A high-order L2 type difference scheme for the time-fractional diffusion equation*

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Abstract

The present paper is devoted to constructing L2 type difference analog of the Caputo fractional derivative. The fundamental features of this difference operator are studied and it is used to construct difference schemes generating approximations of the second and fourth order in space and the $(3 - \alpha)$ th-order in time for the time fractional diffusion equation with variable coefficients. Stability of the schemes under consideration as well as their convergence with the rate equal to the order of the approximation error are proven. The received results are supported by the numerical computations performed for some test problems.

Keywords: fractional diffusion equation, finite difference method, stability, convergence

1. Introduction

A significant growth of the researches' attention to the fractional differential equations has been noticed lately. It is brought about by many effective applications of fractional calculation to various branches of science and engineering [1, 2, 3, 4, 5, 6]. For instance, we cannot dispense with mathematical language of fractional derivatives when it comes to the description of the physical process of statistical transfer which, as it is well known, brings us to diffusion equations of fractional orders [7, 8].

Let us consider the time fractional diffusion equation with variable coefficients

$$\partial_{0t}^{\alpha} u(x,t) = \mathcal{L}u(x,t) + f(x,t), \ 0 < x < l, \ 0 < t \le T, \tag{1}$$

$$u(0,t) = 0$$
, $u(l,t) = 0$, $0 \le t \le T$, $u(x,0) = u_0(x)$, $0 \le x \le l$, (2)

where

$$\partial_{0t}^{\alpha} u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{\partial u(x,\eta)}{\partial \eta} (t-\eta)^{-\alpha} d\eta, \quad 0 < \alpha < 1$$
 (3)

is the Caputo derivative of order α ,

$$\mathcal{L}u(x,t) = \frac{\partial}{\partial x} \left(k(x,t) \frac{\partial u}{\partial x} \right) - q(x,t)u,$$

 $k(x,t) \ge c_1 > 0$, $q(x,t) \ge 0$ and f(x,t) are given functions.

The time fractional diffusion equation constitutes a linear integro - differential equation. Its solution in many cases cannot be found in an analytical form; as a consequence it is required to apply numerical

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methods. Nevertheless, in contrast to the classical case, when we numerically approximate a time fractional diffusion equation on a certain time layer, we need information about all the previous time layers. That is why algorithms for solving the time fractional diffusion equations are rather labour-consuming even in one - dimensional case. When we pass to two - dimensional and three - dimensional problems, their complexity grows significantly. In this respect constructing stable differential schemes of higher order approximation is a major task.

A common difference approximation of fractional derivative (3) is the so-called L1 method [2, 9] which is specified in the following way

$$\partial_{0t_{j+1}}^{\alpha} u(x,t) = \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^{j} \frac{u(x,t_{s+1}) - u(x,t_s)}{t_{s+1} - t_s} \int_{t}^{t_{s+1}} \frac{d\eta}{(t_{j+1} - \eta)^{\alpha}} + r^{j+1}, \tag{4}$$

where $0 = t_0 < t_1 < \ldots < t_{j+1}$, and r^{j+1} is the local truncation error. In the case of the uniform grid, $\tau = t_{s+1} - t_s$, for all $s = 0, 1, \ldots, j+1$, it was proved that $r^{j+1} = \mathcal{O}(\tau^{2-\alpha})$ [9, 10, 11]. The L1 method has been commonly used to solve the fractional differential equations with the Caputo derivatives [9, 10, 11, 12, 13, 14].

The main idea of the traditional L1 formula for approximating Caputo fractional derivative $\partial_{0t}^{\alpha}f(t)$ of the function f(t) is to replace the integrand f(t) inside the integral by its piecewise linear interpolating polynomial (see [2, 9]). A simple technique for improving the accuracy of L1 formula is to use piecewise high-degree interpolating polynomials instead of the linear interpolating polynomial. In general, the obtained numerical formulae in this way improve the accuracy of L1 formula from the order $2 - \alpha$ to the order $r + 1 - \alpha$, where $r \geq 2$ is the degree of the interpolating polynomial. When such formulae are applied to solve time-fractional PDEs, a key issue is the stability analysis of the corresponding methods for all $\alpha \in (0,1)$.

In [21] a new difference analog of the Caputo fractional derivative with the order of approximation $\mathcal{O}(\tau^{3-\alpha})$, called L1-2 formula, is created. Based on this formula, calculations of difference schemes for the time-fractional sub-diffusion equations in bounded and unbounded spatial domains and the fractional ODEs are performed. In [15] the Caputo time-fractional derivative is discretized by a $(3-\alpha)$ th-order numerical formula (called the L2 formula in this paper) which is constructed using piecewise quadratic interpolating polynomials. By developing a technique of discrete energy analysis, a full theoretical analysis of the stability and convergence of the method is carried out for all $\alpha \in (0,1)$.

Using piecewise quadratic interpolating polynomials, In [22] a numerical formula (called $L2-1_{\sigma}$ formula) to approximate the Caputo fractional derivative $\partial_{0t}^{\alpha}f(t)$ at a special points with the numerical accuracy of order $3-\alpha$ was derived. Then some finite difference methods based on the $L2-1_{\sigma}$ formula were proposed for solving the time-fractional diffusion equation. In [23, 24] $L2-1_{\sigma}$ formula was generalized and applied for solving the multi-term, distributed and variable order time-fractional diffusion equations.

Difference schemes of the heightened order of approximation such as the compact difference scheme [13, 16, 17, 18, 15] and spectral method [10, 19, 20] were used to enhance the spatial accuracy of fractional diffusion equations.

By means of the energy inequality method, a priori estimates for the solution of the Dirichlet, Robin and non-local boundary value problems for the diffusion-wave equation with the Caputo fractional derivative have been found in [14, 25, 26].

In the present paper we construct L2 type difference analog of the fractional Caputo derivative with the order of approximation $\mathcal{O}(\tau^{3-\alpha})$ for each $\alpha \in (0,1)$. Features of the found difference operator are investigated. Difference schemes of the second and fourth order of approximation in space and the $(3-\alpha)$ th-order in time for the time fractional diffusion equation with variable coefficients are built. By means of the method of energy inequalities, the stability and convergence of these schemes are proven. Numerical computations of some test problems confirming reliability of the obtained results are implemented. The method can be without difficulty expanded to other time fractional partial differential equations with other boundary conditions.

2. The L2 type fractional numerical differentiation formula

In this section we study a difference analog of the Caputo fractional derivative with the approximation order $\mathcal{O}(\tau^{3-\alpha})$ and explore its fundamental features.

We consider the uniform grid $\bar{\omega}_{\tau} = \{t_j = j\tau, j = 0, 1, \dots, M; T = \tau M\}$. For the Caputo fractional derivative of the order $\alpha, 0 < \alpha < 1$, of the function $u(t) \in \mathcal{C}^3[0,T]$ at the fixed point $t_{j+1}, j \in \{1, 2, \dots, M-1\}$ the following equalities are valid

$$\partial_{0t_{j+1}}^{\alpha} u(t) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t_{j+1}} \frac{u'(\eta)d\eta}{(t_{j+1}-\eta)^{\alpha}}$$

$$= \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t_2} \frac{u'(\eta)d\eta}{(t_{j+1}-\eta)^{\alpha}} + \frac{1}{\Gamma(1-\alpha)} \sum_{s=2}^{j} \int_{t_s}^{t_{s+1}} \frac{u'(\eta)d\eta}{(t_{j+1}-\eta)^{\alpha}}.$$
 (5)

On each interval $[t_{s-1}, t_s]$ $(1 \le s \le j)$, applying the quadratic interpolation $\Pi_{2,s}u(t)$ of u(t) that uses three points $(t_{s-1}, u(t_{s-1}))$, $(t_s, u(t_s))$ and $(t_{s+1}, u(t_{s+1}))$, we arrive at

$$\Pi_{2,s}u(t) = u(t_{s-1})\frac{(t-t_s)(t-t_{s+1})}{2\tau^2} - u(t_s)\frac{(t-t_{s-1})(t-t_{s+1})}{\tau^2} + u(t_{s+1})\frac{(t-t_{s-1})(t-t_s)}{2\tau^2},$$

$$(\Pi_{2,s}u(t))' = u_{t,s} + u_{\bar{t}t,s}(t-t_{s+1/2}),$$
(6)

and

$$u(t) - \Pi_{2,s}u(t) = \frac{u'''(\bar{\xi}_s)}{6}(t - t_{s-1})(t - t_s)(t - t_{s+1}), \tag{7}$$

where $t \in [t_{s-1}, t_{s+1}], \ \bar{\xi}_s \in (t_{s-1}, t_{s+1}), \ t_{s-1/2} = t_s - 0.5\tau, \ u_{t,s} = (u(t_{s+1}) - u(t_s))/\tau, \ u_{\bar{t},s} = (u(t_s) - u(t_{s-1}))/\tau.$

