



A new difference scheme for the time fractional diffusion equation

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ABSTRACT

In this paper we construct a new difference analog of the Caputo fractional derivative (called the L_2 -1 $_{\sigma}$ formula). The basic properties of this difference operator are investigated and on its basis some difference schemes generating approximations of the second and fourth order in space and the second order in time for the time fractional diffusion equation with variable coefficients are considered. Stability of the suggested schemes and also their convergence in the grid L_2 -norm with the rate equal to the order of the approximation error are proved. The obtained results are supported by the numerical calculations carried out for some test problems.

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1. Introduction

Recently a noticeable growth of the attention of researches to the fractional differential equations has been observed. It is caused by numerous effective applications of fractional calculation to various areas of science and engineering [1–6]. For example, mathematical language of fractional derivatives is irreplaceable for the description of the physical process of statistical transfer and, as it is known, leads to diffusion equations of fractional orders [7,8].

Consider the time fractional diffusion equation with variable coefficients

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

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

where

$$\partial_{0t}^{\alpha} u(x, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x, \eta)}{\partial \eta} (t-\eta)^{-\alpha} d\eta, \quad 0 < \alpha < 1 \quad (3)$$

is the Caputo derivative of the order α ,

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

$k(x, t) \geq c_1 > 0$, $q(x, t) \geq 0$ and $f(x, t)$ are sufficiently smooth functions.

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The time fractional diffusion equation represents a linear integro-differential equation. Its solution not always can be found analytically; therefore it is necessary to use numerical methods. However, unlike the classical case, we require information about all the previous time layers, when numerically approximating a time fractional diffusion equation on a certain time layer. For that reason algorithms for solving the time fractional diffusion equations are rather time-consuming even in one-dimensional case. Upon transition to two-dimensional and three-dimensional problems their complexity considerably increases. In this regard constructing stable differential schemes of higher order approximation is a very important task.

A widespread difference approximation of fractional derivative (3) is the so-called $L1$ method [2,9] which is defined as follows

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

where $0 = t_0 < t_1 < \dots < t_{j+1}$, and r^{j+1} is the local truncation error. In the case of the uniform mesh, $\tau = t_{s+1} - t_s$, for all $s = 0, 1, \dots, j+1$, it was proved that $r^{j+1} = \mathcal{O}(\tau^{2-\alpha})$ [10–12]. The $L1$ method has been widely used for solving the fractional differential equations with Caputo derivatives [10–16].

Difference schemes of the increased order of approximation such as the compact difference scheme [14,17–19] and spectral method [11,20,21] were applied to improve the spatial accuracy of fractional diffusion equations. However, it is rather difficult to get a high-order time approximation due to the singularity of fractional derivatives.

A good approximation of the $L1$ method is observed in case of a nonuniform mesh, when it is refined in a neighborhood of the point t_{j+1} [9]. Though the nonuniform mesh turns out to be more effective in comparison with the uniform one, it does not generate the second order of approximation in all points of the mesh.

In [22] a new difference analog of the Caputo fractional derivative with the order of approximation $\mathcal{O}(\tau^{3-\alpha})$, called $L1-2$ formula, is constructed. On the basis of this formula calculations of difference schemes for the time-fractional sub-diffusion equations in bounded and unbounded spatial domains and the fractional ODEs are carried out. If the stability and convergence of difference schemes from [22] will be strictly proved, then this will undoubtedly be a significant progress in computing the time-fractional partial differential equations.

Using the energy inequality method, a priori estimates for the solution of the Dirichlet and Robin boundary value problems for the diffusion-wave equation with Caputo fractional derivative have been obtained in [15,23].

In this paper a new difference analog of the fractional Caputo derivative with the order of approximation $\mathcal{O}(\tau^{3-\alpha})$ for each $\alpha \in (0, 1)$ is constructed. Properties of the obtained difference operator are studied. Difference schemes of the second and fourth order of approximation in space and the second order in time for the time fractional diffusion equation with variable coefficients are constructed. Using the method of energy inequalities, the stability and convergence of these schemes in the mesh L_2 -norm are proved. Numerical calculations of some test problems confirming reliability of the obtained results are carried out.

2. Family of difference schemes. Stability and convergence

In this section, families of difference schemes in a general form set on a non-uniform time mesh are investigated. A criterion of the stability of the difference schemes in the mesh L_2 -norm is obtained. The convergence of solutions of the difference schemes to the solution of the corresponding differential problem with the rate equal to the order of the approximation error is proved.

2.1. Family of difference schemes

In the rectangle $\bar{Q}_T = \{(x, t) : 0 \leq x \leq l, 0 \leq t \leq T\}$ we introduce the mesh $\bar{\omega}_{h\tau} = \bar{\omega}_h \times \bar{\omega}_\tau$, where $\bar{\omega}_h = \{x_i = ih, i = 0, 1, \dots, N; hN = l\}$, $\bar{\omega}_\tau = \{t_j : 0 = t_0 < t_1 < t_2 < \dots < t_{M-1} < t_M = T\}$.

Basically the family of difference schemes, approximating problem (1)–(2) on the mesh $\bar{\omega}_{h\tau}$, has the form

$$g \Delta_{0t_{j+1}}^\alpha y_i = \Lambda y_i^{(\sigma_{j+1})} + \varphi_i^{j+1}, \quad i = 1, 2, \dots, N-1, \quad j = 0, 1, \dots, M-1, \quad (5)$$

$$y(0, t) = 0, \quad y(l, t) = 0, \quad t \in \bar{\omega}_\tau, \quad y(x, 0) = u_0(x), \quad x \in \bar{\omega}_h, \quad (6)$$

where

$$g \Delta_{0t_{j+1}}^\alpha y_i = \sum_{s=0}^j (y_i^{s+1} - y_i^s) g_s^{j+1}, \quad g_s^{j+1} > 0, \quad (7)$$

is a difference analog of the Caputo derivative of the order α ($0 < \alpha < 1$), Λ is a difference operator approximating the continuous operator \mathcal{L} , such that the operator $-\Lambda$ preserves its positive definiteness ($(-\Lambda y, y) \geq \kappa \|y\|^2$, $\kappa > 0$), for example

$$(\Lambda y)_i = ((ay_{\bar{x}})_x - dy)_i = \frac{a_{i+1}y_{i+1} - (a_{i+1} + a_i)y_i + a_iy_{i-1}}{h^2} - d_iy_i, \quad (8)$$

a , d and φ are the mesh functions approximating k , q and f , respectively, $y^{(\sigma_{j+1})} = \sigma_{j+1}y^{j+1} + (1 - \sigma_{j+1})y^j$, $0 \leq \sigma_{j+1} \leq 1$, at $j = 0, 1, \dots, M-1$, $y_{\bar{x},i} = (y_i - y_{i-1})/h$, $y_{x,i} = (y_{i+1} - y_i)/h$.

2.2. Stability and convergence

Lemma 1. If $g_j^{j+1} > g_{j-1}^{j+1} > \dots > g_0^{j+1} > 0$, $j = 0, 1, \dots, M-1$ then for any function $v(t)$ defined on the mesh $\bar{\omega}_\tau$ one has the inequalities

$$v^{j+1} g \Delta_{0t}^\alpha v \geq \frac{1}{2} g \Delta_{0t}^\alpha (v^2) + \frac{1}{2g_j^{j+1}} (g \Delta_{0t}^\alpha v)^2, \quad (9)$$

$$v^j g \Delta_{0t}^\alpha v \geq \frac{1}{2} g \Delta_{0t}^\alpha (v^2) - \frac{1}{2(g_j^{j+1} - g_{j-1}^{j+1})} (g \Delta_{0t}^\alpha v)^2, \quad (10)$$

where $g_{-1}^1 = 0$.

Proof. Let us consider the difference

$$\begin{aligned} & v^{j+1} g \Delta_{0t}^\alpha v - \frac{1}{2} g \Delta_{0t}^\alpha (v^2) \\ &= v^{j+1} \sum_{s=0}^j g_s^{j+1} (v^{s+1} - v^s) - \sum_{s=0}^j g_s^{j+1} (v^{s+1} - v^s) \left(\frac{v^{s+1} + v^s}{2} \right) \\ &= \sum_{s=0}^j g_s^{j+1} (v^{s+1} - v^s) \left(v^{j+1} - \frac{v^{s+1} + v^s}{2} \right) \\ &= \sum_{s=0}^j g_s^{j+1} (v^{s+1} - v^s) \left(\frac{1}{2} (v^{s+1} - v^s) + \sum_{k=s+1}^j (v^{k+1} - v^k) \right) \\ &= \frac{1}{2} \sum_{s=0}^j g_s^{j+1} (v^{s+1} - v^s)^2 + \sum_{k=1}^j (v^{k+1} - v^k) \sum_{s=0}^{k-1} g_s^{j+1} (v^{s+1} - v^s). \end{aligned} \quad (11)$$

Here we consider the sums to be equal to zero if the upper summation index is less than the lower one.

