

## A SECOND ORDER APPROXIMATION FOR THE CAPUTO FRACTIONAL DERIVATIVE

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ABSTRACT. When  $0 < \alpha < 1$ , the approximation for the Caputo derivative

$$y^{(\alpha)}(x) = \frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} y(x-kh) + O(h^{2-\alpha}),$$

where  $\sigma_0^{(\alpha)} = 1, \sigma_n^{(\alpha)} = (n-1)^{1-\alpha} - n^{1-\alpha}$  and

$$\sigma_k^{(\alpha)} = (k-1)^{1-\alpha} - 2k^{1-\alpha} + (k+1)^{1-\alpha}, \quad (k = 1 \cdots, n-1),$$

has accuracy  $O(h^{2-\alpha})$ . We use the expansion of  $\sum_{k=0}^n k^\alpha$  to determine an approximation for the fractional integral of order  $2-\alpha$  and the second order approximation for the Caputo derivative

$$y^{(\alpha)}(x) = \frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \delta_k^{(\alpha)} y(x-kh) + O(h^2),$$

where  $\delta_k^{(\alpha)} = \sigma_k^{(\alpha)}$  for  $2 \leq k \leq n$ ,

$$\delta_0^{(\alpha)} = \sigma_0^{(\alpha)} - \zeta(\alpha-1), \delta_1^{(\alpha)} = \sigma_1^{(\alpha)} + 2\zeta(\alpha-1), \delta_2^{(\alpha)} = \sigma_2^{(\alpha)} - \zeta(\alpha-1),$$

and  $\zeta(s)$  is the Riemann zeta function. The numerical solutions of the fractional relaxation and subdiffusion equations are computed.

### 1. INTRODUCTION

Fractional differential equations are used for modeling complex diffusion processes in science and engineering [1–5]. The Caputo fractional derivatives are important as a tool for describing nature as well as for their relation to integer order derivatives and special functions. The Caputo derivative of order  $\alpha$ , when  $0 < \alpha < 1$ , is defined as the convolution of the power function  $x^{-\alpha}$  and the first derivative of the function on the interval  $[0, x]$

$$y^{(\alpha)}(x) = D^\alpha y(x) = \frac{d^\alpha y(x)}{dx^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^x \frac{y'(\xi)}{(x-\xi)^\alpha} d\xi.$$

When the function  $y(x)$  is defined on the interval  $(-\infty, x]$ , the lower limit of the integral in the definition of Caputo derivative is  $-\infty$ . The Caputo derivative of the

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constant function 1 is zero, and

$$D^\alpha D^{1-\alpha} y(x) = y'(x).$$

While the integer order derivatives describe the local behavior of a function, the fractional derivative  $y^{(\alpha)}(x)$  depends on the values of the function on the interval  $[0, x]$ . One approach for discretizing the Caputo derivative is to divide the interval to subintervals of small length and approximate the values of the function on each subinterval with a Lagrange polynomial. Let  $x_n = nh$  and  $y_n = y(x_n) = y(nh)$ , where  $h > 0$  is a small number. The Lagrange polynomial for the function  $y'(x)$  at the midpoint  $x_{k-0.5}$  of the interval  $[x_{k-1}, x_k]$  is the value of  $y'(x_{k-0.5})$ .

Approximation (1) for the Caputo fractional derivative is a commonly used approximation for numerical solutions of ordinary and partial fractional differential equations [6-8].

$$\begin{aligned} \Gamma(1-\alpha)y^{(\alpha)}(x_n) &= \int_0^{x_n} \frac{y'(\xi)}{(x_n-\xi)^\alpha} d\xi \approx \sum_{k=1}^n \int_{x_{k-1}}^{x_k} \frac{y'(x_{k-0.5})}{(x_n-\xi)^\alpha} d\xi \\ &\approx \sum_{k=1}^n \frac{y(x_k) - y(x_{k-1})}{h} \int_{(k-1)h}^{kh} \frac{1}{(nh-\xi)^\alpha} d\xi \\ &= \sum_{k=1}^n \frac{y_k - y_{k-1}}{h} \frac{((n-k+1)h)^{1-\alpha} - ((n-k)h)^{1-\alpha}}{1-\alpha}. \end{aligned}$$

Let  $\rho_k^{(\alpha)} = (n-k+1)^{1-\alpha} - (n-k)^{1-\alpha}$ .

$$\begin{aligned} \Gamma(2-\alpha)h^\alpha y_n^{(\alpha)} &\approx \sum_{k=1}^n \rho_k^{(\alpha)} (y_k - y_{k-1}) = \sum_{k=1}^n y_k \rho_k^{(\alpha)} - \sum_{k=1}^n y_{k-1} \rho_k^{(\alpha)} \\ &= \rho_n^{(\alpha)} y_n + \sum_{k=1}^{n-1} y_k (\rho_k^{(\alpha)} - \rho_{k-1}^{(\alpha)}) - \rho_1^{(\alpha)} y_0. \end{aligned}$$

Then

$$y_n^{(\alpha)} \approx \frac{1}{\Gamma(2-\alpha)h^\alpha} \left( \rho_n^{(\alpha)} y_n + \sum_{k=1}^{n-1} y_{n-k} (\rho_{n-k}^{(\alpha)} - \rho_{n-k+1}^{(\alpha)}) - \rho_1^{(\alpha)} y_0 \right).$$

Let  $\sigma_0^{(\alpha)} = \rho_n^{(\alpha)} = 1$ ,  $\sigma_n^{(\alpha)} = -\rho_1^{(\alpha)} = (n-1)^{1-\alpha} - n^{1-\alpha}$  and

$$\sigma_k^{(\alpha)} = \rho_{n-k}^{(\alpha)} - \rho_{n-k+1}^{(\alpha)} = (k+1)^{1-\alpha} - 2k^{1-\alpha} + (k-1)^{1-\alpha},$$

for  $k = 1, 2, \dots, n-1$ . Denote

$$\mathcal{A}_h y_n = \sum_{k=0}^n \sigma_k^{(\alpha)} y_{n-k}.$$

We obtain the approximation for the Caputo derivative

$$y_n^{(\alpha)} \approx \frac{1}{\Gamma(2-\alpha)h^\alpha} \mathcal{A}_h y_n. \quad (1)$$

Approximation (1) has accuracy  $O(h^{2-\alpha})$  when  $y \in C^2[0, x_n]$  ([9]).