In (5), we make use of $\Pi_{2,s}u(t)$ in order to approximate u(t) on the interval $[t_{s-1},t_s]$ $(1 \le s \le j)$. In view of the equality

$$\int_{t_{s-1}}^{t_s} (\eta - t_{s-1/2})(t_{j+1} - \eta)^{-\alpha} d\eta = \frac{\tau^{2-\alpha}}{1-\alpha} b_{j-s+1}^{(\alpha)}, \quad 1 \le s \le j$$
(8)

with

$$b_l^{(\alpha)} = \frac{1}{2-\alpha} \left[(l+1)^{2-\alpha} - l^{2-\alpha} \right] - \frac{1}{2} \left[(l+1)^{1-\alpha} + l^{1-\alpha} \right], \quad l \ge 0,$$

from (5) and (6) we get the difference analog of the Caputo fractional derivative of order α (0 < α < 1) for the function u(t), at the points t_{j+1} (j = 1, 2, ...), in this form:

$$\partial_{0t_{j+1}}^{\alpha} u(\eta) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t_2} \frac{u'(\eta)d\eta}{(t_{j+1}-\eta)^{\alpha}} + \frac{1}{\Gamma(1-\alpha)} \sum_{s=2}^{j} \int_{t_s}^{t_{s+1}} \frac{u'(\eta)d\eta}{(t_{j+1}-\eta)^{\alpha}}$$

$$\approx \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t_{2}} \frac{(\Pi_{2,1}u(\eta))' d\eta}{(t_{j+1}-\eta)^{\alpha}} + \frac{1}{\Gamma(1-\alpha)} \sum_{s=2}^{j} \int_{t_{s}}^{t_{s+1}} \frac{(\Pi_{2,s}u(\eta))' d\eta}{(t_{j+1}-\eta)^{\alpha}}$$

$$= \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t_{2}} \frac{u_{t,1} + u_{\bar{t}t,1}(\eta - t_{3/2})}{(t_{j+1} - \eta)^{\alpha}} d\eta$$

$$+ \frac{1}{\Gamma(1-\alpha)} \sum_{s=2}^{j} \int_{t_{s}}^{t_{s+1}} \frac{u_{t,s} + u_{\bar{t}t,s}(\eta - t_{s+1/2})}{(t_{j+1} - \eta)^{\alpha}} d\eta$$

$$= \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \left((a_{j}^{(\alpha)} - b_{j}^{(\alpha)} - b_{j-1}^{(\alpha)}) u_{t,0} + (a_{j-1}^{(\alpha)} + b_{j-1}^{(\alpha)} + b_{j}^{(\alpha)}) u_{t,1} \right)$$

$$+ \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=2}^{j} (-b_{j-s}^{(\alpha)} u_{t,s-1} + (a_{j-s}^{(\alpha)} + b_{j-s}^{(\alpha)}) u_{t,s})$$

$$= \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \left((a_{j}^{(\alpha)} - b_{j}^{(\alpha)} - b_{j-1}^{(\alpha)}) u_{t,0} + (a_{j-1}^{(\alpha)} + b_{j-1}^{(\alpha)} + b_{j}^{(\alpha)} - b_{j-2}^{(\alpha)}) u_{t,1} \right)$$

$$+ \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \left(\sum_{s=2}^{j-1} (-b_{j-s-1}^{(\alpha)} + a_{j-s}^{(\alpha)} + b_{j-s}^{(\alpha)}) u_{t,s} + (a_{0}^{(\alpha)} + b_{0}^{(\alpha)}) u_{t,j} \right) =$$

$$= \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{j} c_{j-s}^{(\alpha)} u_{t,s} = \Delta_{0t_{j+1}}^{\alpha} u_{t,s}$$

$$(9)$$

where

$$a_l^{(\alpha)} = (l+1)^{1-\alpha} - l^{1-\alpha}, \quad l \ge 0;$$

for j = 1

$$c_s^{(\alpha)} = \begin{cases} a_0^{(\alpha)} + b_0^{(\alpha)} + b_1^{(\alpha)}, & s = 0, \\ a_1^{(\alpha)} - b_1^{(\alpha)} - b_0^{(\alpha)}, & s = 1, \end{cases}$$
(10)

for j=2

$$c_s^{(\alpha)} = \begin{cases} a_0^{(\alpha)} + b_0^{(\alpha)}, & s = 0, \\ a_1^{(\alpha)} + b_1^{(\alpha)} + b_2^{(\alpha)} - b_0^{(\alpha)}, & s = 1, \\ a_2^{(\alpha)} - b_2^{(\alpha)} - b_1^{(\alpha)}, & s = 2, \end{cases}$$
(11)

and for $j \geq 3$,

$$c_s^{(\alpha)} = \begin{cases} a_0^{(\alpha)} + b_0^{(\alpha)}, & s = 0, \\ a_s^{(\alpha)} + b_s^{(\alpha)} - b_{s-1}^{(\alpha)}, & 1 \le s \le j - 2, \\ a_{j-1}^{(\alpha)} + b_{j-1}^{(\alpha)} + b_j^{(\alpha)} - b_{j-2}^{(\alpha)}, & s = j - 1, \\ a_j^{(\alpha)} - b_j^{(\alpha)} - b_{j-1}^{(\alpha)}, & s = j. \end{cases}$$
(12)

We name the fractional numerical differentiation formula (9) for the Caputo fractional derivative of order α (0 < α < 1) the L2 formula.

Lemma 2.1. For any $\alpha \in (0,1), j = 1, 2, ..., M-1 \text{ and } u(t) \in C^3[0, t_{i+1}]$

$$|\partial_{0t_{j+1}}^{\alpha} u - \Delta_{0t_{j+1}}^{\alpha} u| = \mathcal{O}(\tau^{3-\alpha}). \tag{13}$$

Proof. Let $\partial_{0t_{j+1}}^{\alpha}u - \Delta_{0t_{j+1}}^{\alpha}u = R_0^2 + R_2^{j+1}$, where

$$R_0^2 = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_2} \frac{u'(\eta)d\eta}{(t_{j+1}-\eta)^{\alpha}} - \frac{1}{\Gamma(1-\alpha)} \int_0^{t_2} \frac{(\Pi_{2,1}u(\eta))'d\eta}{(t_{j+1}-\eta)^{\alpha}}$$

$$\begin{split} &= \frac{1}{\Gamma(1-\alpha)} \int\limits_{0}^{t_{2}} \frac{(u(\eta) - \Pi_{2,1}u(\eta))' d\eta}{(t_{j+1} - \eta)^{\alpha}} = -\frac{\alpha}{\Gamma(1-\alpha)} \int\limits_{0}^{t_{2}} \frac{(u(\eta) - \Pi_{2,1}u(\eta)) d\eta}{(t_{j+1} - \eta)^{\alpha+1}} \\ &= -\frac{\alpha}{6\Gamma(1-\alpha)} \int\limits_{0}^{t_{2}} u'''(\bar{\xi}_{1}) \eta(\eta - t_{1}) (\eta - t_{2}) (t_{j+1} - \eta)^{-\alpha-1} d\eta, \\ &R_{2}^{j+1} = \frac{1}{\Gamma(1-\alpha)} \sum_{s=2}^{j} \int\limits_{t_{s}}^{t_{s+1}} \frac{u'(\eta) d\eta}{(t_{j+1} - \eta)^{\alpha}} - \frac{1}{\Gamma(1-\alpha)} \sum_{s=2}^{j} \int\limits_{t_{s}}^{t_{s+1}} \frac{(\Pi_{2,s}u(\eta))' d\eta}{(t_{j+1} - \eta)^{\alpha}} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=2}^{j} \int\limits_{t_{s}}^{t_{s+1}} (u(\eta) - \Pi_{2,s}u(\eta))' (t_{j+1} - \eta)^{-\alpha} d\eta \\ &= -\frac{\alpha}{\Gamma(1-\alpha)} \sum_{s=2}^{j} \int\limits_{t_{s}}^{t_{s+1}} (u(\eta) - \Pi_{2,s}u(\eta)) (t_{j+1} - \eta)^{-\alpha-1} d\eta \\ &= -\frac{\alpha}{6\Gamma(1-\alpha)} \sum_{s=2}^{j} \int\limits_{t_{s}}^{t_{s+1}} u'''(\bar{\xi}_{s}) (\eta - t_{s-1}) (\eta - t_{s}) (\eta - t_{s+1}) (t_{j+1} - \eta)^{-\alpha-1} d\eta, \end{split}$$

