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A Family of Transformed Difference Schemes for Nonlinear Time-Fractional Equations

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Abstract: In this paper, we present a class of finite difference methods for numerically solving fractional differential equations. Such numerical schemes are developed based on the change in variable and piecewise interpolations. Error analysis of the numerical schemes is obtained by using a Grönwall-type inequality. Numerical examples are given to confirm the theoretical results.

Keywords: time-fractional parabolic problems; change in variable; convergence; optimal error estimates; linearized schemes

1. Introduction

We aim to develop a family of effective numerical methods for solving the following nonlinear time-fractional differential equations:

$$D_*^\alpha y = f(t, y(t)), \quad y(0) = y_0, \quad t \in (0, T], \quad (1)$$

where $0 < \alpha < 1$, D_*^α is the differential operator in sense of Caputo, given by

$$D_*^\alpha y = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-r)^{-\alpha} y'(r) dr.$$

The fractional differential equations provide a powerful tool to describe many natural phenomena in the fields of physics [1–3], economics [4] and biology [5].

Developing and analyzing highly effective numerical methods for fractional differential equations has been one of the hot topics. The widely used numerical methods are the L1 schemes [6–13] and L2-schemes [14–16]. Such schemes are developed by using piecewise interpolations. The optimal convergence results of L1-type schemes for time-dependent partial equations can be obtained by using the fractional Grönwall type inequalities [17–19]. Moreover, L1-type schemes can be accelerated by using sum-of-exponentials approximations [20–22]. Other widely used schemes are the so-called backward differentiation formula (BDF) convolution quadrature (CQ) methods. The CQ methods were originally proposed in [23,24] and further investigated in [25–27]. That aside, some transformed finite difference methods were constructed based on some change in variables [28–30]. More numerical schemes as well as their numerical analysis can be found in an incomplete list of references [31–33].

It is widely accepted that Equation (1) is equivalent to the following Volterra integral equation [34]:

$$y(t) = y_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-r)^{\alpha-1} f(r, y(r)) dr. \quad (2)$$

Here and below, we always assume that the function f is Lipschitz continuous with respect to the second argument on a suitable set G and the Lipschitz constant is L . Moreover,



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suppose $f \in C^3(G)$. Then, there exists a function $\psi \in C^2[0, T]$ and some $c_1, c_2, \dots, c_J \in \mathbb{R}$ and $d_1, d_2, \dots, d_J \in \mathbb{R}$ such that the solution to Equation (1) can be given by (see, e.g., [35–38])

$$y(t) = \psi(t) + \sum_{j=1}^J c_j t^{j\alpha} + \sum_{j=1}^J d_j t^{1+j\alpha}, \quad (3)$$

where $J := \lceil 2/\alpha \rceil - 1$. Clearly, the typical solution to the problem in Equation (1) has an initial layer at the beginning, and y_t blows up as $t \rightarrow 0^+$. In this paper, we aim to present effective numerical schemes to solve the fractional problems, taking the initial layer into account.

The new numerical schemes are developed based on the following changes in variables:

$$t = s^{\eta/\alpha}, \quad \eta \in \mathbb{N}^+, \quad (4)$$

Equations (1) or (2) is equivalent to the following integral equation:

$$\begin{aligned} y(s^{\eta/\alpha}) &= y_0 + \frac{1}{\Gamma(\alpha)} \int_0^{s^{\eta/\alpha}} (s^{\eta/\alpha} - r)^{\alpha-1} f(r, y(r)) dr \\ &= y_0 + \frac{1}{\Gamma(\alpha)} \int_0^s (s^{\eta/\alpha} - u^{\eta/\alpha})^{\alpha-1} f(u^{\eta/\alpha}, y(u^{\eta/\alpha})) \frac{\eta}{\alpha} u^{\eta/\alpha-1} du \\ &= y_0 + \frac{\eta}{\Gamma(1+\alpha)} \int_0^s (s^{\eta/\alpha} - r^{\eta/\alpha})^{\alpha-1} r^{\eta/\alpha-1} f(r^{\eta/\alpha}, y(r^{\eta/\alpha})) dr, \end{aligned} \quad (5)$$

Furthermore, let

$$z(s) = y(s^{\eta/\alpha}), \quad (6)$$

Equation (5) becomes

$$z(s) = y_0 + \frac{\eta}{\Gamma(1+\alpha)} \int_0^s (s^{\eta/\alpha} - r^{\eta/\alpha})^{\alpha-1} r^{\eta/\alpha-1} f(r^{\eta/\alpha}, z(r)) dr, \quad 0 \leq s \leq T^{\alpha/\eta}. \quad (7)$$

Then, the solution to Equation (7) has the form

$$z(s) = \psi(s^{\eta/\alpha}) + \sum_{j=1}^J c_j s^{j\eta} + \sum_{j=1}^J d_j s^{\frac{\eta(1+j\alpha)}{\alpha}}, \quad (8)$$

where $\psi \in C^2[0, T]$. Clearly, by the changes in variables, the initial layer will vanish, and the exact solution will become smoother. Then, the idea of developing effective numerical methods for solving Equation (1) is as follows:

- Apply the change in Equation (4) with a suitable parameter η to obtain Equation (7) and its regularity of the solution.
- Develop numerical methods based on the smoothness of the solution to Equation (7).
- Recover the numerical solution by using the simple inverse change $y(s) = z(s^{\alpha/\eta})$.

The rest of the paper is organized as follows. In Section 2, we present a family of new numerical schemes and investigate the numerical schemes' convergence results. In Section 3, we present some numerical results to confirm the theoretical findings. Finally, our conclusions are presented in Section 4.