The numbers  $\sigma_k^{(\alpha)}$  have the following properties:

$$\sigma_0^{(\alpha)} > 0, \quad \sigma_1^{(\alpha)} < \sigma_2^{(\alpha)} < \dots < \sigma_k^{(\alpha)} < \dots < 0, \quad \sum_{k=0}^{\infty} \sigma_k^{(\alpha)} = 0.$$

TABLE 1. Error and order of approximation (1) for  $y(x) = \cos x$  on the interval  $[0, 1]$ , when  $\alpha = 0.6$ .

$h$	<i>Error</i>	<i>Ratio</i>	<i>Order</i>
0.05	0.0023484	2.69618	1.43092
0.025	0.000878437	2.67338	1.41867
0.0125	0.000330265	2.65979	1.41131
0.00625	0.000124548	2.65171	1.40692
0.003125	0.0000470549	2.64687	1.40429

Approximation (1) and its modifications have been successfully used for numerical solutions of fractional differential equations, as well as in proofs of the convergence of numerical methods. One disadvantage of (1) is that when the order of the Caputo fractional derivative  $\alpha \approx 1$ , its accuracy decreases to  $O(h)$ . The numerical solutions of multidimensional partial fractional differential equations require a large number of computations, when the approximation has accuracy  $O(h)$ .

In section 4, we determine the second order approximation (4) for the Caputo derivative by modifying the first three coefficients of (1) with values of the Riemann zeta function. Approximation (4) has accuracy  $O(h^2)$  for all values of  $\alpha$  between 0 and 1. The ordinary fractional differential equation

$$y^{(\alpha)} + By = F(t), \quad (2)$$

is called relaxation equation when  $0 < \alpha < 1$ , and oscillation equation when  $1 < \alpha < 2$ . In section 5 we compare the numerical solutions for the relaxation and the time-fractional subdiffusion equations for discretizations (1) and (4). We observe a noticeable improvement of the accuracy of the numerical solutions using approximation (4) for Caputo derivative, especially when  $\alpha \approx 1$ .

When  $y(x)$  is a sufficiently differentiable function, the integral in the definition of the Caputo derivative has a singularity at the endpoint  $x$ . Sidi [10] discusses approximations for integrals with singularities.

The sum of the powers of the first  $n - 1$  integers has expansion [11]

$$\sum_{k=1}^{n-1} k^\alpha = \zeta(-\alpha) + \frac{n^{\alpha+1}}{\alpha+1} \sum_{m=0}^{\infty} \binom{\alpha+1}{m} \frac{B_m}{n^m}, \quad (3)$$

where  $\alpha \neq -1$  and  $B_m$  are the Bernoulli numbers. In section 3, we use expansion (3) to determine a second order approximation (6) for the left Riemann sums and the fractional integral of order  $2 - \alpha$ . In section 4 we determine the second order approximation for the Caputo derivative (4) from (6), using discrete integration by parts and second order backward difference approximation for the second derivative.

## 2. PRELIMINARIES

In this section we introduce the basic definitions and facts used in the paper. The fractional integral of order  $\alpha$  is defined as the convolution of the function  $y(x)$  and the power function  $x^{\alpha-1}$  on the interval  $[0, x]$

$$J^\alpha y(x) = \frac{1}{\Gamma(\alpha)} \int_0^x \frac{y(\xi)}{(x-\xi)^{1-\alpha}} d\xi,$$

where  $\alpha > 0$ . The fractional integral of order  $\alpha$  is often denoted as  $y^{(-\alpha)}(x)$ . The value of the fractional integral of order  $\alpha$  of the constant function 1 is  $x^\alpha/\Gamma(\alpha+1)$ . The Caputo derivative is defined as the composition of  $y'(x)$  with a fractional integral of order  $1-a$ . In Claim 1, we represent the Caputo derivative with the composition of the second derivative  $y''(x)$  and a fractional integral of order  $2-\alpha$

$$y^{(\alpha)}(x) = J^{1-\alpha}y'(x) = J^{2-\alpha}y''(x) + \frac{y'(0)x^{1-\alpha}}{\Gamma(2-\alpha)}.$$

The composition of fractional integrals satisfies

$$J^\alpha J^\beta y(x) = J^\beta J^\alpha y(x) = J^{\alpha+\beta}y(x).$$

The composition of the Caputo derivative and the fractional integral of order  $\alpha$ , when  $0 < \alpha < 1$ , has properties

$$D^\alpha J^\alpha y(x) = y(x), \quad J^\alpha D^\alpha y(x) = y(x) - y(0).$$

In Theorem 3 we use the expansion of the sum of the powers of the first  $n-1$  integers (3), to determine the second order approximation for the fractional integral of order  $2-\alpha$

$$\frac{h^{2-\alpha}}{\Gamma(2-\alpha)} \sum_{k=1}^n k^{1-\alpha} y(x-kh) \approx J^{2-\alpha}y(x) + \frac{y(0)}{2\Gamma(2-\alpha)}x^{1-\alpha}h + \frac{\zeta(\alpha-1)}{\Gamma(2-\alpha)}y(x)h^{2-\alpha},$$

where  $h = x/n$ , and  $\zeta(s)$  is the Riemann zeta function, defined as the analytic continuation of the function

$$\zeta(s) = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \cdots + \frac{1}{n^s} + \cdots = \sum_{n=1}^{\infty} n^{-s} \quad (Re(s) > 1).$$