Next we estimate the errors R_0^2 and R_2^{j+1} : For j=1 we have

$$\begin{aligned} \left| R_0^2 \right| &= \frac{\alpha}{6\Gamma(1-\alpha)} \left| \int_0^{t_2} u'''(\bar{\xi}_1) \eta(\eta - t_1) (\eta - t_2) (t_2 - \eta)^{-\alpha - 1} d\eta \right| \\ &\leq \frac{\alpha M_3 \tau^2}{3\Gamma(1-\alpha)} \int_0^{t_2} (t_2 - \eta)^{-\alpha} d\eta = \frac{2^{1-\alpha} \alpha M_3}{3\Gamma(2-\alpha)} \tau^{3-\alpha}, \end{aligned}$$

For $j \geq 2$ we have

$$\begin{split} \left|R_0^2\right| &= \frac{\alpha}{6\Gamma(1-\alpha)} \left|\int\limits_0^{t_2} u'''(\bar{\xi}_1) \eta(\eta-t_1)(\eta-t_2)(t_{j+1}-\eta)^{-\alpha-1} d\eta \right| \\ &\leq \frac{2\sqrt{3}\alpha M_3 \tau^3}{54\Gamma(1-\alpha)} \int\limits_0^{t_2} (t_{j+1}-\eta)^{-\alpha-1} d\eta = \frac{\sqrt{3}M_3 \tau^{3-\alpha}}{27\Gamma(1-\alpha)} \left((j-1)^{-\alpha}-(j+1)^{-\alpha}\right) \leq \frac{\sqrt{3}(1-3^{-\alpha})M_3}{27\Gamma(1-\alpha)} \tau^{3-\alpha}, \\ \left|R_2^{j+1}\right| &= \frac{\alpha}{6\Gamma(1-\alpha)} \left|\sum_{s=2}^j \int\limits_{t_s}^{t_{s+1}} u'''(\bar{\xi}_s)(\eta-t_{s-1})(\eta-t_s)(\eta-t_{s+1})(t_{j+1}-\eta)^{-\alpha-1} d\eta \right| \\ &\leq \frac{2\sqrt{3}\alpha M_3 \tau^3}{54\Gamma(1-\alpha)} \sum_{s=2}^{j-1} \int\limits_{t_s}^{t_{s+1}} (t_{j+1}-\eta)^{-\alpha-1} d\eta + \frac{\alpha M_3 \tau^2}{3\Gamma(1-\alpha)} \int\limits_{t_j}^{t_{j+1}} (t_{j+1}-\eta)^{-\alpha} d\eta \\ &= \frac{\sqrt{3}\alpha M_3 \tau^3}{27\Gamma(1-\alpha)} \int\limits_{t_2}^{t_j} (t_{j+1}-\eta)^{-\alpha-1} d\eta + \frac{\alpha M_3 \tau^2}{3\Gamma(1-\alpha)} \int\limits_{t_j}^{t_{j+1}} (t_{j+1}-\eta)^{-\alpha} d\eta \end{split}$$

$$= \frac{\sqrt{3}M_3\tau^3}{27\Gamma(1-\alpha)} \left(\tau^{-\alpha} - t_{j-1}^{-\alpha}\right) + \frac{\alpha M_3\tau^2}{3\Gamma(1-\alpha)} \frac{\tau^{1-\alpha}}{1-\alpha} \le \left(\frac{\sqrt{3}}{9} + \frac{\alpha}{(1-\alpha)}\right) \frac{M_3}{3\Gamma(1-\alpha)} \tau^{3-\alpha}.$$

2.1. Fundamental features of the new L2 fractional numerical differentiation formula.

Lemma 2.2. For all $\alpha \in (0,1)$ and s = 1, 2, 3, ...

$$\frac{1-\alpha}{(s+1)^{\alpha}} < a_s < \frac{1-\alpha}{s^{\alpha}},\tag{14}$$

$$\frac{\alpha(1-\alpha)}{(s+2)^{\alpha+1}} < a_s - a_{s+1} < \frac{\alpha(1-\alpha)}{s^{\alpha+1}},\tag{15}$$

$$\frac{\alpha(1-\alpha)}{12(s+1)^{\alpha+1}} < b_s < \frac{\alpha(1-\alpha)}{12s^{\alpha+1}},\tag{16}$$

Proof. The validity of Lemma 2.2 follows from the following equalities:

$$a_{s} = (1 - \alpha) \int_{0}^{1} \frac{d\xi}{(s + \xi)^{\alpha}},$$

$$a_{s} - a_{s+1} = \alpha(1 - \alpha) \int_{0}^{1} d\eta \int_{0}^{1} \frac{d\xi}{(s + \xi + \eta)^{\alpha+1}},$$

$$b_{s} = \frac{\alpha(1 - \alpha)}{2^{2-\alpha}} \int_{0}^{1} \eta d\eta \int_{2s+1-\eta}^{2s+1+\eta} \frac{d\xi}{\xi^{\alpha+1}}.$$

For j = 1 we have

$$c_0^{(\alpha)} = \frac{2+\alpha}{2^{\alpha}(2-\alpha)}, \quad c_1^{(\alpha)} = \frac{2-3\alpha}{2^{\alpha}(2-\alpha)}, \quad c_0^{(\alpha)} + 3c_1^{(\alpha)} = \frac{2^{3-\alpha}(1-\alpha)}{2-\alpha} > 0.$$

For $j \geq 2$, the next lemma shows properties of the coefficient $c_s^{(\alpha)}$ defined in (11) and (12)

Lemma 2.3. For any $\alpha \in (0,1)$ and $c_s^{(\alpha)}$ $(0 \le s \le j, j \ge 2)$ the following inequalities are valid

$$\frac{11}{16} \cdot \frac{1-\alpha}{(j+1)^{\alpha}} < c_j^{(\alpha)} < \frac{1-\alpha}{j^{\alpha}},\tag{17}$$

$$c_0^{(\alpha)} > c_2^{(\alpha)} > c_3^{(\alpha)} > \dots > c_{j-2}^{(\alpha)} > c_{j-1}^{(\alpha)} > c_j^{(\alpha)},$$
 (18)

$$c_0^{(\alpha)} + 3c_1^{(\alpha)} - 4c_2^{(\alpha)} > 0.$$
 (19)

Proof. For $j \geq 2$ we get

$$c_{j}^{(\alpha)} = a_{j}^{(\alpha)} - b_{j}^{(\alpha)} - b_{j-1}^{(\alpha)} < a_{j}^{(\alpha)} < \frac{1 - \alpha}{j^{\alpha}}.$$

$$c_{j}^{(\alpha)} = a_{j}^{(\alpha)} - b_{j}^{(\alpha)} - b_{j-1}^{(\alpha)} > \frac{1 - \alpha}{(j+1)^{\alpha}} - \frac{\alpha(1-\alpha)}{12j^{\alpha+1}} - \frac{\alpha(1-\alpha)}{12(j-1)^{\alpha+1}}.$$

$$= \frac{1-\alpha}{(j+1)^{\alpha}} \left(1 - \frac{\alpha}{12} \cdot \left(\frac{j+1}{j} \right)^{\alpha} \cdot \frac{1}{j} - \frac{\alpha}{12} \cdot \left(\frac{j+1}{j-1} \right)^{\alpha} \cdot \frac{1}{j-1} \right)$$

$$> \frac{1-\alpha}{(j+1)^{\alpha}} \left(1 - \frac{1}{12} \cdot \frac{3}{2} \cdot \frac{1}{2} - \frac{1}{12} \cdot 3 \right) = \frac{11}{16} \cdot \frac{1-\alpha}{(j+1)^{\alpha}}$$