2. Construction of the Numerical Methods

In this section, we develop some numerical methods and present the numerical results based on the change in variable. Here and below, we always set the step size $h = \frac{T^{\alpha/\eta}}{N}$, with N being a given integer and $s_i = ih$, $i = 0, 1, 2, \dots, N$. In what follows, we will present two numerical methods for solving Equation (7).

2.1. First-Order Accurate Methods

In this subsection, we present a numerical method based on the following change in variable:

$$t = s^{1/\alpha}$$

With Equations (7) and (8), one can check that its solution $z(s) \in C[0, T]$ with the change in variable. Therefore, we propose a first-order accurate method based on the product rectangle rule for every interval; in other words, we propose

$$\int_{s_{m-1}}^{s_m} (s_i^{1/\alpha} - r^{1/\alpha})^{\alpha-1} r^{1/\alpha-1} f(r^{1/\alpha}, z(r)) dr \approx f(s_m^{1/\alpha}, z(s_m)) \int_{s_{m-1}}^{s_m} (s_i^{1/\alpha} - r^{1/\alpha})^{\alpha-1} r^{1/\alpha-1} dr.$$

Then, it follows from Equation (7) that

$$\begin{aligned} z(s_i) &= z_0 + \frac{1}{\Gamma(1+\alpha)} \sum_{m=1}^i \int_{s_{m-1}}^{s_m} (s_i^{1/\alpha} - r^{1/\alpha})^{\alpha-1} r^{1/\alpha-1} f(r^{1/\alpha}, z(r)) dr \\ &= z_0 + \frac{1}{\Gamma(1+\alpha)} \sum_{m=1}^i f(s_m^{1/\alpha}, z(s_m)) \int_{s_{m-1}}^{s_m} (s_i^{1/\alpha} - r^{1/\alpha})^{\alpha-1} r^{1/\alpha-1} dr + R_1^i \\ &= z_0 + \frac{1}{\Gamma(1+\alpha)} \sum_{m=1}^i a_m^i f(s_m^{1/\alpha}, z(s_m)) + R_1^i, \end{aligned} \quad (9)$$

where $z_0 = y_0$ and the truncation error is

$$R_1^i = \frac{1}{\Gamma(1+\alpha)} \sum_{m=1}^i \int_{s_{m-1}}^{s_m} (s_i^{1/\alpha} - r^{1/\alpha})^{\alpha-1} r^{1/\alpha-1} \left(f(r^{1/\alpha}, z(r)) - f(s_m^{1/\alpha}, z(s_m)) \right) dr = \mathcal{O}(h),$$

while the coefficients are

$$a_m^i = \int_{s_{m-1}}^{s_m} (s_i^{1/\alpha} - r^{1/\alpha})^{\alpha-1} r^{1/\alpha-1} dr. \quad (10)$$

Let z_i be a numerical approximation to $z(s_i)$. By replacing $z(s_i)$ with z_i and omitting the truncation error R_i , we have the following numerical scheme:

$$\text{Scheme I: } z_i = z_0 + \frac{1}{\Gamma(1+\alpha)} \sum_{m=1}^i a_m^i f(s_m^{1/\alpha}, z_m). \quad (11)$$

Scheme I is an implicit method. At each step, iterative processes are required to solve the nonlinear equations. In order to reduce the computational cost, a linearized scheme can be developed as follows:

$$\text{Scheme II: } z_i = z_0 + \frac{1}{\Gamma(1+\alpha)} \sum_{m=1}^i a_m^i f(s_m^{1/\alpha}, z_{m-1}). \quad (12)$$

The convergence results of the proposed schemes rely heavily on the following lemmas:

Lemma 1 ([39]). Let x_i , $0 \leq i \leq N$ be a sequence of non-negative real numbers. If

$$x_i \leq \psi_i + Mh^{\sigma+1-\alpha\beta} \sum_{j=0}^{i-1} \frac{j^\sigma x_j}{(i^\beta - j^\beta)^\alpha}, \quad 0 \leq i \leq N,$$

where $0 < \alpha < 1$, $1 \leq \beta \leq \sigma + 1$, $\sigma \geq 0$, M is a positive constant, and ψ_i , $0 \leq i \leq N$, is a monotonic increasing sequence of non-negative real numbers, then

$$x_i \leq \psi_i \sum_{n=0}^{\infty} \left(\frac{M(ih)^{\sigma+1-\alpha\beta}}{\beta} \right)^n \hat{B}_n(\alpha, \beta, \sigma), \quad 0 \leq i \leq N.$$

$$\hat{B}_n(\alpha, \beta, \sigma) = \begin{cases} 1, & n = 0, \\ \Pi_{l=1}^n B\left(\frac{l}{\beta}(\sigma + 1 - \alpha\beta) + \alpha, (1 - \alpha)\right), & n \geq 1, \end{cases}$$

where B is the Beta function.

When $\sigma + 1 - \beta = 0$, the following is true:

$$x_i \leq \psi_i E_{1-\alpha} \left(\frac{M\Gamma(1-\alpha)}{\beta} (ih)^{\beta(1-\alpha)} \right), \quad 0 \leq i \leq N,$$

where $E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+k\alpha)}$ is the Mittag-Leffler function.

Now, we have the following convergence results:

Theorem 1. Suppose $f \in \mathcal{C}^3(G)$. Then, the schemes in Equations (11) and (12) are first-order accurate.