In the special case of (3), when  $\alpha = -1$ , the sums of the harmonic series have expansion [11]

$$\sum_{k=1}^{n-1} \frac{1}{k} \approx \ln n + \gamma - \frac{1}{2n} - \sum_{s=1}^{\infty} \frac{B_{2m}}{2m} \frac{1}{n^{2m}},$$

where  $\gamma \approx 0.5772$  is the Euler-Mascheroni constant and  $B_{2m}$  are the Bernoulli numbers. In section 4 we use the approximation for the fractional integral (6), to determine the second order approximations for the Caputo fractional derivative

$$\begin{aligned} y^{(\alpha)}(x) &= \frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} y(x-kh) - \frac{\zeta(\alpha-1)}{\Gamma(2-\alpha)} y''(x) h^{2-\alpha} + O(h^2), \\ y^{(\alpha)}(x) &= \frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \delta_k^{(\alpha)} y(x-kh) + O(h^2). \end{aligned} \quad (4)$$

The numbers  $\delta_k^{(\alpha)}$  are computed from the coefficients  $\sigma_k^{(\alpha)}$  of (1) by

$$\begin{aligned} \delta_0^{(\alpha)} &= \sigma_0^{(\alpha)} - \zeta(\alpha-1), \quad \delta_1^{(\alpha)} = \sigma_1^{(\alpha)} + 2\zeta(\alpha-1), \quad \delta_2^{(\alpha)} = \sigma_2^{(\alpha)} - \zeta(\alpha-1), \\ \delta_k^{(\alpha)} &= \sigma_k^{(\alpha)} \quad (k = 2, 3, \dots, n). \end{aligned}$$

The values of the Riemann zeta function satisfy [13]

$$\zeta(s) = \frac{1}{1-2^{1-s}} \sum_{n=0}^{\infty} \frac{1}{2^{n+1}} \sum_{k=0}^n (-1)^k \binom{n}{k} (k+1)^{-s},$$

for all  $s \in \mathbb{C}$ , and the functional equation

$$\zeta(s) = 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(1-s) \zeta(1-s).$$

From the functional equation for the Riemann zeta function we obtain a representation of  $\zeta(\alpha-1)/\Gamma(2-\alpha)$

$$\frac{\zeta(\alpha-1)}{\Gamma(2-\alpha)} = -2^{\alpha-1} \pi^{\alpha-2} \cos\left(\frac{\pi\alpha}{2}\right) \zeta(2-\alpha).$$

### 3. APPROXIMATION FOR THE FRACTIONAL INTEGRAL OF ORDER $2-\alpha$

In this section we determine a second order approximation (6) for the fractional integral of order  $2-\alpha$ , when  $0 < \alpha < 1$

$$J^{2-\alpha}y(x) = \frac{1}{\Gamma(2-\alpha)} \int_0^x (x-\xi)^{1-\alpha} y(\xi) d\xi.$$

Approximation (6) uses the left Riemann sums of a uniform partition of the interval  $[0, x]$ , and the values of  $y(0)$  and  $y(x)$ . The Caputo derivative  $y^{(\alpha)}(x) = J^{1-\alpha}y'(x)$  is defined as the composition of the fractional integral of order  $1-\alpha$  and the first derivative  $y'(x)$ . In Claim 1 we use integration by parts to express the Caputo derivative as a composition of the fractional integral of order  $2-\alpha$  and the second derivative  $y''(x)$ .

**Claim 1.** *Let  $y \in C^2[0, x]$ , and  $0 < \alpha < 1$ .*

$$\Gamma(2-\alpha)y^{(\alpha)}(x) = \Gamma(2-\alpha)J^{2-\alpha}y''(x) + y'(0)x^{1-\alpha}.$$

*Proof.* From the properties of the composition of fractional integrals and Caputo derivatives

$$J^{2-\alpha}y''(x) = J^{1-\alpha}J^1y''(x) = J^{1-\alpha}(y'(x) - y'(0)).$$

Then

$$\begin{aligned} y^{(\alpha)}(x) &= J^{1-\alpha}y'(x) = J^{2-\alpha}y''(x) + J^{1-\alpha}y'(0), \\ y^{(\alpha)}(x) &= J^{2-\alpha}y''(x) + \frac{y'(0)x^{1-\alpha}}{\Gamma(2-\alpha)}. \end{aligned}$$

□

Let  $x = nh$ , where  $n$  is a positive integer. Consider the partition  $\mathcal{P}_h$  of the interval  $[0, x]$  to  $n$  subintervals of length  $h$ . Denote by  $\mathcal{L}_{y,h}^{(\alpha)}$  and  $\mathcal{T}_{y,h}^{(\alpha)}$  the left Riemann sum and the Trapezoidal sum of the function  $(x-\xi)^{1-\alpha}y(\xi)$ .

$$\begin{aligned} \mathcal{L}_{y,h}^{(\alpha)} &= h \sum_{m=0}^n (x-mh)^{1-\alpha} y(mh) = h \sum_{m=0}^{n-1} (nh-mh)^{1-\alpha} y(mh), \\ \mathcal{T}_{y,h}^{(\alpha)} &= \frac{h}{2} \left( (nh)^{1-\alpha} f(0) + 2 \sum_{m=1}^{n-1} (nh-mh)^{1-\alpha} y(mh) \right). \end{aligned}$$

Substitute  $k = n - m$

$$\begin{aligned} \mathcal{L}_{y,h}^{(\alpha)} &= h^{2-\alpha} \sum_{k=1}^n k^{1-\alpha} y(x-kh), \\ \mathcal{T}_{y,h}^{(\alpha)} &= \frac{y(0)}{2} x^{1-\alpha} h + h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} y(x-kh). \end{aligned}$$

The numbers  $\mathcal{L}_{y,h}^{(\alpha)}$  and  $\mathcal{T}_{y,h}^{(\alpha)}$  are approximations for  $\Gamma(2-\alpha)J^{(2-\alpha)}y(x)$  and

$$\mathcal{L}_{y,h}^{(\alpha)} - \mathcal{T}_{y,h}^{(\alpha)} = \frac{y(0)}{2}x^{1-\alpha}h. \quad (5)$$

Now we use (3), to determine a second order approximation for the left Riemann sums of the constant function  $y(x) = 1$ .