Let us introduce the following notation: $\sum_{s=0}^k g_s^{j+1} (v^{s+1} - v^s) = w^{k+1}$, then $v^1 - v^0 = (g_0^{j+1})^{-1} w^1$, $v^{k+1} - v^k = (g_k^{j+1})^{-1} (w^{k+1} - w^k)$, $k = 1, 2, \dots, j$, and rewrite the equality (11) as

$$\begin{aligned} & \frac{1}{2} (g_0^{j+1})^{-1} (w^1)^2 + \frac{1}{2} \sum_{k=1}^j (g_k^{j+1})^{-1} (w^{k+1} - w^k)^2 + \sum_{k=1}^j (g_k^{j+1})^{-1} (w^{k+1} - w^k) w^k \\ &= \frac{1}{2} (g_0^{j+1})^{-1} (w^1)^2 + \frac{1}{2} \sum_{k=1}^j (g_k^{j+1})^{-1} ((w^{k+1})^2 - (w^k)^2) \\ &= \frac{1}{2} (g_j^{j+1})^{-1} (w^{j+1})^2 + \frac{1}{2} \sum_{k=0}^{j-1} \frac{g_{k+1}^{j+1} - g_k^{j+1}}{g_{k+1}^{j+1} g_k^{j+1}} (w^{k+1})^2 \geq \frac{1}{2} (g_j^{j+1})^{-1} (w^{j+1})^2, \end{aligned}$$

which is valid since $g_{k+1}^{j+1} - g_k^{j+1} > 0$, $k = 0, 1, \dots, j-1$.

Let us prove now the inequality (10). Since $v^j = v^{j+1} - (v^{j+1} - v^j)$, one obtains

$$\begin{aligned} & v^j g \Delta_{0t}^\alpha v - \frac{1}{2} g \Delta_{0t}^\alpha (v^2) + \frac{1}{2(g_j^{j+1} - g_{j-1}^{j+1})} (g \Delta_{0t}^\alpha v)^2 \\ &= v^{j+1} g \Delta_{0t}^\alpha v - \frac{1}{2} g \Delta_{0t}^\alpha (v^2) + \frac{1}{2(g_j^{j+1} - g_{j-1}^{j+1})} (g \Delta_{0t}^\alpha v)^2 - (v^{j+1} - v^j) g \Delta_{0t}^\alpha v \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2}(g_j^{j+1})^{-1}(w^{j+1})^2 + \frac{1}{2} \sum_{k=0}^{j-1} \frac{g_{k+1}^{j+1} - g_k^{j+1}}{g_{k+1}^{j+1} g_k^{j+1}} (w^{k+1})^2 \\
&\quad + \frac{1}{2(g_j^{j+1} - g_{j-1}^{j+1})} (w^{j+1})^2 - (g_j^{j+1})^{-1} (w^{j+1} - w^j) w^{j+1} \\
&= \frac{g_{j-1}^{j+1}}{2g_j^{j+1} (g_j^{j+1} - g_{j-1}^{j+1})} \left(w^{j+1} + \frac{g_j^{j+1} - g_{j-1}^{j+1}}{g_{j-1}^{j+1}} w^j \right)^2 + \frac{1}{2} \sum_{k=0}^{j-2} \frac{g_{k+1}^{j+1} - g_k^{j+1}}{g_{k+1}^{j+1} g_k^{j+1}} (w^{k+1})^2 \geq 0.
\end{aligned}$$

The proof of Lemma 1 is completed. \square

Corollary 1. If $g_j^{j+1} > g_{j-1}^{j+1} > \dots > g_0^{j+1} > 0$ and $\frac{g_j^{j+1}}{2g_j^{j+1} - g_{j-1}^{j+1}} \leq \sigma_{j+1} \leq 1$, where $j = 0, 1, \dots, M-1$, $g_{-1}^1 = 0$, then for any function $v(t)$ defined on the mesh $\bar{\omega}_\tau$ one has the inequality

$$(\sigma_{j+1} v^{j+1} + (1 - \sigma_{j+1}) v^j)_g \Delta_{0t_{j+1}}^\alpha v \geq \frac{1}{2} g \Delta_{0t_{j+1}}^\alpha (v^2). \quad (12)$$

Theorem 1. If

$$g_j^{j+1} > g_{j-1}^{j+1} > \dots > g_0^{j+1} \geq c_2 > 0, \quad \frac{g_j^{j+1}}{2g_j^{j+1} - g_{j-1}^{j+1}} \leq \sigma_{j+1} \leq 1,$$

where $j = 0, 1, \dots, M-1$, $g_{-1}^1 = 0$, then the difference scheme (5)–(6) is unconditionally stable and its solution satisfies the following a priori estimate:

$$\|y^{j+1}\|_0^2 \leq \|y^0\|_0^2 + \frac{1}{2\kappa c_2} \max_{0 \leq j \leq M} \|\varphi^j\|_0^2, \quad (13)$$

where $(y, v) = \sum_{i=1}^{N-1} y_i v_i h$, $\|y\|_0^2 = (y, y)$.

Proof. Taking the inner product of Eq. (5) with $y^{(\sigma_{j+1})}$, we have

$$(y^{(\sigma_{j+1})}, g \Delta_{0t_{j+1}}^\alpha y) - (y^{(\sigma_{j+1})}, \Lambda y^{(\sigma_{j+1})}) = (y^{(\sigma_{j+1})}, \varphi^{j+1}). \quad (14)$$

Using inequality (12) and the positive definiteness of operator $A = -\Lambda$ from identity (14) one obtains

$$\frac{1}{2} g \Delta_{0t_{j+1}}^\alpha \|y\|_0^2 + \kappa \|y^{(\sigma_{j+1})}\|_0^2 \leq \varepsilon \|y^{(\sigma_{j+1})}\|_0^2 + \frac{1}{4\varepsilon} \|\varphi^{j+1}\|_0^2, \quad \varepsilon > 0. \quad (15)$$

From (15), at $\varepsilon = \kappa$ we get

$$g \Delta_{0t_{j+1}}^\alpha \|y\|_0^2 \leq \frac{1}{2\kappa} \|\varphi^{j+1}\|_0^2. \quad (16)$$

Let us rewrite inequality (16) in the form

$$g_j^{j+1} \|y^{j+1}\|_0^2 \leq \sum_{s=1}^j (g_s^{j+1} - g_{s-1}^{j+1}) \|y^s\|_0^2 + g_0^{j+1} \|y^0\|_0^2 + \frac{1}{2\kappa} \|\varphi^{j+1}\|_0^2. \quad (17)$$

Noticing that $g_0^{j+1} \geq c_2 > 0$, we get

$$g_j^{j+1} \|y^{j+1}\|_0^2 \leq \sum_{s=1}^j (g_s^{j+1} - g_{s-1}^{j+1}) \|y^s\|_0^2 + g_0^{j+1} \left(\|y^0\|_0^2 + \frac{1}{2\kappa c_2} \|\varphi^{j+1}\|_0^2 \right). \quad (18)$$

Denote

$$E = \|y^0\|_0^2 + \frac{1}{2\kappa c_2} \max_{0 \leq j \leq M} \|\varphi^j\|_0^2.$$

The inequality (18) is reduced to

$$g_j^{j+1} \|y^{j+1}\|_0^2 \leq \sum_{s=1}^j (g_s^{j+1} - g_{s-1}^{j+1}) \|y^s\|_0^2 + g_0^{j+1} E. \quad (19)$$

It is obvious that at $j = 0$ the a priori estimate (13) follows from (19). Let us prove that (13) holds for $j = 1, 2, \dots$ by using the mathematical induction method. For this purpose, let us assume that the a priori estimate (13) takes place for all $j = 0, 1, \dots, k - 1$:

$$\|y^{j+1}\|_0^2 \leq E, \quad j = 0, 1, \dots, k - 1.$$

From (19) at $j = k$ one has

$$\begin{aligned} g_k^{k+1} \|y^{k+1}\|_0^2 &\leq \sum_{s=1}^k (g_s^{k+1} - g_{s-1}^{k+1}) \|y^s\|_0^2 + g_0^{k+1} E \\ &\leq \sum_{s=1}^k (g_s^{k+1} - g_{s-1}^{k+1}) E + g_0^{k+1} E = g_k^{k+1} E. \end{aligned} \quad (20)$$

The proof of Theorem 1 is completed. \square

A priori estimate (13) implies the stability of difference scheme (5)–(6).