Proof. Let $e_i = z(s_i) - z_i$. Subtracting Equation (11) from Equation (9) gives

$$\begin{aligned} |e_i| &= \left| e_0 + \frac{1}{\Gamma(1+\alpha)} \sum_{m=1}^i a_m^i (f(s_m^{1/\alpha}, z(s_m)) - f(s_m^{1/\alpha}, z_m)) + R_1^i \right| \\ &\leq |e_0| + \frac{L}{\Gamma(1+\alpha)} \sum_{m=1}^i a_m^i |e_i| + |R_1^i|. \end{aligned} \quad (13)$$

It follows from Equation (10) that, for $1 \leq m \leq i-1$, we have

$$a_m^i = \int_{s_{m-1}}^{s_m} \frac{r^{\frac{1}{\alpha}-1}}{(s_i^{\frac{1}{\alpha}} - r^{\frac{1}{\alpha}})^{1-\alpha}} = h \frac{\zeta^{\frac{1}{\alpha}-1}}{(s_i^{\frac{1}{\alpha}} - \zeta^{\frac{1}{\alpha}})^{1-\alpha}} \quad (14)$$

$$\leq h \frac{s_m^{\frac{1}{\alpha}-1}}{(s_i^{\frac{1}{\alpha}} - s_m^{\frac{1}{\alpha}})^{1-\alpha}} = h \frac{m^{\frac{1}{\alpha}-1}}{(i^{\frac{1}{\alpha}} - m^{\frac{1}{\alpha}})^{\alpha-1}}, \quad (15)$$

where ζ belongs to the interval $[s_{m-1}, s_m]$ and the mean value theorem of the integral is used. Noting that

$$a_i^i = (s_i^{1/\alpha} - s_{i-1}^{1/\alpha})^\alpha = \zeta^{1/\alpha-1} h, \quad (\zeta \in (s_{i-1}, s_i)). \quad (16)$$

then $a_i^i |e^i|$ can be absorbed by the left-hand side of the inequality when h is sufficiently small. By combining Equations (14) and (15) with the truncation error R_1^i , we can obtain

$$\begin{aligned} |e_i| &\leq |e_0| + \frac{C_0 L}{\Gamma(1+\alpha)} \sum_{m=1}^{i-1} h \frac{m^{\frac{1}{\alpha}-1}}{(i^{\frac{1}{\alpha}} - m^{\frac{1}{\alpha}})^{1-\alpha}} + \frac{L}{\Gamma(1+\alpha)} \zeta^{\frac{1}{\alpha}-1} h + C_2 h \\ &\leq C_3 h + \frac{C_0 L}{\Gamma(1+\alpha)} \sum_{m=1}^{i-1} h \frac{m^{\frac{1}{\alpha}-1}}{(i^{\frac{1}{\alpha}} - m^{\frac{1}{\alpha}})^{1-\alpha}}, \end{aligned}$$

where C_2 and C_3 are two constants independent on h . When applying Lemma 1, the above inequality yields that

$$e_i \leq C_3 h E_{1-\alpha} \left(\frac{\alpha C_0 \Gamma(1-\alpha)}{\Gamma(1+\alpha)} (ih)^{\frac{1-\alpha}{\alpha}} \right).$$

Now, we conclude that Scheme I is first-order accurate. The convergence of Scheme II can be obtained in a similar fashion. $\square$

2.2. Second-Order Accurate Methods

In this subsection, we present the numerical methods based on the following change in variable:

$$t = s^{2/\alpha}.$$

Again, through Equations (7) and (8), one can check that its solution $z(s) \in C^2[0, T]$ with the change in variable. Therefore, we propose a second-order accurate method based on the product trapezoidal quadrature rule; in other words, we have

$$\begin{aligned} & \int_{s_m}^{s_{m+1}} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} f(r^{2/\alpha}, z(r)) dr \\ & \approx \int_{s_m}^{s_{m+1}} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \left(\frac{s_{m+1} - r}{h} f(s_m^{2/\alpha}, z(s_m)) + \frac{r - s_m}{h} f(s_{m+1}^{2/\alpha}, z(s_{m+1})) \right) dr. \end{aligned}$$

Then, it follows from Equation (7) again that

$$\begin{aligned} z(s_i) &= z_0 + \frac{2}{\Gamma(1+\alpha)} \sum_{m=0}^{i-1} \int_{s_m}^{s_{m+1}} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} f(r^{2/\alpha}, z(r)) dr \\ &= z_0 + \frac{2}{\Gamma(1+\alpha)} \sum_{m=0}^{i-1} \int_{s_m}^{s_{m+1}} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \left(\frac{s_{m+1} - r}{h} f(s_m^{2/\alpha}, z(s_m)) + \right. \\ & \quad \left. \frac{r - s_m}{h} f(s_{m+1}^{2/\alpha}, z(s_{m+1})) \right) dr + R_2^i \\ &= z_0 + \frac{2}{\Gamma(1+\alpha)} \sum_{m=0}^i b_m^i f(s_m^{2/\alpha}, z(s_m)) + R_2^i, \end{aligned} \quad (17)$$

where the truncation error is

$$\begin{aligned} R_2^i &= \frac{2}{\Gamma(1+\alpha)} \sum_{m=0}^{i-1} \int_{s_m}^{s_{m+1}} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \left(f(r^{2/\alpha}, z(r)) - \frac{s_{m+1} - r}{h} f(s_m^{2/\alpha}, z(s_m)) - \right. \\ & \quad \left. \frac{r - s_m}{h} f(s_{m+1}^{2/\alpha}, z(s_{m+1})) \right) dr = \mathcal{O}(h^2), \end{aligned}$$