**Lemma 2.** *Let  $x = nh$ , where  $n$  is a positive integer.*

$$\mathcal{L}_{1,h}^{(\alpha)} = \frac{x^{2-\alpha}}{2-\alpha} + \frac{1}{2}x^{1-\alpha}h + \zeta(\alpha-1)h^{2-\alpha} + O(h^2).$$

*Proof.* Consider the first terms of (3)

$$\begin{aligned} \sum_{k=1}^{n-1} k^{1-\alpha} &= \frac{n^{2-\alpha}}{2-\alpha} - \frac{n^{1-\alpha}}{2} + \zeta(\alpha-1) + O\left(\frac{1}{n^\alpha}\right), \\ \sum_{k=1}^n k^{1-\alpha} &= \frac{n^{2-\alpha}}{2-\alpha} + \frac{n^{1-\alpha}}{2} + \zeta(\alpha-1) + O\left(\frac{1}{n^\alpha}\right). \end{aligned}$$

Multiply by  $h^{2-\alpha}$

$$h^{2-\alpha} \sum_{k=1}^n k^{1-\alpha} = \frac{x^{2-\alpha}}{2-\alpha} + \frac{1}{2}x^{1-\alpha}h + \zeta(\alpha-1)h^{2-\alpha} + O\left(\frac{h^{2-\alpha}}{n^\alpha}\right).$$

We have that  $h^{2-\alpha}/n^\alpha = h^2/x^\alpha$ . Hence

$$\mathcal{L}_{1,h}^{(\alpha)} = \frac{x^{2-\alpha}}{2-\alpha} + \frac{1}{2}x^{1-\alpha}h + \zeta(\alpha-1)h^{2-\alpha} + O(h^2).$$

□

In the next theorem we determine a second order approximation for the left Riemann sums of the fractional integral  $J^{2-\alpha}y(x)$  when the function  $y(x)$  is a polynomial.

**Theorem 3.** *Let  $x = nh$  and  $y(x)$  be a polynomial.*

$$\mathcal{L}_{y,h}^{(\alpha)} = \Gamma(2-\alpha)J^{2-\alpha}y(x) + \frac{y(0)}{2}x^{1-\alpha}h + \zeta(\alpha-1)y(x)h^{2-\alpha} + O(h^2). \quad (6)$$

*Proof.* Let  $y(\xi)$  be a polynomial of degree  $m$ . The Taylor polynomial for  $y(\xi)$  of degree  $m$  at the point  $\xi = x$  is equal to  $y(\xi)$ .

$$y(\xi) = p_0 + p_1(x-\xi) + \cdots + p_m(x-\xi)^m = p_0 + \sum_{k=1}^m p_k(x-\xi)^k.$$

Denote

$$y_0(\xi) = y(\xi) - y(x) = \sum_{k=1}^m p_k(x-\xi)^k.$$

The function  $(x-\xi)^{1-\alpha}y_0(\xi)$  has a bounded derivative on the interval  $[0, x]$ . The trapezoidal approximation  $\mathcal{T}_{y_0,h}^{(\alpha)}$  is a second order approximation for the fractional integral  $\Gamma(2-\alpha)J^{(2-\alpha)}y_0(x)$ . From Lemma 2 and (5)

$$\mathcal{T}_{1,h}^{(\alpha)} = \frac{x^{2-\alpha}}{2-\alpha} + \zeta(\alpha-1)h^{2-\alpha} + O(h^2).$$

Then

$$\mathcal{T}_{y,h}^{(\alpha)} = \mathcal{T}_{y_0,h}^{(\alpha)} + p_0 \mathcal{T}_{1,h}^{(\alpha)} = \Gamma(2-\alpha)J^{2-\alpha}y_0(x) + \frac{p_0}{2-\alpha}x^{2-\alpha} + p_0\zeta(\alpha-1)h^{2-\alpha} + O(h^2).$$

We have that  $y(x) = p_0$  and  $J^{2-\alpha}1 = x^{2-\alpha}/\Gamma(3-\alpha)$ ,

$$\Gamma(2-\alpha)J^{2-\alpha}y(x) = \Gamma(2-\alpha)J^{2-\alpha}y_0(x)(x) + \frac{p_0}{2-\alpha}x^{2-\alpha}.$$

Hence

$$\mathcal{T}_{y,h}^{(\alpha)} = \mathcal{L}_{y,h}^{(\alpha)} - \frac{y(0)}{2}x^{1-\alpha}h = \Gamma(2-\alpha)J^{2-\alpha}y(x) + y(x)\zeta(\alpha-1)h^{2-\alpha} + O(h^2).$$

□

In Theorem 3 we showed that (6) is a second order approximation for the left Riemann sums and the fractional integral of order  $2 - \alpha$ , when the function  $y(x)$  is a polynomial. From the Weierstrass Approximation Theorem every sufficiently differentiable function and its derivatives on the interval  $[0, x]$  are uniform limit of polynomials. The class of functions for which Theorem 3 holds includes functions with bounded derivatives. In section 4, we present a proof for the second order approximation (4) of the Caputo derivative.

TABLE 2. Error and order of approximation (6) for  $y(x) = \cos x$  (left) and  $y(x) = \ln(x + 1)$  (right) on the interval  $[0, 1]$ , when  $\alpha = 0.4$ .

$h$	<i>Error</i>	<i>Order</i>	$h$	<i>Error</i>	<i>Order</i>
0.05	0.00011853	1.95822	0.05	0.00020451	1.98580
0.025	0.00003019	1.97331	0.025	0.00005145	1.99083
0.0125	$7.63 \times 10^{-6}$	1.98275	0.0125	0.00001292	1.99400
0.00625	$1.92 \times 10^{-6}$	1.98876	0.00625	$3.24 \times 10^{-6}$	1.99606
0.003125	$4.83 \times 10^{-7}$	1.99264	0.003125	$8.11 \times 10^{-7}$	1.99740

#### 4. SECOND ORDER APPROXIMATION FOR THE CAPUTO DERIVATIVE

In this section we use approximation (6) to determine a second order discretization for the Caputo derivative of order  $\alpha$ , by modifying the first three coefficients of approximation (1) with the value of the Riemann zeta function at the point  $\alpha - 1$ .