Theorem 2. If the conditions of Theorem 1 are satisfied and difference scheme (5)–(6) has the approximation order $\mathcal{O}(N^{-r_1} + M^{-r_2})$, where r_1 and r_2 are some known positive numbers, then the solution of difference scheme (5)–(6) converges to the solution of differential problem (1)–(2) in the mesh L_2 -norm with the rate equal to the order of the approximation error $\mathcal{O}(N^{-r_1} + M^{-r_2})$.

Proof. Let us introduce the error $z = y - u$ and substitute it into (5)–(6). Then we obtain the problem for the error

$$g \Delta_{0t}^\alpha z_i = \Lambda z_i^{(\sigma_{j+1})} + \psi_i^{j+1}, \quad i = 1, \dots, N - 1, \quad j = 0, 1, \dots, M - 1, \quad (21)$$

$$z(0, t) = 0, \quad z(l, t) = 0, \quad t \in \bar{\omega}_\tau, \quad z(x, 0) = 0, \quad x \in \bar{\omega}_h, \quad (22)$$

where $\psi_i^{j+1} = \Lambda u_i^{(\sigma_{j+1})} - g \Delta_{0t}^\alpha u_i + \varphi_i^{j+1}$, $\psi_i^{j+1} = \mathcal{O}(N^{-r_1} + M^{-r_2})$.

Since the conditions of Theorem 1 are fulfilled, then a priori estimate (13) holds true for the solution of problem (21)–(22) and, therefore, the following inequality takes place

$$\|z\|_0 \leq \frac{1}{\sqrt{2\kappa c_2}} \max_{0 \leq j \leq M} \|\psi^j\|_0 = \mathcal{O}(N^{-r_1} + M^{-r_2}),$$

which implies the convergence in the mesh L_2 -norm with the rate $\mathcal{O}(N^{-r_1} + M^{-r_2})$. \square

3. A new L_2 -1 σ fractional numerical differentiation formula

In this section a difference analog of the Caputo fractional derivative with the approximation order $\mathcal{O}(\tau^{3-\alpha})$ is constructed and its basic properties are investigated.

Let us consider the uniform mesh $\bar{\omega}_\tau = \{t_j = j\tau, \quad j = 0, 1, \dots, M; \quad T = \tau M\}$. Let $\sigma = 1 - \frac{\alpha}{2}$, then for the Caputo fractional derivative of the order α , $0 < \alpha < 1$, of the function $u(t) \in C^3[0, T]$ at the fixed point $t_{j+\sigma}$, $j \in \{0, 1, \dots, M - 1\}$ the following equalities hold

$$\begin{aligned} \partial_{0t_{j+\sigma}}^\alpha u(t) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{j+\sigma}} \frac{u'(\eta) d\eta}{(t_{j+\sigma} - \eta)^\alpha} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} \frac{u'(\eta) d\eta}{(t_{j+\sigma} - \eta)^\alpha} + \frac{1}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{u'(\eta) d\eta}{(t_{j+\sigma} - \eta)^\alpha}. \end{aligned} \quad (23)$$

As in [22], on each interval $[t_{s-1}, t_s]$ ($1 \leq s \leq j$), denoting the quadratic interpolation $\Pi_{2,s}u(t)$ of $u(t)$ using three points $(t_{s-1}, u(t_{s-1}))$, $(t_s, u(t_s))$ and $(t_{s+1}, u(t_{s+1}))$, we get

$$\begin{aligned} \Pi_{2,s}u(t) &= u(t_{s-1}) \frac{(t - t_s)(t - t_{s+1})}{2\tau^2} - u(t_s) \frac{(t - t_{s-1})(t - t_{s+1})}{\tau^2} + u(t_{s+1}) \frac{(t - t_{s-1})(t - t_s)}{2\tau^2}, \\ (\Pi_{2,s}u(t))' &= u_{t,s} + u_{\bar{t},s}(t - t_{s+1/2}) = u_{t,s-1} + u_{\bar{t},s}(t - t_{s-1/2}), \end{aligned} \quad (24)$$

and

$$u(t) - \Pi_{2,s}u(t) = \frac{u'''(\bar{\xi}_s)}{6} (t - t_{s-1})(t - t_s)(t - t_{s+1}), \quad (25)$$

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 (23), we use $\Pi_{2,s}u(t)$ to approximate $u(t)$ on the interval $[t_{s-1}, t_s]$ ($1 \leq s \leq j$). Taking into account the equality

$$\int_{t_{s-1}}^{t_s} (\eta - t_{s-1/2})(t_{j+\sigma} - \eta)^{-\alpha} d\eta = \frac{\tau^{2-\alpha}}{1-\alpha} b_{j-s+1}^{(\alpha, \sigma)}, \quad 1 \leq s \leq j \quad (26)$$

with

$$b_l^{(\alpha, \sigma)} = \frac{1}{2-\alpha} [(l+\sigma)^{2-\alpha} - (l-1+\sigma)^{2-\alpha}] - \frac{1}{2} [(l+\sigma)^{1-\alpha} + (l-1+\sigma)^{1-\alpha}],$$

$l \geq 1$, from (23) and (24) we obtain the difference analog of the Caputo fractional derivative of the order α ($0 < \alpha < 1$) for the function $u(t)$ in the following form:

$$\begin{aligned} \partial_{0t_{j+\sigma}}^\alpha u(\eta) &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} \frac{u'(\eta) d\eta}{(t_{j+\sigma} - \eta)^\alpha} + \frac{1}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{u'(\eta) d\eta}{(t_{j+\sigma} - \eta)^\alpha} \\ &\approx \frac{1}{\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} \frac{(\Pi_{2,s}u(\eta))' d\eta}{(t_{j+\sigma} - \eta)^\alpha} + \frac{u_{t,j}}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{d\eta}{(t_{j+\sigma} - \eta)^\alpha} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} \frac{u_{t,s-1} + u_{\bar{t},s}(\eta - t_{s-1/2}) d\eta}{(t_{j+\sigma} - \eta)^\alpha} + \frac{u_{t,j}}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{d\eta}{(t_{j+\sigma} - \eta)^\alpha} \\ &= \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \left(\sum_{s=1}^j (a_{j-s+1}^{(\alpha, \sigma)} u_{t,s-1} + b_{j-s+1}^{(\alpha, \sigma)} u_{\bar{t},s} \tau) + a_0^{(\alpha, \sigma)} u_{t,j} \right) \\ &= \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \left(\sum_{s=1}^j (a_{j-s+1}^{(\alpha, \sigma)} u_{t,s-1} + b_{j-s+1}^{(\alpha, \sigma)} (u_{t,s} - u_{t,s-1})) + a_0^{(\alpha, \sigma)} u_{t,j} \right) \\ &= \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{s=0}^j c_{j-s}^{(\alpha, \sigma)} u_{t,s} = \Delta_{0t_{j+\sigma}}^\alpha u, \end{aligned} \quad (27)$$

where

$$\begin{aligned} a_0^{(\alpha, \sigma)} &= \sigma^{1-\alpha}, \quad a_l^{(\alpha, \sigma)} = (l+\sigma)^{1-\alpha} - (l-1+\sigma)^{1-\alpha}, \quad l \geq 1; \\ c_0^{(\alpha, \sigma)} &= a_0^{(\alpha, \sigma)}, \text{ for } j=0; \text{ and for } j \geq 1, \\ c_s^{(\alpha, \sigma)} &= \begin{cases} a_0^{(\alpha, \sigma)} + b_1^{(\alpha, \sigma)}, & s=0, \\ a_s^{(\alpha, \sigma)} + b_{s+1}^{(\alpha, \sigma)} - b_s^{(\alpha, \sigma)}, & 1 \leq s \leq j-1, \\ a_j^{(\alpha, \sigma)} - b_j^{(\alpha, \sigma)}, & s=j. \end{cases} \end{aligned} \quad (28)$$

We call the fractional numerical differentiation formula (27) for the Caputo fractional derivative of order α ($0 < \alpha < 1$) the $L2-1_\sigma$ formula.