and the coefficient is

$$\begin{aligned} b_0^i &= \int_{s_0}^{s_1} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \frac{s_1 - r}{h} dr = \frac{1}{2} s_i^2 - \frac{1}{2} (s_i^{2/\alpha} - s_1^{2/\alpha})^\alpha - \frac{1}{h} \int_{s_0}^{s_1} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha} dr \\ &= \frac{1}{2} s_i^2 - \frac{1}{2} (s_i^{2/\alpha} - s_1^{2/\alpha})^\alpha - \frac{\alpha}{2h} \int_{s_0}^{s_1} (s_i^{2/\alpha} - u)^{\alpha-1} u^{\alpha/2} du \\ &= \frac{1}{2} s_i^2 - \frac{1}{2} (s_i^{2/\alpha} - s_1^{2/\alpha})^\alpha - \frac{\alpha s_i^{2/\alpha+1}}{2h} \int_0^{(s_1/s_i)^{2/\alpha}} (1-r)^{\alpha-1} r^{\alpha/2} dr \\ &= \frac{1}{2} s_i^2 - \frac{1}{2} (s_i^{2/\alpha} - s_1^{2/\alpha})^\alpha - \frac{\alpha s_i^{2/\alpha+1}}{2h} \mathbf{B}(i-2/\alpha, \alpha/2 + 1, \alpha), \end{aligned}$$

where $\mathbf{B}(i^{-2/\alpha}, \alpha/2 + 1, \alpha)$ is the product of an incomplete beta function and beta function. For $1 \leq m \leq i - 1$, we have

$$\begin{aligned} b_m^i &= \int_{s_m}^{s_{m+1}} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \left(\frac{s_{m+1} - r}{h} \right) dr + \int_{s_{m-1}}^{s_m} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \left(\frac{r - s_{m-1}}{h} \right) dr \\ &= \frac{m+1}{2} \left((s_i^{2/\alpha} - s_m^{2/\alpha})^\alpha - (s_i^{2/\alpha} - s_{m+1}^{2/\alpha})^\alpha \right) - \frac{m-1}{2} \left((s_i^{2/\alpha} - s_{m-1}^{2/\alpha})^\alpha - (s_i^{2/\alpha} - s_m^{2/\alpha})^\alpha \right) \\ &\quad - \frac{\alpha s_i^{2+1}}{2h} \int_{(s_m/s_i)^{2/\alpha}}^{(s_{m+1}/s_i)^{2/\alpha}} (1-r)^{\alpha-1} r^{\alpha/2} dr + \frac{\alpha s_i^{2+1}}{2h} \int_{(s_{m-1}/s_i)^{2/\alpha}}^{(s_m/s_i)^{2/\alpha}} (1-r)^{\alpha-1} r^{\alpha/2} dr \\ &= \frac{m+1}{2} \left((s_i^{2/\alpha} - s_m^{2/\alpha})^\alpha - (s_i^{2/\alpha} - s_{m+1}^{2/\alpha})^\alpha \right) - \frac{m-1}{2} \left((s_i^{2/\alpha} - s_{m-1}^{2/\alpha})^\alpha - (s_i^{2/\alpha} - s_m^{2/\alpha})^\alpha \right) \\ &\quad - \frac{\alpha s_i^{2+1}}{2h} \mathbf{B}((m+1/i)^{2/\alpha}, \alpha/2 + 1, \alpha) + 2 \frac{\alpha s_i^{2+1}}{2h} \mathbf{B}((m/i)^{2/\alpha}, \alpha/2 + 1, \alpha) \\ &\quad - \frac{\alpha s_i^{2+1}}{2h} \mathbf{B}((m-1/i)^{2/\alpha}, \alpha/2 + 1, \alpha). \end{aligned}$$

In addition, we have

$$\begin{aligned} b_i^i &= \int_{s_{i-1}}^{s_i} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \frac{s_i - s_{i-1}}{h} dr \\ &= \frac{\alpha s_i^{2+1}}{2h} \mathbf{B}(1, \frac{\alpha}{2} + 1, \alpha) - \frac{\alpha s_i^{2+1}}{2h} \mathbf{B}((i-1/i)^{2/\alpha}, \frac{\alpha}{2} + 1, \alpha) - \frac{i-1}{2} (s_i^{2/\alpha} - s_{i-1}^{2/\alpha})^\alpha. \end{aligned}$$

Again, by replacing $z(s_i)$ with z_i and omitting the truncation error R_i in Equation (9), we have the following numerical scheme:

$$\text{Scheme III: } z_i = z_0 + \frac{2}{\Gamma(1+\alpha)} \sum_{m=0}^i b_m^i f(s_m^{2/\alpha}, z_m). \quad (18)$$

By applying the Newton linearized method to approximate the nonlinear term, we have the following linearized scheme:

$$\text{Scheme IV: } z_i = z_0 + \frac{2}{\Gamma(1+\alpha)} \sum_{m=0}^{i-1} b_m^i f(s_m^{2/\alpha}, z_m) + \frac{2}{\Gamma(1+\alpha)} b_i^i \left(f(s_i^{2/\alpha}, z_{i-1}) + f_2(s_i^{2/\alpha}, z_{i-1})(z_i - z_{i-1}) \right). \quad (19)$$

$$\text{where } f_2(s_i^{2/\alpha}, z_{i-1}) = \left. \frac{\partial}{\partial y} f(s, y) \right|_{s=s_i^{2/\alpha}, y=z_{i-1}}.$$

By applying the extrapolation to approximate the nonlinear term, we obtain the following linearized scheme:

$$\begin{aligned} \text{Scheme V: } z_0 &= z_0, \\ z_1 &= z_0 + \frac{2}{\Gamma(1+\alpha)} b_0^1 f(s_0^{2/\alpha}, z_0) + \frac{2}{\Gamma(1+\alpha)} b_1^1 \left(f(s_1^{2/\alpha}, z_0) + f_2(s_1^{2/\alpha}, z_0)(z_1 - z_0) \right), \\ z_i &= z_0 + \frac{2}{\Gamma(1+\alpha)} \sum_{m=0}^{i-1} b_m^i f(s_m^{2/\alpha}, z_m) + \frac{2}{\Gamma(1+\alpha)} b_i^i f(s_i^{2/\alpha}, 2z_{i-1} - z_{i-2}), \quad i \geq 2. \end{aligned} \quad (20)$$

Next, we have the following convergence results:

Theorem 2. Suppose $f \in C^3(G)$. Then, the schemes in Equations (18)–(20) are second-order accurate.