Inequality (17) is proved. Let us prove inequality (18).

$$c_0^{(\alpha)} - c_2^{(\alpha)} \ge a_0^{(\alpha)} - a_2^{(\alpha)} + b_0^{(\alpha)} - b_2^{(\alpha)} + b_1^{(\alpha)} - b_3^{(\alpha)} > 0,$$

For $j \geq 5$, $2 \leq s \leq j-3$ we have

$$\begin{split} c_s^{(\alpha)} - c_{s+1}^{(\alpha)} &= a_s^{(\alpha)} - a_{s+1}^{(\alpha)} - b_{s-1}^{(\alpha)} + 2b_s^{(\alpha)} - b_{s+1}^{(\alpha)} \\ &= \frac{1}{2 - \alpha} \left(-(s+2)^{2-\alpha} + 3(s+1)^{2-\alpha} - 3s^{2-\alpha} + (s-1)^{2-\alpha} \right) \\ &- \frac{1}{2} \left(-(s+2)^{1-\alpha} + 3(s+1)^{1-\alpha} - 3s^{1-\alpha} + (s-1)^{1-\alpha} \right) \\ &= \alpha (1 - \alpha) \int\limits_0^1 dz_1 \int\limits_0^1 dz_2 \int\limits_0^1 \frac{dz_3}{(s-1+z_1+z_2+z_3)^{\alpha+1}} \\ &- \frac{\alpha (1-\alpha)(1+\alpha)}{2} \int\limits_0^1 dz_1 \int\limits_0^1 dz_2 \int\limits_0^1 \frac{dz_2}{(s-1+z_1+z_2+z_3)^{\alpha+2}} \\ &= \alpha (1-\alpha) \int\limits_0^1 dz_1 \int\limits_0^1 dz_2 \int\limits_0^1 \frac{\left(1 - \frac{1+\alpha}{2} \cdot \frac{1}{s-1+z_1+z_2+z_3}\right)}{(s-1+z_1+z_2+z_3)^{\alpha+1}} dz_3 \\ &> \frac{\alpha (1-\alpha)}{(s+2)^{\alpha+1}} \left(1 - \frac{1+\alpha}{2} \int\limits_0^1 dz_1 \int\limits_0^1 dz_2 \int\limits_0^1 \frac{dz_3}{1+z_1+z_2+z_3} \right). \end{split}$$

Since

$$\int_{0}^{1} dz_{1} \int_{0}^{1} dz_{2} \int_{0}^{1} \frac{dz_{3}}{1 + z_{1} + z_{2} + z_{3}} = \frac{1}{2} \left(44 \ln 2 - 27 \ln 3 \right) < \frac{1}{2},$$

$$c_{s}^{(\alpha)} - c_{s+1}^{(\alpha)} > \frac{\alpha(1 - \alpha)}{(s+2)^{\alpha+1}} \left(1 - \frac{1 + \alpha}{4} \right) > \frac{\alpha(1 - \alpha)}{2(s+2)^{\alpha+1}} > 0.$$

For $j \geq 4$ we get

$$\begin{split} c_{j-2}^{(\alpha)} - c_{j-1}^{(\alpha)} &= a_{j-2}^{(\alpha)} - a_{j-1}^{(\alpha)} - b_{j-3}^{(\alpha)} + 2b_{j-2}^{(\alpha)} - b_{j-1}^{(\alpha)} - b_{j}^{(\alpha)} \\ &> \frac{\alpha(1-\alpha)}{2j^{\alpha+1}} - b_{j}^{(\alpha)} > \frac{\alpha(1-\alpha)}{2j^{\alpha+1}} - \frac{\alpha(1-\alpha)}{12j^{\alpha+1}} = \frac{5\alpha(1-\alpha)}{12j^{\alpha+1}} > 0. \end{split}$$

For $j \geq 3$ we have

$$c_{j-1}^{(\alpha)} - c_{j}^{(\alpha)} = a_{j-1}^{(\alpha)} - a_{j}^{(\alpha)} - b_{j-2}^{(\alpha)} + 2b_{j-1}^{(\alpha)} + 2b_{j}^{(\alpha)}$$

$$> a_{j-1}^{(\alpha)} - a_{j}^{(\alpha)} - b_{j-2}^{(\alpha)} + 2b_{j-1}^{(\alpha)} - b_{j}^{(\alpha)} > \frac{\alpha(1-\alpha)}{2(j+1)^{\alpha+1}} > 0.$$

Inequality (18) is proved.

For j = 2 we get

$$c_0^{(\alpha)} + 3c_1^{(\alpha)} - 4c_2^{(\alpha)} = a_0^{(\alpha)} + 3a_1^{(\alpha)} - 4a_2^{(\alpha)} - 2b_0^{(\alpha)} + 7b_1^{(\alpha)} + 7b_2^{(\alpha)}$$

$$> a_0^{(\alpha)} - a_1^{(\alpha)} - 2b_0^{(\alpha)} = 3 - 2^{1-\alpha} - \frac{2}{2-\alpha}.$$

Since, for any function $f(x) \in C^2[0,1]$, if f(0) = 0, f(1) = 0 and f''(x) < 0 for all $x \in (0,1)$ then f(x) > 0 for all $x \in (0,1)$, we have

$$c_0^{(\alpha)} + 3c_1^{(\alpha)} - 4c_2^{(\alpha)} > f(\alpha) = 3 - 2^{1-\alpha} - \frac{2}{2-\alpha} > 0$$
 for all $\alpha \in (0,1)$.

For j = 3 we get

$$\begin{split} c_0^{(\alpha)} + 3c_1^{(\alpha)} - 4c_2^{(\alpha)} &= a_0^{(\alpha)} + 3a_1^{(\alpha)} - 4a_2^{(\alpha)} - 2b_0^{(\alpha)} + 7b_1^{(\alpha)} - 4b_2^{(\alpha)} - 4b_3^{(\alpha)} \\ &> a_0^{(\alpha)} - a_1^{(\alpha)} - 2b_0^{(\alpha)} + 4(a_1^{(\alpha)} - a_2^{(\alpha)} - b_3^{(\alpha)}) > 3 - 2^{1-\alpha} - \frac{2}{2-\alpha} > 0. \end{split}$$

Lemma 2.4. For any real constants c_0, c_1 such that $c_0 \ge \max\{c_1, -3c_1\}$, and $\{v_j\}_{j=0}^{j=M}$ the following inequality holds

$$v_{j+1}(c_0v_{j+1} - (c_0 - c_1)v_j - c_1v_{j-1}) \ge E_{j+1} - E_j, \quad j = 1, \dots, M-1,$$
 (20)

where

$$E_{j} = \left(\frac{1}{2}\sqrt{\frac{c_{0} - c_{1}}{2}} + \frac{1}{2}\sqrt{\frac{c_{0} + 3c_{1}}{2}}\right)^{2}v_{j}^{2} + \left(\sqrt{\frac{c_{0} - c_{1}}{2}}v_{j} - \left(\frac{1}{2}\sqrt{\frac{c_{0} - c_{1}}{2}} + \frac{1}{2}\sqrt{\frac{c_{0} + 3c_{1}}{2}}\right)v_{j-1}\right)^{2}, \quad j = 1, 2, \dots, M.$$

Proof. The proof of Lemma 2.4 immediately follows from the next equality

$$v_{j+1} \left(c_0 v_{j+1} - (c_0 - c_1) v_j - c_1 v_{j-1} \right) - E_{j+1} + E_j$$

$$= \left(\left(\frac{1}{2} \sqrt{\frac{c_0 - c_1}{2}} - \frac{1}{2} \sqrt{\frac{c_0 + 3c_1}{2}} \right) v_{j+1} - \sqrt{\frac{c_0 - c_1}{2}} v_j + \left(\frac{1}{2} \sqrt{\frac{c_0 - c_1}{2}} + \frac{1}{2} \sqrt{\frac{c_0 + 3c_1}{2}} \right) v_{j-1} \right)^2 \ge 0.$$

Lemma 2.5. [22] If $g_j^{j+1} \ge g_{j-1}^{j+1} \ge \ldots \ge g_0^{j+1} > 0$, $j = 0, 1, \ldots, M-1$ then for any function v(t) defined on the grid $\overline{\omega}_{\tau}$ one has the inequalities

$$v^{j+1}{}_{g}\Delta^{\alpha}_{0t_{j+1}}v \ge \frac{1}{2}{}_{g}\Delta^{\alpha}_{0t_{j+1}}(v^2) + \frac{1}{2g_j^{j+1}} \left({}_{g}\Delta^{\alpha}_{0t_{j+1}}v\right)^2, \tag{21}$$

where

$$_{g}\Delta_{0t_{j+1}}^{\alpha}y_{i} = \sum_{s=0}^{j} (y_{i}^{s+1} - y_{i}^{s}) g_{s}^{j+1},$$

is a difference analog of the Caputo fractional derivative of the order α (0 < α < 1).