Lemma 2. For any $\alpha \in (0, 1)$ and $u(t) \in \mathcal{C}^3[0, t_{j+1}]$

$$|\partial_{0t_{j+\sigma}}^\alpha u - \Delta_{0t_{j+\sigma}}^\alpha u| = \mathcal{O}(\tau^{3-\alpha}). \quad (29)$$

Proof. Let $\partial_{0t_{j+\sigma}}^\alpha u - \Delta_{0t_{j+\sigma}}^\alpha u = R_1^j + R_j^{j+\sigma}$, where

$$\begin{aligned} R_1^j &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} \frac{u'(\eta) d\eta}{(t_{j+\sigma} - \eta)^\alpha} - \frac{1}{\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} \frac{(\Pi_{2,s}u(\eta))' d\eta}{(t_{j+\sigma} - \eta)^\alpha} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} (u(\eta) - \Pi_{2,s}u(\eta))' (t_{j+\sigma} - \eta)^{-\alpha} d\eta \end{aligned}$$

$$\begin{aligned}
&= -\frac{\alpha}{\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} (u(\eta) - \Pi_{2,s}u(\eta))(t_{j+\sigma} - \eta)^{-\alpha-1} d\eta \\
&= -\frac{\alpha}{6\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} u'''(\xi_s)(\eta - t_{s-1})(\eta - t_s)(\eta - t_{s+1})(t_{j+\sigma} - \eta)^{-\alpha-1} d\eta, \\
R_j^{j+\sigma} &= \frac{1}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{u'(\eta)d\eta}{(t_{j+\sigma} - \eta)^\alpha} - \frac{u_{t,j}}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{d\eta}{(t_{j+\sigma} - \eta)^\alpha} \\
&= \frac{1}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{(u'(\eta) - u_{t,j})d\eta}{(t_{j+\sigma} - \eta)^\alpha} \\
&= \frac{1}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{(u'(t_{j+1/2}) - u_{t,j})d\eta}{(t_{j+\sigma} - \eta)^\alpha} + \frac{u''(t_{j+1/2})}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{(\eta - t_{j+1/2})d\eta}{(t_{j+\sigma} - \eta)^\alpha} + \mathcal{O}(\tau^{3-\alpha}) \\
&= \frac{u''(t_{j+1/2})}{\Gamma(1-\alpha)} \int_{t_j}^{t_{j+\sigma}} \frac{(\eta - t_{j+1/2})d\eta}{(t_{j+\sigma} - \eta)^\alpha} + \mathcal{O}(\tau^{3-\alpha}).
\end{aligned}$$

We estimate the error R_1^j similarly to [22]:

$$\begin{aligned}
|R_1^j| &\leq \frac{\alpha|u'''(\xi)|}{6\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} (\eta - t_{s-1})(t_s - \eta)(t_{s+1} - \eta)(t_{j+\sigma} - \eta)^{-\alpha-1} d\eta \\
&\leq \frac{\alpha|u'''(\xi)|\tau^3}{3\Gamma(1-\alpha)} \sum_{s=1}^j \int_{t_{s-1}}^{t_s} (t_{j+\sigma} - \eta)^{-\alpha-1} d\eta = \frac{\alpha|u'''(\xi)|\tau^3}{3\Gamma(1-\alpha)} \int_0^{t_j} (t_{j+\sigma} - \eta)^{-\alpha-1} d\eta \\
&= \frac{|u'''(\xi)|\tau^3}{3\Gamma(1-\alpha)} \left(\frac{1}{\sigma^\alpha \tau^\alpha} - \frac{1}{(j+\sigma)^\alpha \tau^\alpha} \right) \leq \frac{|u'''(\xi)|}{3\sigma^\alpha \Gamma(1-\alpha)} \tau^{3-\alpha}, \quad \xi \in (0, t_j).
\end{aligned}$$

Since

$$\int_{t_j}^{t_{j+\sigma}} \frac{(\eta - t_{j+1/2})d\eta}{(t_{j+\sigma} - \eta)^\alpha} = \frac{\tau t_\sigma^{1-\alpha}(2\sigma + \alpha - 2)}{2(1-\alpha)(2-\alpha)} = 0$$

the error $|R_j^{j+\sigma}| = \mathcal{O}(\tau^{3-\alpha})$. Lemma 2 is proved. \square

3.1. Basic properties of the new $L2-1_\sigma$ fractional numerical differentiation formula

Lemma 3. For all $s = 1, 2, \dots$ and $0 < \alpha < 1$ the following inequalities hold

$$\frac{1}{2} < \kappa_s < \frac{1}{2-\alpha},$$

where

$$\kappa_s = \frac{(s+\sigma)^{2-\alpha} - (s-1+\sigma)^{2-\alpha} - (2-\alpha)(s-1+\sigma)^{1-\alpha}}{(2-\alpha)((s+\sigma)^{1-\alpha} - (s-1+\sigma)^{1-\alpha})}.$$

Proof. Let us consider two functions

$$f_\alpha(x) = \frac{(x+1)^{2-\alpha} - x^{2-\alpha} - (2-\alpha)x^{1-\alpha}}{(2-\alpha)((x+1)^{1-\alpha} - x^{1-\alpha})} = \int_0^1 \frac{(z+x)^{1-\alpha} - x^{1-\alpha}}{(1+x)^{1-\alpha} - x^{1-\alpha}} dz, \quad x > 0$$

and

$$g_\alpha(z, x) = \frac{(z+x)^{1-\alpha} - x^{1-\alpha}}{(1+x)^{1-\alpha} - x^{1-\alpha}} = \frac{z \int_0^1 \frac{d\xi}{(x+z\xi)^\alpha}}{\int_0^1 \frac{d\xi}{(x+\xi)^\alpha}}, \quad 0 < z < 1, \quad x > 0.$$

For all $x > 0$ and $0 < z < 1$ the following inequalities hold

$$\int_0^1 \frac{d\xi}{(x+\xi)^\alpha} < \int_0^1 \frac{d\xi}{(x+z\xi)^\alpha} < \int_0^1 \frac{d\xi}{(zx+z\xi)^\alpha} = z^{-\alpha} \int_0^1 \frac{d\xi}{(x+\xi)^\alpha}.$$

Therefore, for the function $g_\alpha(z, x)$ for all $x > 0$ and $0 < z < 1$ the inequalities

$$z < g_\alpha(z, x) < z^{1-\alpha} \quad (30)$$

are valid.

Integrating (30) with respect to z from 0 to 1, we get the inequalities

$$\frac{1}{2} < f_\alpha(x) < \frac{1}{2-\alpha},$$

which hold for all $x > 0$. Lemma 3 is proved. \square

Corollary 2. For any α ($0 < \alpha < 1$), it holds $b_s^{(\alpha, \sigma)} > 0$, $s \geq 1$.

The latter follows from the equality

$$b_s^{(\alpha, \sigma)} = [(s+\sigma)^{1-\alpha} - (s-1+\sigma)^{1-\alpha}] \left(\kappa_s - \frac{1}{2} \right).$$

Lemma 4. For any α ($0 < \alpha < 1$) and $c_s^{(\alpha, \sigma)}$ ($0 \leq s \leq j$, $j \geq 1$) defined in (28), it holds

$$c_j^{(\alpha, \sigma)} > \frac{1-\alpha}{2} (j+\sigma)^{-\alpha}, \quad (31)$$

$$c_0^{(\alpha, \sigma)} > c_1^{(\alpha, \sigma)} > c_2^{(\alpha, \sigma)} > \dots > c_{j-1}^{(\alpha, \sigma)} > c_j^{(\alpha, \sigma)}, \quad (32)$$

$$(2\sigma-1)c_0^{(\alpha, \sigma)} - \sigma c_1^{(\alpha, \sigma)} > 0, \quad (33)$$

where $\sigma = 1 - \alpha/2$.