Denote by  $\Delta_h^1 y_n$  and  $\Delta_h^2 y_n$  the forward difference and the central difference of the function  $y(x)$  at the point  $x_n = nh$ .

$$\Delta_h^1 y_n = y_{n+1} - y_n,$$

$$\Delta_h^2 y_n = y_{n+1} - 2y_n + y_{n-1}.$$

When  $y(x)$  is a sufficiently differentiable function

$$y'_{n+0.5} = \frac{\Delta_h^1 y_n}{h} + O(h^2), \quad y''_n = \frac{\Delta_h^2 y_n}{h^2} + O(h^2).$$

**Lemma 4.**

$$\mathcal{A}_h y_n = \sum_{k=1}^{n-1} k^{1-\alpha} \Delta_h^2 y_{n-k} + n^{1-\alpha} \Delta_h^1 y_0.$$

*Proof.*

$$\begin{aligned} \mathcal{A}_h y_n &= \sum_{k=0}^n \sigma_k^{(\alpha)} y_{n-k} = \sigma_0^{(\alpha)} y_n + \sum_{k=1}^{n-1} \sigma_k^{(\alpha)} y_{n-k} + \sigma_n^{(\alpha)} y_0 \\ &= y_n + \sum_{k=1}^{n-1} \left( (k-1)^{1-\alpha} - 2k^{1-\alpha} + (k+1)^{1-\alpha} \right) y_{n-k} + \sigma_n^{(\alpha)} y_0 \\ &= y_n + \sum_{k=1}^{n-1} (k-1)^{1-\alpha} y_{n-k} - 2 \sum_{k=1}^{n-1} k^{1-\alpha} y_{n-k} + \sum_{k=1}^{n-1} (k+1)^{1-\alpha} y_{n-k} + \sigma_n^{(\alpha)} y_0. \end{aligned}$$

Substitute  $K = k - 1$  in the first sum and  $K = k + 1$  in the third sum

$$\mathcal{A}_h y_n = y_n + \sum_{K=1}^{n-2} K^{1-\alpha} y_{n-K-1} - 2 \sum_{k=1}^{n-1} k^{1-\alpha} y_{n-k} + \sum_{K=2}^n K^{1-\alpha} y_{n-K+1} + \sigma_n^{(\alpha)} y_0.$$

We have that

$$\begin{aligned} \sum_{k=1}^{n-2} k^{1-\alpha} y_{n-k-1} &= \sum_{k=1}^{n-1} k^{1-\alpha} y_{n-k-1} - (n-1)^{1-\alpha} y_0, \\ y_n + \sum_{k=2}^n k^{1-\alpha} y_{n-k+1} &= \sum_{k=1}^n k^{1-\alpha} y_{n-k+1} = \sum_{k=1}^{n-1} k^{1-\alpha} y_{n-k+1} + n^{1-\alpha} y_1. \end{aligned}$$

Then

$$\mathcal{A}_h y_n = \sum_{k=1}^{n-1} k^{1-\alpha} (y_{n-k+1} - 2y_{n-k} + y_{n-k-1}) + n^{1-\alpha} (y_1 - y_0),$$

because  $\sigma_n^{(\alpha)} = (n-1)^{1-\alpha} - n^{1-\alpha}$ .  $\square$

**Lemma 5.** *Suppose that  $y(x)$  is sufficiently differentiable function on  $[0, nh]$*

$$\frac{1}{h^\alpha} \mathcal{A}_h y_n = h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} y''_{n-k} + (nh)^{1-\alpha} y'_{0.5} + O(h^2).$$

*Proof.* From Lemma 4

$$\frac{1}{h^\alpha} \mathcal{A}_h y_n = \sum_{k=1}^{n-1} k^{1-\alpha} \Delta_h^2 y_{n-k} + n^{1-\alpha} \Delta_h^1 y_0 = h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} \frac{\Delta_h^2}{h^2} y_{n-k} + n^{1-\alpha} h^{1-\alpha} \frac{\Delta_h^1 y_0}{h},$$

$$\frac{1}{h^\alpha} \mathcal{A}_h y_n = h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} (y''_{n-k} + O(h^2)) + (nh)^{1-\alpha} (y'_{0.5} + O(h^2)),$$

$$\frac{1}{h^\alpha} \mathcal{A}_h y_n = h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} y''_{n-k} + (nh)^{1-\alpha} y'_{0.5} + O(h^2) \left( (nh)^{1-\alpha} + h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} \right).$$

The number  $(nh)^{1-\alpha} \sim O(1)$  is bounded. From (3) we have

$$h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} \sim h^{2-\alpha} O(n^{2-\alpha}) \sim O(1).$$



Therefore

$$\frac{1}{h^\alpha} \mathcal{A}_h y_n = h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} y''_{n-k} + (nh)^{1-\alpha} y'_{0.5} + O(h^2).$$

□

**Theorem 6.** *Let  $y$  be a polynomial and  $x = nh$ .*

$$\frac{1}{h^\alpha} \mathcal{A}_h y(x) = \Gamma(2 - \alpha) y_n^{(\alpha)} + \zeta(\alpha - 1) y''(x) h^{2-\alpha} + O(h^2).$$

*Proof.* From Lemma 5

$$\begin{aligned} \frac{1}{h^\alpha} \mathcal{A}_h y(x) &= h^{2-\alpha} \sum_{k=1}^{n-1} k^{1-\alpha} y''_{n-k} + (nh)^{1-\alpha} y'_{0.5} + O(h^2) = \\ &= h^{2-\alpha} \sum_{k=1}^n k^{1-\alpha} y''_{n-k} - h^{2-\alpha} n^{1-\alpha} y''_0 + x^{1-\alpha} y'_{0.5} + O(h^2). \end{aligned}$$