Lemma 2.6. For any function v(t) defined on the grid $\overline{\omega}_{\tau}$ one has the inequality

$$v_{j+1} \Delta_{0t_{j+1}}^{\alpha} v \ge \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left(E_{j+1} - E_j \right) + \frac{1}{2} \bar{\Delta}_{0t_{j+1}}^{\alpha} v^2 = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left(\mathcal{E}_{j+1} - \mathcal{E}_j \right) - \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)} \bar{c}_j^{(\alpha)} v_0^2, \tag{22}$$

where

$$\bar{\Delta}_{0t_{j+1}}^{\alpha}v = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^{j} \bar{c}_{j-s}^{(\alpha)}(v_{s+1}-v_{s}), \quad j=1,2,\ldots,M,$$

$$\bar{c}_{0}^{(\alpha)} = c_{2}^{(\alpha)}, \quad \bar{c}_{1}^{(\alpha)} = c_{2}^{(\alpha)}, \quad \bar{c}_{s}^{(\alpha)} = c_{s}^{(\alpha)}, \quad s=2,3,\ldots,j,$$

$$for \quad j=1,2,3,\ldots,M, \quad E_{j} = E_{j}(c_{0}^{(\alpha)}-c_{2}^{(\alpha)},c_{1}^{(\alpha)}-c_{2}^{(\alpha)}),$$

$$\mathcal{E}_{j} = E_{j} + \frac{1}{2} \sum_{s=0}^{j-1} \bar{c}_{j-1-s}^{(\alpha)}v_{s+1}^{2}.$$

Proof. For j = 1 we have

$$v_{2}\Delta_{0t_{2}}^{\alpha}v = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}v_{2}\left(c_{0}^{(\alpha)}(v_{2}-v_{1}) + c_{1}^{(\alpha)}(v_{1}-v_{0})\right)$$

$$= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}v_{2}\left((c_{0}^{(\alpha)}-c_{2}^{(\alpha)})v_{2} - (c_{0}^{(\alpha)}-c_{1}^{(\alpha)})v_{1} - (c_{1}^{(\alpha)}-c_{2}^{(\alpha)})v_{0}\right)$$

$$+ \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}c_{2}^{(\alpha)}\left(v_{2}^{2}-v_{2}v_{0}\right)$$

$$\geq \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\left(E_{2}-E_{1}\right) + \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)}c_{2}^{(\alpha)}\left(v_{2}^{2}-v_{0}^{2}\right)$$

$$= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\left(E_{2}-E_{1}\right) + \frac{1}{2}\bar{\Delta}_{0t_{2}}^{\alpha}v^{2}.$$

For j = 2, 3, ..., M - 1 we have

$$v_{j+1}\Delta_{0t_{j+1}}^{\alpha}v = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}v_{j+1}\sum_{s=0}^{j}c_{j-s}^{(\alpha)}(v_{s+1}-v_{s})$$

$$\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}v_{j+1}\left((c_{0}^{(\alpha)}-c_{2}^{(\alpha)})(v_{j+1}-v_{j})+(c_{1}^{(\alpha)}-c_{2}^{(\alpha)})(v_{j}-v_{j-1})\right)+v_{j+1}\bar{\Delta}_{0t_{j+1}}^{\alpha}v$$

$$=\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}v_{j+1}\left((c_{0}^{(\alpha)}-c_{2}^{(\alpha)})v_{j+1}-(c_{0}^{(\alpha)}-c_{1}^{(\alpha)})v_{j}-(c_{1}^{(\alpha)}-c_{2}^{(\alpha)})v_{j-1}\right)+v_{j+1}\bar{\Delta}_{0t_{j+1}}^{\alpha}v$$

$$\geq \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\left(E_{j+1}-E_{j}\right)+\frac{1}{2}\bar{\Delta}_{0t_{j+1}}^{\alpha}v^{2}.$$

In addition, the following equality holds

$$\bar{\Delta}_{0t_{j+1}}^{\alpha}v^2 = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\sum_{s=0}^{j}\bar{c}_{j-s}^{(\alpha)}(v_{s+1}^2-v_s^2) = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{s=0}^{j}\bar{c}_{j-s}^{(\alpha)}v_{s+1}^2 - \sum_{s=0}^{j-1}\bar{c}_{j-1-s}^{(\alpha)}v_{s+1}^2 - \bar{c}_{j}^{(\alpha)}v_0^2\right).$$

3. A difference scheme for the time fractional diffusion equation

In this section for problem (1)–(2) a difference scheme with the approximation order $\mathcal{O}(h^2 + \tau^{3-\alpha})$ is constructed. The stability of the constructed difference scheme as well as its convergence in the grid L_2 - norm with the rate equal to the order of the approximation error is proved. The obtained results are supported with numerical calculations carried out for a test example.

3.1. Derivation of the difference scheme

Lemma 3.1. [22] For any functions $k(x) \in \mathcal{C}_x^3$ and $v(x) \in \mathcal{C}_x^4$ the following equality holds true:

$$\frac{d}{dx}\left(k(x)\frac{d}{dx}v(x)\right)\Big|_{x=x_i} = \frac{k(x_{i+1/2})v(x_{i+1}) - (k(x_{i+1/2}) + k(x_{i-1/2}))v(x_i) + k(x_{i-1/2})v(x_{i-1})}{h^2} + \mathcal{O}(h^2).$$
(23)

Let $u(x,t) \in \mathcal{C}^{4,3}_{x,t}$ be a solution of problem (1)–(2). Then we consider equation (1) for $(x,t)=(x_i,t_{j+1}) \in \overline{Q}_T$, $i=1,2,\ldots,N-1,\ j=1,2,\ldots,M-1$:

$$\partial_{0t_{i+1}}^{\alpha} u = \mathcal{L}u(x,t)|_{(x_i,t_{i+1})} + f(x_i,t_{j+1}). \tag{24}$$

On the basis of Lemmas 2.1 and 3.1 we have

$$\partial_{0t_{j+1}}^{\alpha} u = \Delta_{0t_{j+\sigma}}^{\alpha} u + \mathcal{O}(\tau^{3-\alpha})$$

$$\mathcal{L}u(x,t)|_{(x_i,t_{i+1})} = \Lambda u(x_i,t_{j+1}) + \mathcal{O}(h^2),$$

where the difference operator Λ is defined as follows

$$(\Lambda y)_i = ((ay_{\bar{x}})_x - dy)_i = \frac{a_{i+1}y_{i+1} - (a_{i+1} + a_i)y_i + a_iy_{i-1}}{h^2} - d_iy_i,$$
$$y_{\bar{x},i} = \frac{y_i - y_{i-1}}{h}, \quad y_{x,i} = \frac{y_{i+1} - y_i}{h},$$

with the coefficients $a_i^{j+1} = k(x_{i-1/2}, t_{j+1}), \ d_i^{j+1} = q(x_i, t_{j+1}).$ Let $\varphi_i^{j+1} = f(x_i, t_{j+1}),$ then we get the difference scheme with the approximation order $\mathcal{O}(h^2 + \tau^{3-\alpha})$:

$$\Delta_{0t_{j+1}}^{\alpha} y_i = \Lambda y_i^{j+1} + \varphi_i^{j+1}, \quad i = 1, 2, \dots, N-1, \quad j = 1, 2, \dots, M-1, \tag{25}$$

$$y(0,t) = 0, \quad y(l,t) = 0, \quad t \in \overline{\omega}_{\tau}, \quad y(x,0) = u_0(x), \quad x \in \overline{\omega}_h,$$
 (26)

Remark. We assume that the solution y_i^1 is found with the order of accuracy $\mathcal{O}(h^4 + \tau^{3-\alpha})$. For example, we can use L1-formula and solve problem (1.2)-(1.4) on the time layer $[0,\tau]$ with step $\tau_1 = \mathcal{O}(\tau^{\frac{3-\alpha}{2-\alpha}})$.