Proof. For $j \geq 1$ we get

$$\begin{aligned} c_j^{(\alpha, \sigma)} &= a_j^{(\alpha, \sigma)} - b_j^{(\alpha, \sigma)} = ((j+\sigma)^{1-\alpha} - (j-1+\sigma)^{1-\alpha}) \left(\frac{3}{2} - \kappa_j \right) \\ &> ((j+\sigma)^{1-\alpha} - (j-1+\sigma)^{1-\alpha}) \left(\frac{3}{2} - \frac{1}{2-\alpha} \right) \\ &> \frac{1-\alpha}{2} \int_0^1 \frac{d\eta}{(j+\sigma-\eta)^\alpha} > \frac{1-\alpha}{2} (j+\sigma)^{-\alpha}. \end{aligned}$$

Inequality (31) is proved. Let us prove inequality (32).

For $1 \leq s \leq j-2$ ($j \geq 3$) we have

$$\begin{aligned} c_s^{(\alpha, \sigma)} - c_{s+1}^{(\alpha, \sigma)} &= a_s^{(\alpha, \sigma)} - a_{s+1}^{(\alpha, \sigma)} + 2b_{s+1}^{(\alpha, \sigma)} - b_s^{(\alpha, \sigma)} - b_{s+2}^{(\alpha, \sigma)} \\ &= \frac{1}{2} ((s+2+\sigma)^{1-\alpha} - 3(s+1+\sigma)^{1-\alpha} + 3(s+\sigma)^{1-\alpha} - (s-1+\sigma)^{1-\alpha}) \\ &\quad + \frac{1}{2-\alpha} (-(s+2+\sigma)^{2-\alpha} + 3(s+1+\sigma)^{2-\alpha} - 3(s+\sigma)^{2-\alpha} + (s-1+\sigma)^{2-\alpha}) \end{aligned}$$

$$\begin{aligned}
&= \frac{\alpha(1-\alpha)(1+\alpha)}{2} \int_0^1 dz_1 \int_0^1 dz_2 \int_0^1 \frac{dz_3}{(s-1+\sigma+z_1+z_2+z_3)^{\alpha+2}} \\
&\quad + \alpha(1-\alpha) \int_0^1 dz_1 \int_0^1 dz_2 \int_0^1 \frac{dz_3}{(s-1+\sigma+z_1+z_2+z_3)^{\alpha+1}} \\
&> \frac{\alpha(1-\alpha)(1+\alpha)}{2} (s+2+\sigma)^{-\alpha-2} + \alpha(1-\alpha)(s+2+\sigma)^{-\alpha-1} > 0.
\end{aligned}$$

For $s = j - 1$ ($j \geq 2$) we get

$$\begin{aligned}
c_s^{(\alpha,\sigma)} - c_{s+1}^{(\alpha,\sigma)} &= c_{j-1}^{(\alpha,\sigma)} - c_j^{(\alpha,\sigma)} = a_{j-1}^{(\alpha,\sigma)} - a_j^{(\alpha,\sigma)} + 2b_j^{(\alpha,\sigma)} - b_{j-1}^{(\alpha,\sigma)} \\
&> a_{j-1}^{(\alpha,\sigma)} - a_j^{(\alpha,\sigma)} + 2b_j^{(\alpha,\sigma)} - b_{j-1}^{(\alpha,\sigma)} - b_{j+1}^{(\alpha,\sigma)} \\
&> \frac{\alpha(1-\alpha)(1+\alpha)}{2} (j+1+\sigma)^{-\alpha-2} + \alpha(1-\alpha)(j+1+\sigma)^{-\alpha-1} > 0.
\end{aligned}$$

For inequality (32) it remains to prove the case $s = 0$, that is $c_0^{(\alpha,\sigma)} > c_1^{(\alpha,\sigma)}$ which obviously follows from (33). It is enough to prove inequality (33).

For $j = 1$ we get

$$\begin{aligned}
(2\sigma - 1)c_0^{(\alpha,\sigma)} - \sigma c_1^{(\alpha,\sigma)} &= (2\sigma - 1)(a_0^{(\alpha,\sigma)} + b_1^{(\alpha,\sigma)}) - \sigma(a_1^{(\alpha,\sigma)} - b_1^{(\alpha,\sigma)}) \\
&= \left(\frac{2\sigma - 1}{2\sigma} - \frac{2\sigma - 1}{2} \right) (1 + \sigma)^{1-\alpha} = \frac{(2\sigma - 1)(1 - \sigma)}{2\sigma} (1 + \sigma)^{1-\alpha} > 0.
\end{aligned}$$

For $j \geq 2$ we get

$$\begin{aligned}
(2\sigma - 1)c_0^{(\alpha,\sigma)} - \sigma c_1^{(\alpha,\sigma)} &= (2\sigma - 1)(a_0^{(\alpha,\sigma)} + b_1^{(\alpha,\sigma)}) - \sigma(a_1^{(\alpha,\sigma)} + b_2^{(\alpha,\sigma)} - b_1^{(\alpha,\sigma)}) \\
&= \frac{4\sigma - 1}{2\sigma} (1 + \sigma)^{1-\alpha} - (2 + \sigma)^{1-\alpha} = (1 + \sigma)^{1-\alpha} \left(\frac{4\sigma - 1}{2\sigma} - \left(1 + \frac{1}{1 + \sigma} \right)^{1-\alpha} \right) \\
&> (1 + \sigma)^{1-\alpha} \left(\frac{4\sigma - 1}{2\sigma} - 1 - \frac{1 - \alpha}{1 + \sigma} \right) = \frac{(2\sigma - 1)(1 - \sigma)}{2\sigma(1 + \sigma)^\alpha} > 0.
\end{aligned}$$

Here we used the inequality $(1 + t)^\gamma < 1 + \gamma t$ which is valid for all $t > 0$ and $0 < \gamma < 1$. Lemma 4 is proved. \square

3.2. Test example

In this subsection, the validity and numerical accuracy of the new presented $L2-1_\sigma$ formula (27) are demonstrated by a test example.

Let us take a positive integer M , let $\tau = 1/(M - 1 + \sigma)$ and denote

$$E_{L2-1_\sigma}^M(\tau) = |\partial_{0t}^\alpha f(t) - \Delta_{0t_{M-1+\sigma}}^\alpha f(t)|.$$

Example. Let $f(t) = t^{4+\alpha}$, $0 < \alpha < 1$. Compute the α -order Caputo fractional derivative of $f(t)$ at $t = t_{M-1+\sigma} = 1$ numerically.

The exact solution is given by

$$\partial_{0t}^\alpha t^{4+\alpha} \Big|_{t=1} = \frac{\Gamma(5 + \alpha)}{24}.$$

Taking different temporal stepsizes $M = 10, 20, 40, 80, 160, 320, 640, 1280, 2560, 5120$, we compute the example using $L2-1_\sigma$ formula (27) and compare the results with those obtained with the help of the $L1-2$ formula in [22]. Table 1 lists the computational errors and numerical convergence order (CO) at $t_{M-1+\sigma} = 1$ with different parameters $\alpha = 0.9, 0.5, 0.1$.

4. A second order difference scheme for the time fractional diffusion equation

In this section for problem (1)–(2) a difference scheme with the approximation order $\mathcal{O}(h^2 + \tau^2)$ is constructed. The stability of the constructed difference scheme as well as its convergence in the mesh 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.

Table 1

Computational errors and convergence order with different temporal stepsizes.