Proof. Let $e_i = z(s_i) - z_i$. Subtracting Equation (11) from Equation (9) gives

$$\begin{aligned} |e_i| &= \left| e_0 + \frac{1}{\Gamma(1+\alpha)} \sum_{m=1}^i b_m^i (f(s_m^{1/\alpha}, z_m) - f(s_m^{1/\alpha}, z_m)) + R_2^i \right| \\ &\leq |e_0| + \frac{L}{\Gamma(1+\alpha)} \sum_{m=1}^i b_m^i |e_i| + |R_2^i|. \end{aligned} \quad (21)$$

Now, we present some estimates for the coefficients b_m^i . First, it holds that

$$b_0^i = \int_{s_0}^{s_1} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \frac{s_1-r}{h} dr = \frac{1}{2} s_i^2 - \frac{1}{2} (s_i^{2/\alpha} - s_1^{2/\alpha})^\alpha \leq C_1 h^2$$

For $1 \leq m \leq i-1$, it holds that

$$\begin{aligned} b_m^i &= \int_{s_m}^{s_{m+1}} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \left(\frac{s_{m+1}-r}{h} \right) dr + \int_{s_{m-1}}^{s_m} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \left(\frac{r-s_{m-1}}{h} \right) dr \\ &= (s_i^{2/\alpha} - \xi_m^{2/\alpha})^{\alpha-1} \xi_m^{2/\alpha-1} (s_{m+1} - \xi_m) + (s_i^{2/\alpha} - \xi_m^{2/\alpha})^{\alpha-1} \xi_m^{2/\alpha-1} (\xi_m - s_{m-1}) \\ &\leq C_2 h^2 (i^{2/\alpha} - m^{2/\alpha})^{\alpha-1} m^{2/\alpha-1}, \end{aligned}$$

where C_2 is a constant independent of h , $\xi_m \in (s_m, s_{m+1})$, and $\xi_m \in (s_{m-1}, s_m)$. Noting that

$$b_i^i = \int_{s_{i-1}}^{s_i} (s_i^{2/\alpha} - r^{2/\alpha})^{\alpha-1} r^{2/\alpha-1} \frac{s_i-r}{h} dr \leq h (s_i^{2/\alpha} - s_{i-1}^{2/\alpha})^{\alpha-1} s_i^{2/\alpha-1}$$

then $b_i^i |e^i|$ can be absorbed by the left-hand side of the inequality when h is sufficiently small.

Now, together with the estimates for b_m^i and Lemma 1, we conclude that Scheme III is second-order accurate. The rest of the results can be obtained in a similar manner. $\square$

3. Applications

In this section, several numerical examples are given to illustrate the convergence results, and the L^∞ norm of the error is computed with different α . All numerical examples are calculated by using the software MATLAB, and $T = 1$.

Example 1. We consider the nonlinear time fractional ODEs as follows:

$$D_*^\alpha u - (u^2 - u) = g, t \in (0, T], \quad (22)$$

where $g(t)$ satisfies the exact solution $u = t + t^\alpha, 0 < \alpha < 1$.

We solve Equation (22) by using Schemes I–V. To verify the numerical errors and convergence orders, we use the temporal step sizes $d_s = 1/1000, 1/2000, 1/3000, 1/4000$ with different α in the first-order scheme. The results presented in Tables 1 and 2 indicate that the convergence order was one, which coincided with our theoretical results. In Tables 3–5, we give the maximum error and the convergence orders for the Newton iterative and Newton linearized methods and the extrapolation skills, respectively. In all these cases, the time steps chosen were $d_s = 1/100, 1/200, 1/400, 1/800$, and we can see from Table 3 that the convergence order was two, which is consistent with the theoretical findings. The results illustrated in Tables 4 and 5 indicate that the numerical experiment performed better than the theoretical conclusions. Here, we also compared our methods with some classical ones, and the results in Table 6 indicate that these methods' orders were α . Moreover, we present the evolution of the maximum norm of the error, and the results found in Figure 1 indicate that our method performed well at the beginning.

Table 1. Errors and orders in temporal direction for Scheme I (Example 1).

N	$\alpha = 0.4$		$\alpha = 0.6$		$\alpha = 0.8$	
	Errors	Orders	Errors	Orders	Errors	Orders
1000	3.4639×10^{-1}	*	6.7655×10^{-3}	*	2.2863×10^{-3}	*
2000	1.3343×10^{-1}	1.3763	3.3359×10^{-3}	1.0201	1.8669×10^{-3}	1.0731
3000	8.3082×10^{-2}	1.1685	2.2133×10^{-3}	1.012	7.0564×10^{-4}	1.0649
4000	6.0391×10^{-2}	1.1088	1.6559×10^{-3}	1.0086	5.2011×10^{-4}	1.0643

Table 2. Errors and orders in temporal direction for Scheme II (Example 1).