3.2. Stability and convergence

Theorem 3.1. The difference scheme (25)–(26) is unconditionally stable and its solution meets the following a priori estimates:

$$\sum_{j=1}^{M-1} \left(\|y^{j+1}\|_0^2 + \|y_{\bar{x}}^{j+1}\|_0^2 \right) \tau \le M_1 \left(\|y^1\|_0^2 + \|y^0\|_0^2 + \sum_{j=1}^{M-1} \|\varphi^{j+1}\|_0^2 \tau \right), \tag{27}$$

where $||y||_0^2 = \sum_{i=1}^N y_i^2 h$, $M_1 > 0$ is a known number independent of h and τ .

Proof. Taking the inner product of the equation (25) with y^{j+1} , we have

$$\left(y^{j+1}, \Delta_{0t_{j+1}}^{\alpha} y\right) - \left(y^{j+1}, \Lambda y^{j+1}\right) = \left(y^{j+1}, \varphi^{j+1}\right). \tag{28}$$

Using Lemma 2.6, we obtain

$$\left(y^{j+1}, \Delta_{0t_{j+1}}^{\alpha} y \right) \ge \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left(E_{j+1} - E_j \right) + \frac{1}{2} \bar{\Delta}_{0t_{j+1}}^{\alpha} ||y||_0^2$$

$$= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left(\mathcal{E}_{j+1} - \mathcal{E}_j \right) - \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)} \bar{c}_j^{(\alpha)} ||y^0||_0^2, \quad j = 1, 2, \dots, M-1,$$

where

$$E_{j} = \left(\frac{1}{2}\sqrt{\frac{c_{0}^{(\alpha)} - c_{1}^{(\alpha)}}{2}} + \frac{1}{2}\sqrt{\frac{c_{0}^{(\alpha)} + 3c_{1}^{(\alpha)} - 4c_{2}^{(\alpha)}}{2}}\right)^{2} \|y^{j}\|_{0}^{2}$$

$$+ \left\| \sqrt{\frac{c_0^{(\alpha)} - c_1^{(\alpha)}}{2}} y^j - \left(\frac{1}{2} \sqrt{\frac{c_0^{(\alpha)} - c_1^{(\alpha)}}{2}} + \frac{1}{2} \sqrt{\frac{c_0^{(\alpha)} + 3c_1^{(\alpha)} - 4c_2^{(\alpha)}}{2}} \right) y^{j-1} \right\|_0^2.$$

$$\mathcal{E}_j = E_j + \frac{1}{2} \sum_{s=0}^{j-1} \bar{c}_{j-1-s}^{(\alpha)} \|y^{s+1}\|_0^2.$$

For the difference operator Λ using Green's first difference formula for the functions vanishing at x = 0 and x = l, we get $(-\Lambda y, y) \ge c_1 ||y_{\bar{x}}||_0^2$.

From (28), using that

$$\left(y^{j+1},\varphi^{j+1}\right) \leq \frac{c_1}{l^2} \|y^{j+1}\|_0^2 + \frac{l^2}{4c_1} \|\varphi^{j+1}\|_0^2 \leq \frac{c_1}{2} \|y_{\bar{x}}^{j+1}]|_0^2 + \frac{l^2}{4c_1} \|\varphi^{j+1}\|_0^2,$$

one obtains the inequality

$$\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left(\mathcal{E}_{j+1} - \mathcal{E}_j \right) + \frac{c_1}{2} \|y_{\bar{x}}^{j+1}\|_0^2 \le \frac{l^2}{4c_1} \|\varphi^{j+1}\|_0^2 + \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)} \bar{c}_j^{(\alpha)} \|y^0\|_0^2. \tag{29}$$

Multiplying inequality (29) by τ and summing the resulting relation over j from 1 to M-1 and taking into account inequality (17), one obtains a priori estimate (27).

The stability and convergence of the difference scheme (25) - (26) follow from the a priori estimate (27).

3.3. Numerical results

Numerical computations are executed for a test problem on the assumption that the function

$$u(x,t) = \sin(\pi x) (t^{3+\alpha} + t^2 + 1)$$

is the exact solution of problem (1)–(2) with the coefficients $k(x,t) = 2 - \cos(xt)$, $q(x,t) = 1 - \sin(xt)$ and l = 1, T = 1.

The errors (z = y - u) and convergence order (CO) in the norms $\|\cdot\|_0$ and $\|\cdot\|_{\mathcal{C}(\bar{\omega}_{h\tau})}$, where $\|y\|_{\mathcal{C}(\bar{\omega}_{h\tau})} = \max_{(x_i,t_j)\in\bar{\omega}_{h\tau}} |y|$, are given in Table 1.

Table 1 demonstrates that as the number of the spatial subintervals and time steps increases, while $h^2 = \tau^{3-\alpha}$, then the maximum error decreases, as it is expected and the convergence order of the approximate scheme is $\mathcal{O}(h^2) = \mathcal{O}(\tau^{3-\alpha})$, where the convergence order is given by the formula: CO= $\log_{\frac{h_1}{h_2}} \frac{||z_1||}{||z_2||}$ (z_i is the error corresponding to h_i).

Table 2 shows that if h = 1/50000, then as the number of time steps of our approximate scheme increases, then the maximum error decreases, as it is expected and the convergence order of time is $\mathcal{O}(\tau^{3-\alpha})$, where the convergence order is given by the following formula: $CO = \log_{\frac{\tau_1}{\tau_2}} \frac{\|z_1\|}{\|z_2\|}$.

4. A compact difference scheme for the time fractional diffusion equation

In this section for problem (1)–(2), we create a compact difference scheme with the approximation order $\mathcal{O}(h^4 + \tau^{3-\alpha})$ in the case when k = k(t) and q = q(t). The stability and convergence of the constructed difference scheme in the grid L_2 - norm with the rate equal to the order of the approximation error are proved. The found results are supported by the numerical calculations implemented for a test example.

Table 1: The error and the convergence order in the norms $\|\cdot\|_0$ and $\|\cdot\|_{C(\bar{\omega}_{h\tau})}$ when decreasing time-grid size for different values of $\alpha = 0.1; 0.5; 0.9, \tau^{3-\alpha} = h^2$.

α	au	h	$\max_{0 \le j \le M} \ z^j\ _0$	CO	$\max_{0 \le j \le M} \ z^j\ _{C(\bar{\omega}_{h\tau})}$	СО	$\max_{0 \le j \le M} \ z_{\bar{x}}^j\ _0$	CO
0.1	1/10	1/29	1.694597e-3		2.387728e-3		5.341255e-2	
	1/20	1/78	2.343539e-4	2.8541	3.304157e-4	2.8533	7.389758e-4	2.8536
	1/40	1/211	3.204204 e-5	2.8707	4.517782e-5	2.8706	1.010417e-4	2.8706
	1/80	1/575	4.316975e-6	2.8918	6.086836e-6	2.8919	1.361321e-5	2.8919
	1/160	1/1571	5.786215e-7	2.8993	8.158422e-7	2.8993	1.824621e-6	2.8993
0.5	1/10	1/18	4.556026e-3		6.401088e-3		1.434106e-2	
	1/20	1/43	8.011052e-4	2.5077	1.129064e-3	2.5032	2.524196e-3	2.5063
	1/40	1/101	1.452643e-4	2.4633	2.047995e-4	2.4628	4.577935e-4	2.4630
	1/80	1/240	2.575571e-5	2.4957	3.631166e-5	2.4957	8.116952e-5	2.4956
	1/160	1/570	4.568945e-6	2.4950	6.441587e-6	2.4949	1.439907e-5	2.4950
0.9	1/10	1/12	1.181474e-2		1.662948e-2		3.707516e-2	
	1/20	1/24	2.931153e-3	2.0110	4.125467e-3	2.0111	9.218339e-3	2.0078
	1/40	1/49	7.018065e-4	2.0623	9.891705e-4	2.0603	2.208378e-3	2.0615
	1/80	1/100	1.678681e-4	2.0637	2.367034e-4	2.0631	5.283157e-4	2.0635
	1/160	1/207	3.921292e-5	2.0979	5.529153e-5	2.0979	1.234141e-4	2.0979