α	M	$E_{L1-2}^M(\tau)$ [22]	$CO_{E_{L1-2}^M}$	$E_{L2-1,\sigma}^M(\tau)$	$CO_{E_{L2-1,\sigma}^M}$
0.9	10	1.070471e−1		1.922978e−2	
	20	2.699702e−2	1.99	4.368964e−3	2.07
	40	6.545547e−3	2.04	1.009364e−3	2.08
	80	1.556707e−3	2.07	2.347614e−4	2.09
	160	3.666902e−4	2.09	5.473732e−5	2.09
	320	8.595963e−5	2.09	1.277246e−5	2.10
	640	2.010152e−5	2.10	2.980723e−6	2.10
	1280	4.694884e−6	2.10	6.955612e−7	2.10
	2560	1.095840e−6	2.10	1.622925e−7	2.10
	5120	2.556990e−7	2.10	3.786340e−8	2.10
0.5	10	1.350657e−2		3.756950e−3	
	20	2.612085e−3	2.37	7.231988e−4	2.33
	40	4.861786e−4	2.43	1.367574e−4	2.38
	80	8.864502e−5	2.46	2.544814e−5	2.42
	160	1.597499e−5	2.47	4.673501e−6	2.44
	320	2.859085e−6	2.48	8.495470e−7	2.46
	640	5.095342e−7	2.49	1.532461e−7	2.47
	1280	9.056389e−8	2.49	2.748687e−8	2.48
	2560	1.606869e−8	2.49	4.909831e−9	2.48
	5120	2.847764e−9	2.50	8.743961e−10	2.49
0.1	10	6.238229e−4		2.686107e−4	
	20	9.663202e−5	2.69	4.492624e−5	2.57
	40	1.444281e−5	2.74	7.204745e−6	2.64
	80	2.111896e−6	2.77	1.119177e−6	2.68
	160	3.043133e−7	2.79	1.696376e−7	2.72
	320	4.338827e−8	2.81	2.522442e−8	2.75
	640	6.136347e−9	2.82	3.694254e−9	2.77
	1280	8.622698e−10	2.83	5.344856e−10	2.79
	2560	1.205229e−10	2.84	7.656497e−11	2.80
	5120	1.676992e−11	2.85	1.087796e−11	2.82

4.1. Derivation of the difference scheme

Lemma 5. For any functions $k_1(x) \in C_x^3$ and $v(x) \in C_x^4$ the following equality is valid:

$$\left. \frac{d}{dx} \left(k_1(x) \frac{d}{dx} v(x) \right) \right|_{x=x_i} = \frac{k_1(x_{i+1/2})v(x_{i+1}) - (k_1(x_{i+1/2}) + k_1(x_{i-1/2}))v(x_i) + k_1(x_{i-1/2})v(x_{i-1}))}{h^2} + \mathcal{O}(h^2). \quad (34)$$

Let $u(x, t) \in C_{x,t}^{4,3}$ be a solution of the problem (1)–(2). Let us consider Eq. (1) for $(x, t) = (x_i, t_{j+\sigma}) \in \overline{Q}_T$, $i = 1, 2, \dots, N - 1$, $j = 0, 1, \dots, M - 1$, $\sigma = 1 - \alpha/2$:

$$\partial_{0t_{j+\sigma}}^\alpha u = \left. \frac{\partial}{\partial x} \left(k(x, t) \frac{\partial u}{\partial x} \right) \right|_{(x_i, t_{j+\sigma})} - q(x_i, t_{j+\sigma})u(x_i, t_{j+\sigma}) + f(x_i, t_{j+\sigma}). \quad (35)$$

Since

$$\begin{aligned} \left. \frac{\partial}{\partial x} \left(k(x, t) \frac{\partial u}{\partial x} \right) \right|_{(x_i, t_{j+\sigma})} &= k(x_i, t_{j+\sigma}) \frac{\partial^2 u}{\partial x^2}(x_i, t_{j+\sigma}) + \frac{\partial k}{\partial x}(x_i, t_{j+\sigma}) \frac{\partial u}{\partial x}(x_i, t_{j+\sigma}) \\ &= k(x_i, t_{j+\sigma}) \left(\sigma \frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1}) + (1 - \sigma) \frac{\partial^2 u}{\partial x^2}(x_i, t_j) \right) \\ &\quad + \frac{\partial k}{\partial x}(x_i, t_{j+\sigma}) \left(\sigma \frac{\partial u}{\partial x}(x_i, t_{j+1}) + (1 - \sigma) \frac{\partial u}{\partial x}(x_i, t_j) \right) + \mathcal{O}(\tau^2) \\ &= \sigma \left(k(x_i, t_{j+\sigma}) \frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1}) + \frac{\partial k}{\partial x}(x_i, t_{j+\sigma}) \frac{\partial u}{\partial x}(x_i, t_{j+1}) \right) \\ &\quad + (1 - \sigma) \left(k(x_i, t_{j+\sigma}) \frac{\partial^2 u}{\partial x^2}(x_i, t_j) + \frac{\partial k}{\partial x}(x_i, t_{j+\sigma}) \frac{\partial u}{\partial x}(x_i, t_j) \right) + \mathcal{O}(\tau^2) \end{aligned}$$

$$= \sigma \frac{\partial}{\partial x} \left(k(x, t_{j+\sigma}) \frac{\partial}{\partial x} u(x, t_{j+1}) \right) \Big|_{x=x_i} + (1-\sigma) \frac{\partial}{\partial x} \left(k(x, t_{j+\sigma}) \frac{\partial}{\partial x} u(x, t_j) \right) \Big|_{x=x_i} + \mathcal{O}(\tau^2),$$

$$q(x_i, t_{j+\sigma})u(x_i, t_{j+\sigma}) = q(x_i, t_{j+\sigma})(\sigma u(x_i, t_{j+1}) + (1-\sigma)u(x_i, t_j)) + \mathcal{O}(\tau^2),$$

by virtue of Lemma 5 we have

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

where the difference operator Λ is defined by formula (8) with the coefficients $a_i^{j+1} = k(x_{i-1/2}, t_{j+\sigma})$, $d_i^{j+1} = q(x_i, t_{j+\sigma})$. Let $\varphi_i^{j+1} = f(x_i, t_{j+\sigma})$, then with regard to Lemma 2 we get the difference scheme with the approximation order $\mathcal{O}(h^2 + \tau^2)$:

$$\Delta_{0t_{j+\sigma}}^\alpha y_i = \Lambda y_i^{(\sigma)} + \varphi_i^{j+1}, \quad i = 1, 2, \dots, N-1, \quad j = 0, 1, \dots, M-1, \quad (36)$$

$$y(0, t) = 0, \quad y(l, t) = 0, \quad t \in \bar{\omega}_\tau, \quad y(x, 0) = u_0(x), \quad x \in \bar{\omega}_h. \quad (37)$$

It is interesting to note that for $\alpha \rightarrow 1$ we obtain the Crank–Nicolson difference scheme.

4.2. Stability and convergence

Theorem 3. The difference scheme (36)–(37) is unconditionally stable and its solution satisfies the following a priori estimate:

$$\|y^{j+1}\|_0^2 \leq \|y^0\|_0^2 + \frac{l^2 T^\alpha \Gamma(1-\alpha)}{4c_1} \max_{0 \leq j \leq M} \|\varphi^j\|_0^2. \quad (38)$$

Proof. For the difference operator Λ using Green's first difference formula and the embedding theorem [24] for the functions vanishing at $x = 0$ and $x = l$, we get $(-\Lambda y, y) \geq \frac{4c_1}{l^2} \|y\|_0^2$, that is for this operator it is possible to take $\kappa = \frac{4c_1}{l^2}$.

Since difference scheme (36)–(37) has the form (5)–(6), where $g_s^{j+1} = \frac{c_{j-s}^{(\alpha, \beta)}}{\tau^\alpha \Gamma(2-\alpha)}$, then Lemma 4 implies validity of the following inequalities:

$$g_0^{j+1} = \frac{c_j^{(\alpha, \beta)}}{\tau^\alpha \Gamma(2-\alpha)} > \frac{1}{2t_{j+\sigma}^\alpha \Gamma(1-\alpha)} > \frac{1}{2T^\alpha \Gamma(1-\alpha)},$$

$$g_j^{j+1} > g_{j-1}^{j+1} > \dots > g_0^{j+1},$$

$$\frac{g_j^{j+1}}{2g_j^{j+1} - g_{j-1}^{j+1}} < \sigma < 1.$$

Therefore, validity of Theorem 3 follows from Theorem 1. Theorem 3 is proved. \square

From Theorem 2 it follows that if the solution and input data of problem (1)–(2) are sufficiently smooth, the solution of difference scheme (36)–(37) converges to the solution of the differential problem with the rate equal to the order of the approximation error $\mathcal{O}(h^2 + \tau^2)$.

4.3. Numerical results

Numerical calculations are performed for a test problem when the function

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

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

The errors ($z = y - u$) and convergence order (CO) in the norms $\|\cdot\|_0$ and $\|\cdot\|_{C(\bar{\omega}_{h\tau})}$, where $\|y\|_{C(\bar{\omega}_{h\tau})} = \max_{(x_i, t_j) \in \bar{\omega}_{h\tau}} |y|$, are given in Table 2.

Table 2 shows that as the number of the spatial subintervals and time steps is increased keeping $h = \tau$, a reduction in the maximum error takes place, as expected and the convergence order of the approximate scheme is $\mathcal{O}(h^2) = \mathcal{O}(\tau^2)$, where the convergence order is given by the formula: $\text{CO} = \log_{h_1/h_2} \frac{\|z_1\|}{\|z_2\|}$ (z_i is the error corresponding to h_i).