Then

$$\frac{1}{h^\alpha} \mathcal{A}_h y(x) = \mathcal{L}_{y'',h}^{(\alpha)} - x^{1-\alpha} (hy''_0 - y'_{0.5}) + O(h^2).$$

From Claim 1 and Theorem 3

$$\mathcal{L}_{y'',h}^{(\alpha)} = \Gamma(2 - \alpha) J^{2-\alpha} y''(x) + \frac{y''(0)}{2} x^{1-\alpha} h + \zeta(\alpha - 1) y''(x) h^{2-\alpha} + O(h^2),$$

$$\Gamma(2 - \alpha) y^{(\alpha)}(x) = \Gamma(2 - \alpha) J^{2-\alpha} y''(x) + y'(0) x^{1-\alpha}.$$

Then

$$\mathcal{L}_{y'',h}^{(\alpha)} = \Gamma(2 - \alpha) y^{(\alpha)}(x) + \zeta(\alpha - 1) y''(x) h^{2-\alpha} - x^{1-\alpha} \left( y'_0 - \frac{y''_0 h}{2} \right) + O(h^2),$$

$$\frac{1}{h^\alpha} \mathcal{A}_h y(x) = \Gamma(2 - \alpha) y^{(\alpha)}(x) + \zeta(\alpha - 1) y''(x) h^{2-\alpha} - x^{1-\alpha} \left( y'_0 + \frac{y''_0 h}{2} - y'_{0.5} \right) + O(h^2).$$

By Taylor's expansion

$$y'_0 + \frac{y''_0 h}{2} - y'_{0.5} = O(h^2).$$

Hence

$$\frac{1}{h^\alpha} \mathcal{A}_h y(x) = \Gamma(2 - \alpha) y^{(\alpha)}(x) + \zeta(\alpha - 1) y''(x) h^{2-\alpha} + O(h^2).$$

□

In Theorem 6 we determined the second order approximation for the Caputo derivative

$$y_n^{(\alpha)} = \frac{1}{\Gamma(2 - \alpha) h^\alpha} \mathcal{A}_h y_n - \frac{\zeta(\alpha - 1)}{\Gamma(2 - \alpha)} y''_n h^{2-\alpha} + O(h^2). \tag{7}$$

**Corollary 7.** *Let  $y(x)$  be a polynomial.*

$$y_n^{(\alpha)} = \frac{1}{\Gamma(2 - \alpha) h^\alpha} \sum_{k=0}^n \delta_k^{(\alpha)} y_{n-k} + O(h^2),$$

where  $\delta_k^{(\alpha)} = \sigma_k^{(\alpha)}$  for  $2 \leq k \leq n$  and

$$\delta_0^{(\alpha)} = \sigma_0^{(\alpha)} - \zeta(\alpha - 1), \delta_1^{(\alpha)} = \sigma_1^{(\alpha)} + 2\zeta(\alpha - 1), \delta_2^{(\alpha)} = \sigma_2^{(\alpha)} - \zeta(\alpha - 1).$$

*Proof.* The second order backward difference approximation for the second derivative  $y_n''$  has accuracy  $O(h)$ .

$$y_n'' = \frac{y_n - 2y_{n-1} + y_{n-2}}{h^2} + O(h).$$

From approximation (7)

$$y_n^{(\alpha)} = \frac{1}{\Gamma(2-\alpha)h^\alpha} \mathcal{A}_h y_n - \frac{\zeta(\alpha-1)}{\Gamma(2-\alpha)} \left( \frac{y_n - 2y_{n-1} + y_{n-2}}{h^2} + O(h) \right) h^{2-\alpha} + O(h^2),$$

$$y_n^{(\alpha)} = \frac{1}{\Gamma(2-\alpha)h^\alpha} \mathcal{A}_h y_n - \frac{\zeta(\alpha-1)}{\Gamma(2-\alpha)h^\alpha} (y_n - 2y_{n-1} + y_{n-2}) + O(h^2),$$

$$y_n^{(\alpha)} = \frac{1}{\Gamma(2-\alpha)h^\alpha} \left( \sum_{k=0}^n \sigma_k^{(\alpha)} y_{n-k} - \zeta(\alpha-1) (y_n - 2y_{n-1} + y_{n-2}) \right) + O(h^2).$$

□

TABLE 3. Error and order of approximation (4) for Caputo derivative of order  $\alpha = 0.25$  and  $y(x) = \cos x$  (left),  $y(x) = \ln(x+1)$  (right) on  $[0, 1]$ .

$h$	<i>Error</i>	<i>Order</i>	$h$	<i>Error</i>	<i>Order</i>
0.05	0.000081955	2.30047	0.05	0.000029455	2.31171
0.025	0.000017556	2.22284	0.025	$6.39 \times 10^{-6}$	2.20475
0.0125	$3.95 \times 10^{-6}$	2.15376	0.0125	$1.46 \times 10^{-6}$	2.13162
0.00625	$9.20 \times 10^{-7}$	2.10073	0.00625	$3.44 \times 10^{-7}$	2.08272
0.003125	$2.20 \times 10^{-7}$	2.06368	0.003125	$8.31 \times 10^{-8}$	2.05103

Denote

$$\mathcal{B}_h y(x) = \sum_{k=0}^n \delta_k^{(\alpha)} y(x - kh).$$

In Corollary 7 we showed that (4) is a second order approximation for the Caputo derivative of polynomials. Now we use the Weierstrass Approximation Theorem to extend the result to differentiable functions.