Table 2: The error and the convergence order in the norms $\|\cdot\|_0$ and $\|\cdot\|_{C(\bar{\omega}_{h\tau})}$ when decreasing time-grid size for different values of $\alpha = 0.3; 0.5; 0.7, h = 1/50000.$

400 01 0	6.00 of 4 = 0.0, 0.0, 0.1, h = 1/00000.									
α	au	$\max_{0 \le j \le M} \ z^j\ _0$	CO	$\max_{0 \le j \le M} \ z^j\ _{C(\bar{\omega}_{h\tau})}$	СО	$\max_{0 \le j \le M} \ z_{\bar{x}}^j] _0$	CO			
0.3	1/10	7.281556e-5		1.036431e-4		2.293180e-4				
	1/20	1.202886e-5	2.5977	1.712493e-5	2.5974	3.787942e-5	2.5978			
	1/40	1.881330e-6	2.6766	2.674734e-6	2.6786	5.928309e-6	2.6757			
	1/80	2.908398e-7	2.6934	4.140875e-7	2.6914	9.159351e-7	2.6943			
0.5	1/10	2.726395e-4		3.880588e-4		8.586014e-4				
	1/20	5.051848e-5	2.4321	7.190513e-5	2.4321	1.590939e-4	2.4321			
	1/40	9.152847e-6	2.4645	1.302443e-5	2.4648	2.882759e-5	2.4643			
	1/80	1.623335e-6	2.4952	2.310709e-6	2.4948	5.112271e-6	2.4954			
0.7	1/10	8.556143e-4		1.217803e-3		2.694425e-3				
	1/20	1.810137e-4	2.2408	2.576392e-4	2.2408	5.700338e-4	2.2408			
	1/40	3.759528e-5	2.2674	5.351332e-5	2.2673	1.183890e-4	2.2675			
	1/80	7.685019e-6	2.2904	1.093830e-5	2.2905	2.420107e-5	2.2903			

4.1. Derivation of the difference scheme

Let a difference scheme be put into a correspondence with differential problem (1)–(2) in the case when k = k(t) and q = q(t):

$$\Delta_{0t_{j+1}}^{\alpha} \mathcal{H}_h y_i = a^{j+1} y_{\bar{x}x,i}^{j+1} - d^{j+1} \mathcal{H}_h y_i^{j+1} + \mathcal{H}_h \varphi_i^{j+1}, \ i = 1, \dots, N-1, \ j = 0, 1, \dots, M-1,$$
 (30)

$$y(0,t) = 0, \quad y(l,t) = 0, \quad t \in \overline{\omega}_{\tau}, \quad y(x,0) = u_0(x), \quad x \in \overline{\omega}_h,$$
 (31)

where $\mathcal{H}_h v_i = v_i + h^2 v_{\bar{x}x,i}/12$, $i = 1, \dots, N-1$, $a^{j+1} = k(t_{j+1})$, $d^{j+1} = q(t_{j+1})$, $\varphi_i^{j+1} = f(x_i, t_{j+1})$. From Lemma 2.1 it follows that if $u \in \mathcal{C}_{x,t}^{6,3}$, then the difference scheme has the approximation order $\mathcal{O}(\tau^{3-\alpha} + h^4)$.

4.2. Stability and convergence

Theorem 4.1. The difference scheme (30)–(31) is unconditionally stable and its solution meets the following a priori estimate:

$$\sum_{j=1}^{M-1} \left(\|\mathcal{H}_h y^{j+1}\|_0^2 + \|y_{\bar{x}}^{j+1}\|_0^2 \right) \tau \le M_2 \left(\|\mathcal{H}_h y^1\|_0^2 + \|\mathcal{H}_h y^0\|_0^2 + \sum_{j=1}^{M-1} \|\mathcal{H}_h \varphi^{j+1}\|_0^2 \tau \right), \tag{32}$$

where $M_2 > 0$ is a known number independent of h and τ .

Proof. Taking the inner product of the equation (30) with $\mathcal{H}_h y^{j+1} = (\mathcal{H}_h y)^{j+1}$, we have

$$(\mathcal{H}_h y^{j+1}, \Delta_{0t_{j+1}}^{\alpha} \mathcal{H}_h y) - a^{j+1} (\mathcal{H}_h y^{j+1}, y_{\bar{x}x}^{j+1})$$

$$+d^{j+1}(\mathcal{H}_h y^{j+1}, \mathcal{H}_h y^{j+1}) = (\mathcal{H}_h y^{j+1}, \mathcal{H}_h \varphi^{j+1}). \tag{33}$$

We transform the terms in identity (33) as

$$(\mathcal{H}_{h}y^{j+1}, \Delta_{0t_{j+1}}^{\alpha}\mathcal{H}_{h}y) \geq \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} (E_{j+1} - E_{j}) + \frac{1}{2} \bar{\Delta}_{0t_{j+\alpha}}^{\alpha} \|\mathcal{H}_{h}y\|_{0}^{2} =$$

$$= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} (\mathcal{E}_{j+1} - \mathcal{E}_{j}) - \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)} \bar{c}_{j}^{(\alpha)} \|\mathcal{H}_{h}y^{0}\|_{0}^{2}, \quad j = 1, 2, \dots, M-1,$$

where

$$\begin{split} E_{j} &= \left(\frac{1}{2}\sqrt{\frac{c_{0}^{(\alpha)} - c_{1}^{(\alpha)}}{2}} + \frac{1}{2}\sqrt{\frac{c_{0}^{(\alpha)} + 3c_{1}^{(\alpha)} - 4c_{2}^{(\alpha)}}{2}}\right)^{2} \|\mathcal{H}_{h}y^{j}\|_{0}^{2} \\ &+ \left\|\sqrt{\frac{c_{0}^{(\alpha)} - c_{1}^{(\alpha)}}{2}} \mathcal{H}_{h}y^{j} - \left(\frac{1}{2}\sqrt{\frac{c_{0}^{(\alpha)} - c_{1}^{(\alpha)}}{2}} + \frac{1}{2}\sqrt{\frac{c_{0}^{(\alpha)} + 3c_{1}^{(\alpha)} - 4c_{2}^{(\alpha)}}{2}}\right) \mathcal{H}_{h}y^{j-1}\right\|_{0}^{2}, \\ &\mathcal{E}_{j} = E_{j} + \frac{1}{2}\sum_{s=0}^{j-1} \bar{c}_{j-1-s}^{(\alpha)} \|\mathcal{H}_{h}y^{s+1}\|_{0}^{2}. \\ &- (\mathcal{H}_{h}y^{j+1}, y_{\bar{x}x}^{j+1}) = -(y^{j+1}, y_{\bar{x}x}^{j+1}) - \frac{h^{2}}{12}\|y_{\bar{x}x}^{j+1}\|_{0}^{2} = \|y_{\bar{x}}^{j+1}\|_{0}^{2} - \frac{1}{12}\sum_{i=1}^{N-1} (y_{\bar{x},i+1}^{j+1} - y_{\bar{x},i}^{j+1})^{2}h \\ &\geq \|y_{\bar{x}}^{j+1}\|_{0}^{2} - \frac{1}{3}\|y_{\bar{x}}^{j+1}\|_{0}^{2} = \frac{2}{3}\|y_{\bar{x}}^{j+1}\|_{0}^{2}, \\ &(\mathcal{H}_{h}y^{j+1}, \mathcal{H}_{h}\varphi^{j+1}) \leq \varepsilon \|\mathcal{H}_{h}y^{j+1}\|_{0}^{2} + \frac{1}{4\varepsilon}\|\mathcal{H}_{h}\varphi^{j+1}\|_{0}^{2} \\ &= \varepsilon \sum_{i=1}^{N-1} \left(\frac{y_{i-1}^{j+1} + 10y_{i}^{j+1} + y_{i+1}^{j+1}}{12}\right)^{2}h + \frac{1}{4\varepsilon}\|\mathcal{H}_{h}\varphi^{j+1}\|_{0}^{2} \\ &\leq \varepsilon \|y^{j+1}\|_{0}^{2} + \frac{1}{4\varepsilon}\|\mathcal{H}_{h}\varphi^{j+1}\|_{0}^{2} \leq \frac{\varepsilon l^{2}}{2}\|y_{\bar{x}}^{j+1}\|_{0}^{2} + \frac{1}{4\varepsilon}\|\mathcal{H}_{h}\varphi^{j+1}\|_{0}^{2}. \end{split}$$

In view of the above-performed transformations, from identity (33) at $\varepsilon = \frac{c_1}{3l^2}$ we get the inequality

$$\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left(\mathcal{E}_{j+1} - \mathcal{E}_{j} \right) + \frac{c_{1}}{2} \|y_{\bar{x}}^{j+1}\|_{0}^{2} \leq \frac{3l^{2}}{4c_{1}} \|\mathcal{H}_{h}\varphi^{j+1}\|_{0}^{2} + \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)} \bar{c}_{j}^{(\alpha)} \|\mathcal{H}_{h}y^{0}\|_{0}^{2}.$$

The following process is similar to the proof of Theorem 3.1, and we leave it out.