N	$\alpha = 0.4$		$\alpha = 0.6$		$\alpha = 0.8$	
	Errors	Orders	Errors	Orders	Errors	Orders
1000	4.3014×10^{-1}	*	2.7604×10^{-2}	*	7.1714×10^{-3}	*
2000	2.7749×10^{-1}	0.6324	1.4006×10^{-2}	0.9788	3.5936×10^{-3}	0.9968
3000	2.0582×10^{-1}	0.7368	9.3831×10^{-3}	0.9879	2.3972×10^{-3}	0.9985
4000	1.6379×10^{-1}	0.7941	1.6559×10^{-3}	1.0086	1.7983×10^{-3}	0.9991

Table 3. Errors and orders in temporal direction for Scheme III (Example 1).

N	$\alpha = 0.4$		$\alpha = 0.6$		$\alpha = 0.8$	
	Errors	Orders	Errors	Orders	Errors	Orders
100	1.8761×10^{-2}	*	7.2753×10^{-5}	*	2.6841×10^{-5}	*
200	3.7660×10^{-3}	2.3167	1.8112×10^{-5}	2.0060	6.6615×10^{-6}	2.0105
400	9.0495×10^{-4}	2.0571	4.5335×10^{-6}	1.9983	1.6600×10^{-6}	2.0046
800	2.2606×10^{-4}	2.0012	1.1354×10^{-6}	1.9974	4.1439×10^{-6}	2.0021

Table 4. Errors and orders in temporal direction for Scheme IV (Example 1).

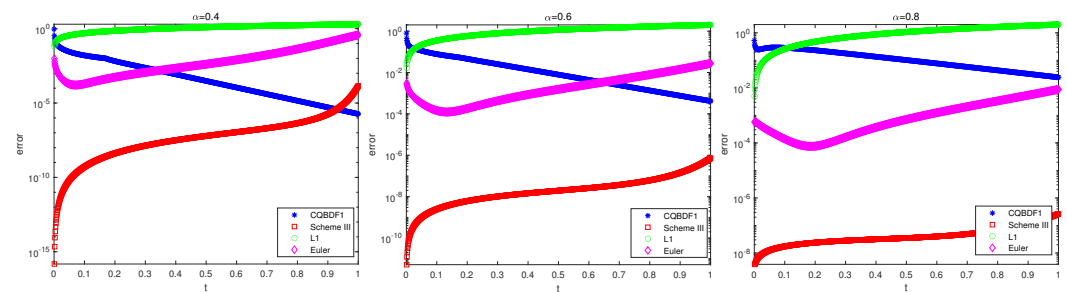
N	$\alpha = 0.4$		$\alpha = 0.6$		$\alpha = 0.8$	
	Errors	Orders	Errors	Orders	Errors	Orders
100	1.5948×10^{-1}	*	2.2079×10^{-3}	*	2.4690×10^{-4}	*
200	3.1524×10^{-2}	2.3388	3.6106×10^{-4}	2.6123	3.8513×10^{-5}	2.6805
400	5.7871×10^{-3}	2.4455	5.8291×10^{-5}	2.6309	6.2528×10^{-6}	2.6228
800	1.0401×10^{-3}	2.4761	9.2534×10^{-6}	2.6552	1.0753×10^{-6}	2.5998

Table 5. Errors and orders in temporal direction for Scheme V (Example 1).

N	$\alpha = 0.4$		$\alpha = 0.6$		$\alpha = 0.8$	
	Errors	Orders	Errors	Orders	Errors	Orders
100	8.7281×10^{-2}	*	1.9757×10^{-3}	*	2.0034×10^{-4}	*
200	2.7388×10^{-2}	1.6721	3.2896×10^{-4}	2.5864	3.1694×10^{-5}	2.6602
400	6.2592×10^{-3}	2.1295	5.3119×10^{-5}	2.6302	5.2614×10^{-6}	2.5907
800	1.2079×10^{-3}	2.3735	8.3960×10^{-6}	2.6615	9.3199×10^{-7}	2.4971

Table 6. Errors and orders in temporal direction.

$\alpha = 0.4$				$\alpha = 0.6$		$\alpha = 0.8$	
	N	Errors	Orders	Errors	Orders	Errors	Orders
Euler	1000	5.8753×10^{-3}	*	2.5839×10^{-3}	*	5.9704×10^{-4}	*
	2000	4.9689×10^{-3}	0.2418	1.7779×10^{-3}	0.5394	3.5089×10^{-4}	0.7668
	4000	4.0802×10^{-3}	0.2843	1.2407×10^{-3}	0.5614	2.0410×10^{-4}	0.7817
	8000	3.2811×10^{-3}	0.3145	8.0860×10^{-4}	0.5752	1.1806×10^{-4}	0.7898
L1	1000	8.3161×10^{-3}	*	2.8395×10^{-3}	*	6.2471×10^{-4}	*
	2000	6.4074×10^{-3}	0.3762	1.8880×10^{-3}	0.5888	3.5977×10^{-4}	0.7961
	4000	4.9231×10^{-3}	0.3802	1.2522×10^{-3}	0.5924	2.0696×10^{-4}	0.7977
	8000	3.7727×10^{-3}	0.3840	8.2909×10^{-4}	0.5949	1.1897×10^{-4}	0.7987
CQBDF1	10	6.6267×10^{-3}	*	1.5370×10^{-3}	*	1.8332×10^{-4}	*
	20	5.1092×10^{-3}	0.3752	1.0393×10^{-3}	0.5646	1.1208×10^{-4}	0.7099
	40	3.9323×10^{-3}	0.3810	6.9808×10^{-4}	0.5741	6.7741×10^{-5}	0.7264
	80	3.0031×10^{-3}	0.3856	4.6667×10^{-4}	0.5810	4.0584×10^{-5}	0.7391

**Figure 1.** Evolution of maximum errors for different methods.

Example 2. We consider the nonlinear time fractional Allen–Cahn equation

$$D_*^\alpha u - u_{xx} - (u - u^3) = g, (x, t) \in \Omega \times (0, T], \quad (23)$$

where $\Omega = [0, \pi]$ and $g(x, t)$ satisfies the exact solution is $u(x, t) = (t + t^\alpha) \sin x$.