Table 3 shows that if $h = 1/1000$, then as the number of time steps of our approximate scheme is increased, a reduction in the maximum error takes place, as expected and the convergence order of time is $\mathcal{O}(\tau^2)$, where the convergence order is given by the following formula: $\text{CO} = \log_{\tau_1/\tau_2} \frac{\|z_1\|}{\|z_2\|}$.

Table 2 L_2 -norm and maximum norm error behavior versus grid size reduction when $\tau = h$.

α	h	$\max_{0 \leq n \leq M} \ z^n\ _0$	CO in $\ \cdot\ _0$	$\ z\ _{C(\bar{\omega}_{h\tau})}$	CO in $\ \cdot\ _{C(\bar{\omega}_{h\tau})}$
0.10	1/160	1.0224e−4		1.4518e−4	
	1/320	2.5558e−5	2.0001	3.6294e−5	2.0000
	1/640	6.3894e−6	2.0000	9.0733e−6	2.0000
0.50	1/160	7.8417e−5		1.1153e−4	
	1/320	1.9604e−5	2.0000	2.7882e−5	2.0000
	1/640	4.9009e−6	2.0000	6.9705e−6	2.0000
0.90	1/160	6.6666e−5		9.4949e−5	
	1/320	1.6669e−5	1.9998	2.3740e−5	1.9999
	1/640	4.1678e−6	1.9998	5.9360e−6	1.9998
0.99	1/160	6.5660e−5		9.3532e−5	
	1/320	1.6415e−5	2.0000	2.3384e−5	1.9999
	1/640	4.1039e−6	1.9999	5.8460e−6	2.0000

Table 3 L_2 -norm and maximum norm error behavior versus τ -grid size reduction when $h = 1/1000$.

α	τ	$\max_{0 \leq n \leq M} \ z^n\ _0$	CO in $\ \cdot\ _0$	$\ z\ _{C(\bar{\omega}_{h\tau})}$	CO in $\ \cdot\ _{C(\bar{\omega}_{h\tau})}$
0.10	1/10	1.9062e−3		2.6962e−3	
	1/20	4.7789e−4	1.9959	6.7593e−4	1.9960
	1/40	1.1779e−4	2.0205	1.6659e−4	2.0206
0.50	1/10	7.6326e−3		1.0795e−2	
	1/20	1.9130e−3	1.9963	2.7058e−3	1.9962
	1/40	4.7697e−4	2.0039	6.7461e−4	2.0039
0.90	1/10	1.0286e−2		1.4547e−2	
	1/20	2.5706e−3	2.0005	3.6357e−3	2.0004
	1/40	6.4066e−4	2.0045	9.0608e−4	2.0045
0.99	1/10	1.0449e−2		1.4777e−2	
	1/20	2.6102e−3	2.0011	3.6915e−3	2.0011
	1/40	6.5050e−4	2.0045	9.1998e−4	2.0045

5. A higher order difference scheme for the time fractional diffusion equation

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

5.1. Derivation of the difference scheme

Let us assign a difference scheme to differential problem (1)–(2) in the case when $k = k(t)$ and $q = q(t)$:

$$\Delta_{0t_{j+\sigma}}^\alpha \mathcal{H}_h y_i = a^{j+1} y_{xx,i}^{(\sigma)} - d^{j+1} \mathcal{H}_h y_i^{(\sigma)} + \mathcal{H}_h \varphi_i^{j+1}, \quad i = 1, \dots, N-1, \quad j = 0, 1, \dots, M-1, \quad (39)$$

$$y(0, t) = 0, \quad y(l, t) = 0, \quad t \in \bar{\omega}_\tau, \quad y(x, 0) = u_0(x), \quad x \in \bar{\omega}_h, \quad (40)$$

where $\mathcal{H}_h v_i = v_i + h^2 v_{xx,i}/12$, $i = 1, \dots, N-1$, $a^{j+1} = k(t_{j+\sigma})$, $d^{j+1} = q(t_{j+\sigma})$, $\varphi_i^{j+1} = f(x_i, t_{j+\sigma})$, $\sigma = 1 - \alpha/2$.

From [9] and Lemma 2 it follows that if $u \in C_{x,t}^{6,3}$, then the difference scheme has the approximation order $\mathcal{O}(\tau^2 + h^4)$.

5.2. Stability and convergence

The difference scheme (39)–(40) differs from (5)–(6) due to the presence of the operator \mathcal{H}_h . However, deriving a priori estimate for the solution of difference scheme (39)–(40) does not differ significantly from proving Theorem 1.

Theorem 4. The difference scheme (39)–(40) is unconditionally stable and its solution satisfies the following a priori estimate:

$$\|\mathcal{H}_h y^{j+1}\|_0^2 \leq \|\mathcal{H}_h y^0\|_0^2 + \frac{l^2 T^\alpha \Gamma(1-\alpha)}{c_1} \max_{0 \leq j \leq M} \|\mathcal{H}_h \varphi^j\|_0^2, \quad (41)$$

Proof. Taking the inner product of Eq. (39) with $\mathcal{H}_h y^{(\sigma)} = (\mathcal{H}_h y)^{(\sigma)}$, we have

$$(\mathcal{H}_h y^{(\sigma)}, \Delta_{0t_{j+\sigma}}^\alpha \mathcal{H}_h y) - a^{j+1} (\mathcal{H}_h y^{(\sigma)}, y_{\bar{x}\bar{x}}^{(\sigma)}) + d^{j+1} (\mathcal{H}_h y^{(\sigma)}, \mathcal{H}_h y^{(\sigma)}) = (\mathcal{H}_h y^{(\sigma)}, \mathcal{H}_h \varphi^{j+1}). \quad (42)$$

Let us transform the terms in identity (42) as

$$\begin{aligned} (\mathcal{H}_h y^{(\sigma)}, \Delta_{0t_{j+\sigma}}^\alpha \mathcal{H}_h y) &\geq \frac{1}{2} \Delta_{0t_{j+\sigma}}^\alpha \|\mathcal{H}_h y\|_0^2, \\ -(\mathcal{H}_h y^{(\sigma)}, y_{\bar{x}\bar{x}}^{(\sigma)}) &= -(y^{(\sigma)}, y_{\bar{x}\bar{x}}^{(\sigma)}) - \frac{h^2}{12} \|y_{\bar{x}\bar{x}}^{(\sigma)}\|_0^2 = \|y_{\bar{x}}^{(\sigma)}\|_0^2 - \frac{1}{12} \sum_{i=1}^{N-1} (y_{\bar{x},i+1}^{(\sigma)} - y_{\bar{x},i}^{(\sigma)})^2 h \\ &\geq \|y_{\bar{x}}^{(\sigma)}\|_0^2 - \frac{1}{3} \|y_{\bar{x}}^{(\sigma)}\|_0^2 = \frac{2}{3} \|y_{\bar{x}}^{(\sigma)}\|_0^2 \geq \frac{8}{3l^2} \|y^{(\sigma)}\|_0^2, \quad \text{where } \|y\|_0^2 = \sum_{i=1}^N y_i^2 h, \\ (\mathcal{H}_h y^{(\sigma)}, \mathcal{H}_h \varphi^{j+1}) &\leq \varepsilon \|\mathcal{H}_h y^{(\sigma)}\|_0^2 + \frac{1}{4\varepsilon} \|\mathcal{H}_h \varphi^{j+1}\|_0^2 \\ &= \varepsilon \sum_{i=1}^{N-1} \left(\frac{y_{i-1}^{(\sigma)} + 10y_i^{(\sigma)} + y_{i+1}^{(\sigma)}}{12} \right)^2 h + \frac{1}{4\varepsilon} \|\mathcal{H}_h \varphi^{j+1}\|_0^2 \leq \varepsilon \|y^{(\sigma)}\|_0^2 + \frac{1}{4\varepsilon} \|\mathcal{H}_h \varphi^{j+1}\|_0^2. \end{aligned}$$

Taking into account the above-performed transformations, from identity (42) at $\varepsilon = \frac{8c_1}{3l^2}$ one arrives at the inequality

$$\Delta_{0t_{j+\sigma}}^\alpha \|\mathcal{H}_h y\|_0^2 \leq \frac{l^2}{8c_1} \|\mathcal{H}_h \varphi^{j+1}\|_0^2.$$

The following process is similar to the proof of Theorem 1, and it is omitted.