The norm $\|\mathcal{H}_h y\|_0$ is equivalent to the norm $\|y\|_0$, which follows from the inequalities

$$\frac{5}{12} \|y\|_0^2 \le \|\mathcal{H}_h y\|_0^2 \le \|y\|_0^2.$$

Using a priori estimate (32), we obtain the convergence result.

Theorem 4.2. Let $u(x,t) \in C_{x,t}^{6,3}$ be the solution of problem (1)–(2) in the case k = k(t), q = q(t), and let $\{y_i^j \mid 0 \le i \le N, 1 \le j \le M\}$ be the solution of difference scheme (30)–(31). Then it holds true that

$$\sqrt{\sum_{j=1}^{M-1} \left(\|z^{j+1}\|_0^2 + \|z_{\bar{x}}^{j+1}\|_0^2 \right) \tau} \le C_R \left(\tau^{3-\alpha} + h^4 \right), \quad 1 \le j \le M,$$

where $z_i^j = u(x_i, t_j) - y_i^j$ and C_R is a positive constant independent of τ and h.

4.3. Numerical results

Numerical calculations are performed for a test problem when the function

$$u(x,t) = \sin(\pi x) (t^{3+\alpha} + t^2 + 1)$$

is the exact solution of the problem (1)–(2) with the coefficients $k(x,t) = 2 - \cos(t)$, $q(x,t) = 1 - \sin(t)$ and l = 1, T = 1.

The errors (z = y - u) and convergence order (CO) in the norms $\|\cdot\|_0$ and $\|\cdot\|_{\mathcal{C}(\bar{\omega}_{h\tau})}$, where $\|y\|_{\mathcal{C}(\bar{\omega}_{h\tau})} = \max_{(x_i,t_j)\in\bar{\omega}_{h\tau}} |y|$, are given in Table 1.

Table 3 shows that as the number of the spatial subintervals and time steps increases keeping $h^4 = \tau^{3-\alpha}$, the maximum error decreases, as it is expected and the convergence order of the compact difference scheme is $\mathcal{O}(h^2) = \mathcal{O}(\tau^{3-\alpha})$, where the convergence order is given by the formula: CO= $\log_{\frac{h_1}{h_2}} \frac{\|z_1\|}{\|z_2\|}$ (z_i is the error corresponding to h_i).

Table 4 demonstrates that if h = 1/2000, then as the number of time steps of our approximate scheme increases, then the maximum error decreases, as it is expected and the convergence order of time is $\mathcal{O}(\tau^{3-\alpha})$, where the convergence order is given by the following formula: $CO = \log_{\frac{\tau_1}{\tau_2}} \frac{\|z_1\|}{\|z_2\|}$.

5. Conclusion

In the current paper we construct a L2 type difference approximation of the Caputo fractional derivative with the approximation order $\mathcal{O}(\tau^{3-\alpha})$. The fundamental features of this difference operator are studied. New difference schemes of the second and fourth approximation order in space and the $3-\alpha$ approximation order in time for the time fractional diffusion equation with variable coefficients are also constructed. The stability and convergence of these schemes with the rate equal to the order of the approximation error are proved. The method can be without difficulty expanded to include other time fractional partial differential equations with other boundary conditions.

Numerical tests entirely corroborating the found theoretical results are implemented. In all the calculations Julia v1.5.1 is used.

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Table 3: The error and the convergence order in the norms $\|\cdot\|_0$ and $\|\cdot\|_{C(\bar{\omega}_{h\tau})}$ when decreasing time-grid size for different values of $\alpha = 0.1; 0.5; 0.9, \tau^{3-\alpha} = (h/2)^4$.

α	au	h	$\max_{0 \le j \le M} \ z^j\ _0$	CO	$\max_{0 \le j \le M} \ z^j\ _{C(\bar{\omega}_{h\tau})}$	CO	$\max_{0 \le j \le M} \ z_{\bar{x}}^j _0$	CO
0.1	1/40	1/29	1.321499e-6		1.866140e-6		4.149581e-6	
	1/80	1/47	1.912169e-7	2.7889	2.702706e-7	2.7875	6.006140e-7	2.7884
	1/160	1/79	2.443382e-8	2.9683	3.454781e-8	2.9677	7.675607e-8	2.9680
	1/320	1/131	3.267337e-9	2.9027	4.620380e-9	2.9025	1.026439e-8	2.9026
	1/640	1/217	4.395804e-10	2.8939	6.216471e-10	2.8938	1.380970e-9	2.8939
0.5	1/40	1/21	1.178052e-5		1.661359e-5		3.697512e-5	
	1/80	1/31	2.241843e-6	2.3936	3.166375e-6	2.3914	7.039944e-6	2.3929
	1/160	1/47	4.096169e-7	2.4523	5.789623e-7	2.4512	1.286610e-6	2.4519
	1/320	1/73	7.195323e-8	2.5091	1.017336e-7	2.5086	2.260303e-7	2.5089
	1/640	1/113	1.268803e-8	2.5036	1.794185e-8	2.5034	3.985934e-8	2.5035
0.9	1/40	1/13	1.470087e-4		2.063859e-4		4.607185e-4	
	1/80	1/19	3.419750e-5	2.1039	4.819739e-5	2.0983	1.073122e-4	2.1020
	1/160	1/29	7.726281e-6	2.1460	1.091058e-5	2.1432	2.426096e-5	2.1451
	1/320	1/41	1.824394e-6	2.0823	2.578190e-6	2.0812	5.730103e-6	2.0820
	1/640	1/59	4.260141e-7	2.0984	6.022614e-7	2.0978	1.338204e-6	2.0982

Table 4: The error and the convergence order in the norms $\|\cdot\|_0$ and $\|\cdot\|_{C(\bar{\omega}_{h\tau})}$ when decreasing time-grid size for different values of $\alpha = 0.3; 0.5; 0.7, h = 1/1000$.

α	au	$\max_{0 \le j \le M} \ z^j\ _0$	CO	$\max_{0 \le j \le M} \ z^j\ _{C(\bar{\omega}_{h\tau})}$	CO	$\max_{0 \le j \le M} \ z_{\bar{x}}^j\ _0$	CO
0.3	1/10	6.155178e-5		8.704736e-5		1.933705e-4	
	1/20	1.016170e-5	2.5986	1.437081e-5	2.5986	3.192392e-5	2.5986
	1/40	1.642526e-6	2.6291	2.322883e-6	2.6291	5.160147e-6	2.6291
	1/80	2.620773e-7	2.6478	3.706331e-7	2.6478	8.233399e-7	2.6478
	1/160	4.147475e-8	2.6596	5.865421e-8	2.6596	1.302967e-7	2.6596
0.5	1/10	2.308509e-4		3.264725e-4		7.252393e-4	
	1/20	4.277465e-5	2.4321	6.049249e-5	2.4321	1.343804e-4	2.4321
	1/40	7.775493e-6	2.4597	1.099620e-5	2.4597	2.442742e-5	2.4597
	1/80	1.398769e-6	2.4747	1.978159e-6	2.4747	4.394362e-6	2.4747
	1/160	2.500909e-6	2.4836	3.536819e-7	2.4836	7.856834e-7	2.4836
0.7	1/10	7.275485e-4		1.028909e-3		2.285660e-3	
	1/20	1.539001e-4	2.2410	2.176477e-4	2.2410	4.834914e-4	2.2410
	1/40	3.192728e-5	2.2691	4.515200 e-5	2.2691	1.003024e-4	2.2691
	1/80	6.558744e-6	2.2832	9.275465e-6	2.2832	2.060489e-5	2.2832
	1/160	1.340380e-6	2.2907	1.895584e-6	2.2907	4.210928e-6	2.2907

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