**Theorem 8.** *Let  $x = nh$  and  $y$  be a sufficiently differentiable function.*

$$y^{(\alpha)}(x) = \frac{1}{\Gamma(2-\alpha)h^\alpha} \mathcal{B}_h y(x) + O(h^2).$$

*Proof.* By the Weierstrass Approximation Theorem every continuous function is a uniform limit of polynomials. Let  $\epsilon > 0$  and  $p_\epsilon(x)$  be a polynomial such that

$$|y'(t) - p_\epsilon(t)| < \epsilon,$$

for all  $t \in [0, x]$ . Define

$$q_\epsilon(t) = y(0) + \int_0^t p_\epsilon(\xi) d\xi.$$

The function  $q_\epsilon(t)$  is polynomial, and  $q_\epsilon'(t) = p_\epsilon(t)$ . We have that

$$|y(t) - q_\epsilon(t)| = \left| \int_0^t (y'(\xi) - p_\epsilon(\xi)) d\xi \right| \leq \int_0^t |y'(\xi) - p_\epsilon(\xi)| d\xi < \int_0^x \epsilon d\xi \leq x\epsilon,$$

for all  $t \in [0, x]$ .

$$\bullet \Gamma(1 - \alpha) \left| y^{(\alpha)}(x) - q_\epsilon^{(\alpha)}(x) \right| = \left| \int_0^x \frac{y'(\xi) - q'_\epsilon(\xi)}{(x - \xi)^\alpha} d\xi \right| \leq \int_0^x \frac{|y'(\xi) - p_\epsilon(\xi)|}{(x - \xi)^\alpha} d\xi,$$

$$\left| y^{(\alpha)}(x) - q_\epsilon^{(\alpha)}(x) \right| < \frac{\epsilon}{\Gamma(1 - \alpha)} \int_0^x (x - \xi)^{-\alpha} d\xi = \frac{\epsilon x^{1-\alpha}}{\Gamma(2 - \alpha)}.$$

Therefore

$$\lim_{\epsilon \rightarrow 0} q_\epsilon^{(\alpha)}(x) = y^{(\alpha)}(x).$$

• Now we estimate  $\mathcal{B}_h(y(x) - q_\epsilon(x))$ .

$$\left| \sum_{k=0}^n \delta_k^{(\alpha)} (y_{n-k} - q_{\epsilon, n-k}) \right| \leq \sum_{k=0}^n |\delta_k^{(\alpha)}| |y_{n-k} - q_{\epsilon, n-k}| \leq x\epsilon \sum_{k=0}^n |\delta_k^{(\alpha)}|.$$

We have that

$$\sum_{k=0}^n |\delta_k^{(\alpha)}| \leq \sum_{k=0}^n |\sigma_k^{(\alpha)}| + 3|\zeta(\alpha - 1)| = 2 - 3\zeta(\alpha - 1).$$

Hence

$$|\mathcal{B}_h(y(x) - q_\epsilon(x))| \leq (2 - 3\zeta(\alpha - 1))x\epsilon,$$

and

$$\lim_{\epsilon \rightarrow 0} \mathcal{B}_h q_\epsilon(x) = \mathcal{B}_h y(x).$$

• From Corollary 7

$$q_\epsilon^{(\alpha)}(x) = \frac{1}{\Gamma(2 - \alpha)h^\alpha} \mathcal{B}_h q_\epsilon(x) + O(h^2).$$

By letting  $\epsilon \rightarrow 0$ , we obtain

$$y^{(\alpha)}(x) = \frac{1}{\Gamma(2 - \alpha)h^\alpha} \mathcal{B}_h y(x) + O(h^2).$$

□

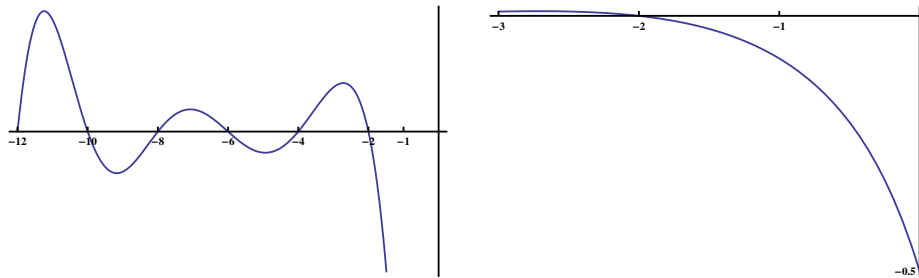


FIGURE 1. Graphs of the Riemann zeta function on the intervals  $[-12, -1]$  and  $[-3, 0]$ .

In Table 3 we compute the error and the numerical order of approximation (4) for the Caputo derivative of the functions  $y(x) = \cos x$  and  $y(x) = \ln(x + 1)$  on the interval  $[0, 1]$ , when  $\alpha = 0.25$ . In Claim 9 and Lemma 10 we discuss the properties of the coefficients  $\sigma_2^{(\alpha)}$  and  $\delta_2^{(\alpha)}$ .

**Claim 9.** Let  $0 < \alpha < 1$

$$-0.1 < \sigma_2^{(\alpha)} < 0.$$

*Proof.* Denote

$$\sigma(\alpha) = -\sigma_2^{(1-\alpha)} = 2^{\alpha+1} - 3^\alpha - 1.$$

The function  $\sigma(\alpha)$  has values  $\sigma(0) = \sigma(1) = 0$ , and

$$\sigma'(\alpha) = \ln 2 \cdot 2^{\alpha+1} - \ln 3 \cdot 3^\alpha.$$

The first derivative of  $\sigma(\alpha)$  is zero when

$$\ln 2 \cdot 2^{\alpha+1} = \ln 3 \cdot 3^\alpha, \quad \left(\frac{3}{2}\right)^\alpha = \frac{2 \cdot \ln 2}{\ln 3}, \quad \alpha = \frac{\ln\left(\frac{2 \cdot \ln 2}{\ln 3}\right)}{\ln(3/2)} \approx 0.5736.$$

The function  $\sigma(\alpha)$  is positive and has a maximum value  $\sigma(0.5736) \approx 0.0985$  on the interval  $[0, 1]$ .  $\square$

The Riemann zeta function has zeroes at the negative even integers and is decreasing on the interval  $[-2, 1]$ . The value of  $\zeta(\alpha - 1)$  is negative, when  $\alpha$  is between 0 and 1. Then  $\delta_0^{(\alpha)} > 0$  and  $\delta_1^{(\alpha)} < 0$ . From the properties of the coefficients of (1), the numbers  $\delta_n^{(\alpha)} = \sigma_n^{(\alpha)}$  are negative, for  $n \geq 3$ .