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

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

Similarly to Theorem 2, we obtain the convergence result. \square

Theorem 5. Assume that $u(x, t) \in C_{x,t}^{6,3}$ is the solution of the problem (1)–(2) in the case $k = k(t)$, $q = q(t)$, and let $\{y_i^j \mid 0 \leq i \leq N, 1 \leq j \leq M\}$ be the solution of the difference scheme (39)–(40). Then it holds that

$$\|u(\cdot, t_j) - y^j\|_0 \leq C_R (\tau^2 + h^4), \quad 1 \leq j \leq M,$$

where C_R is a positive constant independent of τ and h .

5.3. Numerical results

In this subsection we present a test example for a numerical investigation of difference scheme (39)–(40).

Consider the following problem:

$$\partial_{0t}^\alpha u(x, t) = k(t) \frac{\partial^2 u}{\partial x^2}(x, t) - q(t)u(x, t) + f(x, t), \quad 0 < x < 1, \quad 0 < t \leq 1, \quad (43)$$

$$u(0, t) = 0, \quad u(1, t) = 0, \quad 0 \leq t \leq 1, \quad u(x, 0) = 0, \quad 0 \leq x \leq 1, \quad (44)$$

where $k(t) = e^t$, $q(t) = 1 - \sin(2t)$,

$$f(x) = \left[\pi^2 t^2 e^t + t^2 (1 - \sin(2t)) + \frac{2t^{2-\alpha}}{\Gamma(3-\alpha)} \right] \sin(\pi x),$$

whose exact analytical solution reads $u(x, t) = t^2 \sin(\pi x)$.

Table 4 presents the L_2 -norm, the maximum norm errors and the temporal convergence order for $\alpha = 0.75, 0.85, 0.95$. Here we can see that the order of convergence in time is two.

Table 5 shows that if $\tau = 1/20000$ is kept fixed, while h varies, then one obtains the expected fourth-order spatial accuracy.

Table 6 shows that as the number of spatial subintervals and time steps is increased keeping $h^2 = \tau$, a reduction in the maximum error takes place, as expected and the convergence order of the approximate of the scheme is $\mathcal{O}(h^4)$.

In Table 7 for the case $N = \lceil \sqrt{M} \rceil$ the maximum error, the convergence order and CPU time (seconds) are given. For this case we obtain the expected rate of convergence $\mathcal{O}(\tau^2)$.

Table 4 L_2 -norm and maximum norm error behavior versus τ -grid size reduction when $h = 1/100$.

α	τ	$\max_{0 \leq n \leq M} \ z^n\ _0$	CO in $\ \cdot\ _0$	$\ z\ _{C(\bar{\omega}_{h\tau})}$	CO in $\ \cdot\ _{C(\bar{\omega}_{h\tau})}$
0.75	1/10	1.6336e−3		2.3103e−3	
	1/20	4.0889e−4	1.9983	5.7826e−4	1.9983
	1/40	1.0229e−4	1.9990	1.4466e−4	1.9990
	1/80	2.5581e−5	1.9995	3.6177e−5	1.9995
0.85	1/10	1.7130e−3		2.4225e−3	
	1/20	4.2856e−4	1.9989	6.0607e−4	1.9989
	1/40	1.0718e−4	1.9994	1.5158e−4	1.9994
	1/80	2.6801e−5	1.9997	3.7902e−5	1.9997
0.95	1/10	1.7582e−3		2.4865e−3	
	1/20	4.3967e−4	1.9996	6.2179e−4	1.9996
	1/40	1.0993e−4	1.9998	1.5547e−4	1.9998
	1/80	2.7484e−5	1.9999	3.8868e−5	1.9999

Table 5 L_2 -norm and maximum norm error behavior versus h -grid size reduction when $\tau = 1/20000$.

α	h	$\max_{0 \leq n \leq M} \ z^n\ _0$	CO in $\ \cdot\ _0$	$\ z\ _{C(\bar{\omega}_{h\tau})}$	CO in $\ \cdot\ _{C(\bar{\omega}_{h\tau})}$
0.10	1/4	1.1004e−3		1.5562e−3	
	1/8	6.7512e−5	4.0267	9.5476e−5	4.0267
	1/16	4.2000e−6	4.0067	5.9397e−6	4.0067
	1/32	2.6213e−7	4.0021	3.7070e−7	4.0021
0.50	1/4	1.0836e−3		1.5325e−3	
	1/8	6.6485e−5	4.0267	9.4024e−5	4.0267
	1/16	4.1360e−6	4.0067	5.8491e−6	4.0067
	1/32	2.5790e−7	4.0034	3.6472e−7	4.0034
0.90	1/4	1.0654e−3		1.5067e−3	
	1/8	6.5371e−5	4.0266	9.2449e−5	4.0266
	1/16	4.0665e−6	4.0068	5.7510e−6	4.0068
	1/32	2.5346e−7	4.0040	3.5844e−7	4.0040

Table 6 L_2 -norm and maximum norm error behavior versus grid size reduction when $h^2 = \tau$.

α	h	$\max_{0 \leq n \leq M} \ z^n\ _0$	CO in $\ \cdot\ _0$	$\ z\ _{C(\bar{\omega}_{h\tau})}$	CO in $\ \cdot\ _{C(\bar{\omega}_{h\tau})}$
0.10	1/10	2.4349e−5		3.4434e−5	
	1/20	1.5166e−6	4.0049	2.1448e−6	4.0049
	1/40	9.4708e−8	4.0012	1.3394e−7	4.0012
	1/80	5.9180e−9	4.0003	8.3693e−9	4.0003
0.50	1/10	1.4211e−5		2.0097e−5	
	1/20	8.8285e−7	4.0087	1.2485e−6	4.0087
	1/40	5.5094e−8	4.0022	7.7914e−8	4.0022
	1/80	3.4420e−9	4.0006	4.8677e−9	4.0006
0.90	1/10	1.5119e−5		2.1381e−5	
	1/20	9.5080e−7	3.9910	1.3446e−6	3.9911
	1/40	5.9571e−8	3.9965	8.4247e−8	3.9964
	1/80	3.7274e−9	3.9984	5.2714e−9	3.9984

6. Conclusion

In this paper, the stability and convergence of a family of difference schemes approximating the time fractional diffusion equation of a general form is studied. Sufficient conditions for the unconditional stability of such difference schemes are obtained. For proving the stability of a wide class of difference schemes approximating the time fractional diffusion equation, it is simple enough to check the stability conditions obtained in this paper. A new difference approximation of the Caputo fractional derivative with the approximation order $\mathcal{O}(\tau^{3-\alpha})$ is constructed. The basic properties of this difference operator are investigated. New difference schemes of the second and fourth approximation order in space and the second approximation order in time for the time fractional diffusion equation with variable coefficients are constructed as well. The stability and convergence of these schemes in the mesh L_2 -norm with the rate equal to the order of the approximation error are proved. The method can be easily extended to other time fractional partial differential equations with other boundary conditions.

Table 7Maximum norm error behavior versus grid size reduction when $N = \lceil \sqrt{M} \rceil$ and CPU time (seconds).

α	M	$\ z\ _{C(\bar{\omega}_{h\tau})}$	CO in $\ \cdot \ _{C(\bar{\omega}_{h\tau})}$	CPU(s)
0.70	10	2.0986e−3		0.0156
	30	2.1085e−4	2.0916	0.0468
	90	2.3672e−5	1.9905	0.1404
	270	2.6359e−6	1.9980	0.5460
	810	2.9428e−7	1.9956	3.0108
	2430	3.2802e−8	1.9971	22.2925
0.80	10	2.1403e−3		0.0156
	30	2.2690e−4	2.0427	0.0468
	90	2.5342e−5	1.9953	0.1716
	270	2.8146e−6	2.0004	0.5616
	810	3.1383e−7	1.9968	3.2604
	2430	3.4962e−8	1.9976	23.3065
0.90	10	2.2549e−3		0.0156
	30	2.4088e−4	2.0358	0.0468
	90	2.6745e−5	2.0007	0.1404
	270	2.9607e−6	2.0033	0.5460
	810	3.2949e−7	1.9986	3.6670
	2430	3.6670e−8	1.9985	22.7605

Numerical tests completely confirming the obtained theoretical results are carried out. In all the calculations MATLAB is used.

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