Similarly, we solve the time-fractional Allen–Cahn equation by using Scheme III based on a variable transform. We take $M = 1000$ with $N = 8, 16, 32, 64$ to find the maximum of the errors and orders in the temporal direction. Moreover, we consider different spatial step sizes $d_x = \frac{\pi}{M}$, where $M = 8, 16, 32, 64$ with $N = 1000$ for different α . The numerical errors are shown in Tables 7 and 8, respectively, where it can clearly be seen that the convergence orders in the temporal and spatial directions are both two.

Table 7. Errors and orders in temporal direction for Scheme III (Example 2).

$\alpha = 0.4$			$\alpha = 0.6$		$\alpha = 0.8$	
N	Errors	Orders	Errors	Orders	Errors	Orders
8	1.5343×10^{-3}	*	3.4241×10^{-4}	*	7.3544×10^{-4}	*
16	4.3389×10^{-4}	1.8222	8.7884×10^{-5}	1.9459	1.6378×10^{-4}	2.1669
32	1.1709×10^{-4}	1.8897	2.2818×10^{-5}	1.9616	3.8450×10^{-5}	2.0907
64	3.0965×10^{-5}	1.9189	5.8943×10^{-6}	1.9527	9.2644×10^{-6}	2.0532

Table 8. Numerical spatial accuracy of Scheme III for different α (Example 2).

M	$\alpha = 0.4$		$\alpha = 0.6$		$\alpha = 0.8$	
	Errors	Orders	Errors	Orders	Errors	Orders
8	3.4258×10^{-3}	*	3.3368×10^{-3}	*	3.2843×10^{-3}	*
16	8.6220×10^{-4}	1.9903	8.4019×10^{-4}	1.9897	8.2728×10^{-4}	1.9891
32	2.1600×10^{-4}	1.9970	2.1043×10^{-4}	1.9974	2.0720×10^{-4}	1.9974
64	5.4114×10^{-5}	1.9969	5.2643×10^{-5}	1.9990	5.1812×10^{-5}	1.9997

4. Conclusions

In this paper, we presented a family of transformed finite difference methods for numerically solving fractional differential equations while taking the initial singularities of the solutions into account. The convergence results were obtained by using a fractional Grönwall-type inequality. The numerical results were given to illustrate the theoretical results.

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Abbreviations

The following abbreviations are used in this manuscript:

MDPI	Multidisciplinary Digital Publishing Institute
DOAJ	Directory of Open Access Journals
TLA	Three-letter acronym
LD	Linear dichroism

References

- Hilfer, R. *Applications of Fractional Calculus in Physics*; World Scientific: London, UK, 2000.
- Cen, D.; Wang, Z.; Mo, Y. Second order difference schemes for time-fractional KdV-Burgers' equation with initial singularity. *Appl. Math. Lett.* **2021**, *112*, 106829. [\[CrossRef\]](#)
- Li, X.; Wen, J.; Li, D. Mass-and energy-conserving difference schemes for nonlinear fractional Schrödinger equations. *Appl. Math. Lett.* **2021**, *111*, 106686. [\[CrossRef\]](#)
- Fallahgoul, H.; Focardi, S.; Fabozzi, F. Fractional calculus and fractional processes with applications to financial economics. In *Theory and Application*; Academic Press: New York, NY, USA, 2016.
- Koeller, R.C. Applications of fractional calculus to the theory of viscoelasticity. *J. Appl. Mech.* **1984**, *51*, 299–307. [\[CrossRef\]](#)
- Oldham, K.B.; Spanier, J. *The Fractional Calculus*; Academic Press: New York, NY, USA, 1974.
- Zhang, Y.; Sun, Z.; Liao, H. Finite difference methods for time fractional diffusion equations on no-uniform meshes. *J. Comp. Phys.* **2014**, *265*, 195–210. [\[CrossRef\]](#)
- Sun, Z.; Ji, C.; Du, R. A new analytical technique of the L-type difference schemes for time fractional mixed sub-diffusion and diffusion-wave equations. *Appl. Math. Lett.* **2020**, *102*, 106115. [\[CrossRef\]](#)
- Lin, Y.; Xu, C. Finite difference/spectral approximations for the time-fractional diffusion equation. *J. Comput. Phys.* **2007**, *225*, 1533–1552. [\[CrossRef\]](#)
- Jin, B.; Lazarov, R.; Zhou, Z. Error estimates for a semidiscrete finite element method for fractional order parabolic equations. *SIAM J. Numer. Anal.* **2013**, *51*, 445–466. [\[CrossRef\]](#)
- Sun, Z.Z.; Wu, X. A fully discrete difference scheme for a diffusion-wave system. *Appl. Numer. Math.* **2006**, *56*, 193–209. [\[CrossRef\]](#)

