100,$ at time $t=0.75$ (a) Distribution of error, (b) comparison of exact and approximate solution.



(a) (b)

Figure 7. Approximation error obtained with M.F.D method with grid size $1/100\times1/200,$ at time $t=0.75$ (a) Distribution of error, (b) comparison of exact and approximate solution.

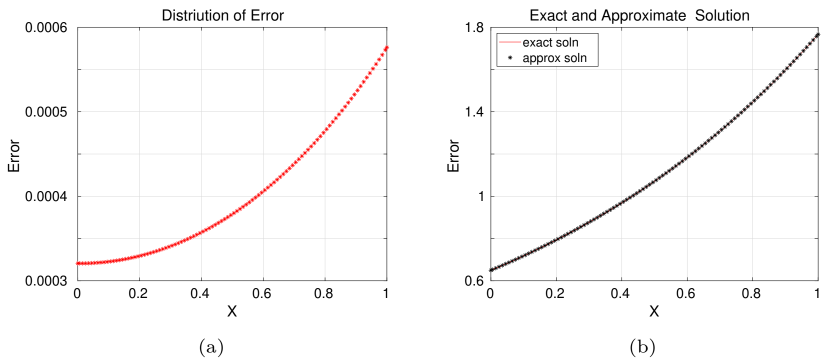


Figure 8. Approximation error obtained with M.F.D method with grid size $1/100 \times 1/300$, at time $t = 0.75$ (a) Distribution of error, (b) comparison of exact and approximate solution.

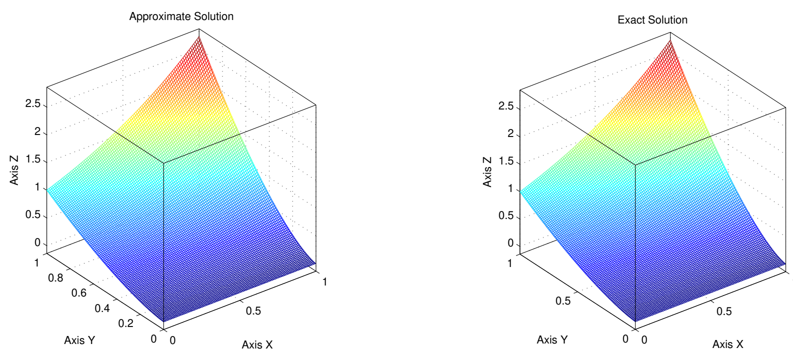


Figure 9. Approximated and exact solutions for a mesh $n = m = 100$

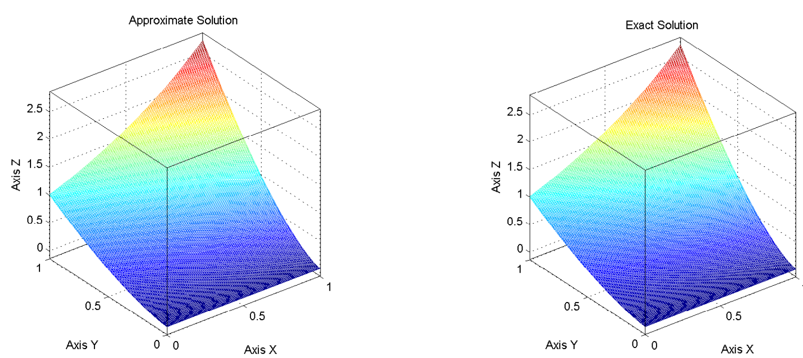


Figure 10. Exact and approximation solution for a mesh $n = m = 200$

5. Conclusions

In this paper, we present the mimetic finite difference method to numerically solve the fractional order diffusion equation in time with mixed boundary conditions,

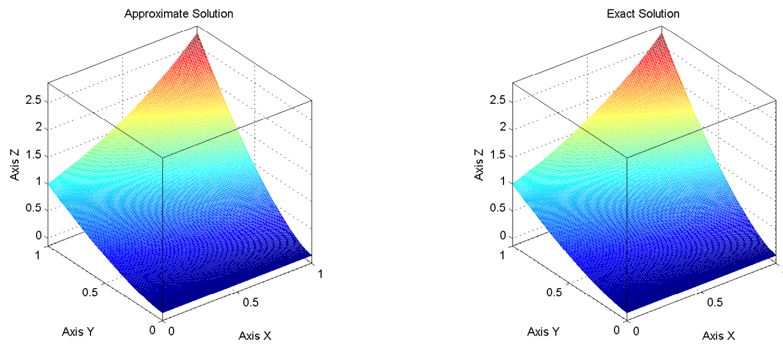


Figure 11. Exact and approximation solution for a mesh $n = m = 300$

characterized mainly by not using ghost points at the boundary of the domain. The result of this method presents an approximation of second order in space and firs order in time.
It is concluded that the approximate error generated between the exact and approximate solution using the method of mimetic finite differences is much better than the error using the approximation method of implicit finite difference, given in [3].

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