12. Chen, X.; Di, Y.; Duan, J.; Li, D. Linearized compact ADI schemes for nonlinear time-fractional Schrödinger equations. *Appl. Math. Lett.* **2018**, *84*, 160–167. [\[CrossRef\]](#)
13. Stynes, M.; Riordan, E.O.; Grace, J.L. Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation. *SIAM J. Numer. Anal.* **2017**, *55*, 1057–1079. [\[CrossRef\]](#)
14. Alikhanov, A.A. A new difference scheme for the time fractional diffusion equation. *J. Comput. Phys.* **2015**, *280*, 424–438. [\[CrossRef\]](#)
15. Ji, C.; Sun, Z. A high-order compact finite difference scheme for the fractional sub-diffusion equation. *J. Sci. Comput.* **2015**, *64*, 959–985. [\[CrossRef\]](#)
16. Zhou, B.; Chen, X.; Li, D. Nonuniform Alikhanov linearized Galerkin finite element methods for nonlinear time-fractional parabolic equations. *J. Sci. Comput.* **2020**, *85*, 39. [\[CrossRef\]](#)
17. Li, D.; Liao, H.; Sun, W.; Wang, J.; Zhang, J. Analysis of L1-Galerkin FEMs for time fractional nonlinear parabolic problems. *Commun. Comput. Phys.* **2018**, *24*, 86–103. [\[CrossRef\]](#)
18. Liao, H.; Li, D.; Zhang, J. Sharp error estimate of the nonuniform L1 formula for linear reaction-subdiffusion equations. *SIAM J. Numer. Anal.* **2018**, *56*, 1112–1133. [\[CrossRef\]](#)
19. Liao, H.; Mclean, W.; Zhang, J. A discrete Grönwall inequality with application to numerical schemes for subdiffusion problems. *SIAM J. Numer. Anal.* **2019**, *57*, 218–237. [\[CrossRef\]](#)
20. Jiang, S.; Zhang, J.; Zhang, Q.; Zhang, Z.Z. Fast evaluation of the Caputo fractional derivative and its applications to fractional diffusion equations. *Commun. Comput. Phys.* **2017**, *21*, 650–678. [\[CrossRef\]](#)
21. Greengard, L.; Strain, J. A fast algorithm for the evaluation of heat potentials. *Commun. Pure Appl. Math.* **1990**, *43*, 949–963. [\[CrossRef\]](#)
22. McLean, W. Fast summation by interval clustering for an evolution equation with memory. *SIAM J. Numer. Anal.* **2012**, *34*, 3039–3056. [\[CrossRef\]](#)
23. Lubich, C. Discretized fractional calculus. *SIAM J. Math. Anal.* **1986**, *17*, 704–719. [\[CrossRef\]](#)
24. Lubich, C. Convolution quadrature and discretized operational calculus. *Numer. Math.* **1988**, *52*, 129–145. [\[CrossRef\]](#)
25. Jin, B.; Li, B.; Zhou, Z. Correction of high-order BDF convolution quadrature for fractional evolution equations. *SIAM J. Comput.* **2017**, *39*, A3129–A3152. [\[CrossRef\]](#)
26. Jin, B.; Li, B.; Zhou, Z. Numerical analysis of nonlinear subdiffusion equations. *SIAM J. Numer. Anal.* **2018**, *56*, 1–23. [\[CrossRef\]](#)
27. Li, D.; She, M.; Sun, H.; Yan, X. A novel discrete fractional Grönwall-type inequality and its application in pointwise-in-time error estimates. *J. Sci. Comput.* **2022**, *91*, 26. [\[CrossRef\]](#)
28. Li, D.; Sun, W.; Wu, C. A novel numerical approach to time-fractional parabolic equations with nonsmooth solutions. *Numer. Math. Theo. Meth. Appl.* **2021**, *14*, 355–376.
29. Qin, H.; Li, D.; Zhang, Z. A novel scheme to capture the initial dramatic evolutions of nonlinear subdiffusion equations. *J. Sci. Comput.* **2021**, *89*, 3. [\[CrossRef\]](#)
30. She, M.; Li, D.; Sun, H. A transformed L1 method for solving the multi-term time-fractional diffusion problem. *Math. Comput. Simu.* **2022**, *193*, 584–606. [\[CrossRef\]](#)
31. Zayernouri, M.; Cao, W.; Zhang, Z.; Karniadakis, G.E. Spectral and discontinuous spectral element methods for fractional delay equations. *SIAM J. Sci. Comput.* **2014**, *36*, B904–B929. [\[CrossRef\]](#)
32. Morgado, M.L.; Ford, N.J.; Lima, P.M. Analysis and numerical methods for fractional differential equations with delay. *J. Comput. Appl. Math.* **2013**, *252*, 159–168. [\[CrossRef\]](#)
33. Kaslik, E.; Sivasundaram, S. Analytical and numerical methods for the stability analysis of linear fractional delay differential equations. *J. Comput. Appl. Math.* **2012**, *236*, 4027–4041. [\[CrossRef\]](#)
34. Diethelm, K.; Ford, N. Analysis of Fractional Differential Equations. *J. Math. Anal. Appl.* **2002**, *265*, 229–248. [\[CrossRef\]](#)
35. Zhang, H.; Zeng, F.; Jiang, X.; Karniadakis, G.E. Convergence analysis of the time-stepping numerical methods for time-fractional nonlinear subdiffusion equations. *Fract. Calc. Appl. Anal.* **2022**, *25*, 453–487. [\[CrossRef\]](#)
36. Cuesta, E.; Lubich, C.; Palencia, C. Convolution quadrature time discretization of fractional diffusion-wave equations. *Math. Comput.* **2006**, *75*, 673–696. [\[CrossRef\]](#)
37. Luchko, Y. Initial-boundary-value problems for the one-dimensional time-fractional diffusion equations. *Fract. Calc. Appl. Anal.* **2012**, *15*, 141–160. [\[CrossRef\]](#)
38. Zhang, H.; Jiang, Y.; Zeng, F. An H_1 convergence of the spectral method for the time-fractional non-linear diffusion equations. *Adv. Comput. Math.* **2021**, *47*, 1–25. [\[CrossRef\]](#)
39. Dixon, J.; McKee, S. Weakly Singular Discrete Gronwall Inequalities. *Z. Fur Angew. Math. Und Mech.* **1986**, *66*, 535–544. [\[CrossRef\]](#)

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