**Lemma 10.** The number  $\delta_2^{(\alpha)}$  is positive when  $0 < \alpha < 1$ .

*Proof.* From the definition of  $\delta_2^{(1-\alpha)}$

$$\delta_2^{(1-\alpha)} = \sigma_2^{(1-\alpha)} - \zeta(-\alpha) = -\sigma(\alpha) - \zeta(-\alpha) = z(\alpha) - \sigma(\alpha).$$

where  $z(\alpha) = -\zeta(-\alpha)$ . The function  $z(\alpha)$  is decreasing on the interval  $[0, 1]$  with values at the endpoints  $z(0) = 0.5$  and  $z(1) = 1/12 = 0.08333$ . The function  $\sigma(\alpha)$  is increasing on the interval  $[0, 0.5736]$  and decreasing on the interval  $[0.5736, 1]$ .

Now we show that the minimum values of  $\delta_2^{(1-\alpha)}$  on the intervals  $[0, 0.8]$  and  $[0.8, 1]$  are positive.

$$\min_{\alpha \in [0, 0.8]} \delta_2^{(1-\alpha)} > \min_{\alpha \in [0, 0.8]} z(\alpha) - \max_{\alpha \in [0, 0.8]} \sigma(\alpha),$$

$$\min_{\alpha \in [0, 0.8]} \delta_2^{(1-\alpha)} > z(0.8) - \sigma(0.5736) \approx 0.122 - 0.0985 = 0.0235.$$

and

$$\min_{\alpha \in [0.8, 1]} \delta_2^{(1-\alpha)} > \min_{\alpha \in [0.8, 1]} z(\alpha) - \max_{\alpha \in [0.8, 1]} \sigma(\alpha),$$

$$\min_{\alpha \in [0.8, 1]} \delta_2^{(1-\alpha)} > z(1) - \sigma(0.8) \approx 0.083 - 0.074 = 0.009.$$

Therefore the numbers  $\delta_2^{(1-\alpha)}$  are positive when  $0 < \alpha < 1$ .  $\square$

5. NUMERICAL EXPERIMENTS

In section 4 we showed that the approximation for the Caputo derivative

$$y_n^{(\alpha)} \approx \frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \delta_k^{(\alpha)} y_n,$$

has accuracy  $O(h^2)$  when  $n \geq 2$ . The numbers  $\delta_k^{(\alpha)}$  satisfy

$$\delta_0^{(\alpha)} > 0, \delta_1^{(\alpha)} < 0, \delta_2^{(\alpha)} > 0, \delta_3^{(\alpha)} < \delta_4^{(\alpha)} < \dots < \delta_k^{(\alpha)} < \dots < 0, \sum_{k=0}^{\infty} \delta_k^{(\alpha)} = 0.$$

In this section we compare the performance of the numerical solutions of the fractional relaxation and time-fractional subdiffusion equations using approximations (1) and (4) for Caputo derivative. From the Mean-Value theorem for the Caputo derivative

$$y(h) - y(0) = \frac{h^\alpha}{\Gamma(1+\alpha)} y^{(\alpha)}(\theta), \quad (0 < \theta < h).$$

The numbers  $\Gamma(1+\alpha)$  and  $\Gamma(2-\alpha)$  are between 0 and 1, when  $0 < \alpha < 1$ .

**Lemma 11.** *Let  $y$  be a sufficiently differentiable function on  $[0, h]$*

$$y(h) - y(0) - h^\alpha \Gamma(2-\alpha) y^{(\alpha)}(h) = O(h^2). \tag{8}$$

*Proof.* From the definition of the Caputo derivative

$$y^{(\alpha)}(h) = \frac{1}{\Gamma(1-\alpha)} \int_0^h \frac{y'(\xi)}{(h-\xi)^\alpha} d\xi.$$

Expand the function  $y'(\xi)$  around  $\xi = 0$

$$y'(\xi) = y'(0) + \xi y''(0) + O(h^2),$$

$$\begin{aligned} \Gamma(1-\alpha) y^{(\alpha)}(h) &= \int_0^h \frac{y'(0) + \xi y''(0) + O(h^2)}{(h-\xi)^\alpha} d\xi = \\ &= y'(0) \int_0^h \frac{1}{(h-\xi)^\alpha} + y''(0) \int_0^h \frac{\xi}{(h-\xi)^\alpha} d\xi + O(h^2) \int_0^h \frac{1}{(h-\xi)^\alpha} d\xi. \end{aligned}$$

We have that

$$\int_0^h \frac{1}{(h-\xi)^\alpha} d\xi = \frac{h^{1-\alpha}}{1-\alpha}, \quad \int_0^h \frac{\xi}{(h-\xi)^\alpha} d\xi = \frac{h^{2-\alpha}}{(1-\alpha)(2-\alpha)}.$$

Then

$$\Gamma(1-\alpha) y^{(\alpha)}(h) = \frac{h^{1-\alpha}}{1-\alpha} y'(0) + \frac{h^{2-\alpha}}{(1-\alpha)(2-\alpha)} y''(0) + O(h^{3-\alpha}),$$

$$\Gamma(2-\alpha) h^\alpha y^{(\alpha)}(h) = h \left( y'(0) + \frac{h}{2-\alpha} y''(0) \right) + O(h^{3-\alpha}),$$

$$\Gamma(2-\alpha) h^\alpha y^{(\alpha)}(h) = h \left( y'(0) + \frac{h}{2} y''(0) \right) + O(h^2),$$

$$\Gamma(2-\alpha) h^\alpha y^{(\alpha)}(h) = h y' \left( \frac{h}{2} \right) + O(h^2) = y(h) - y(0) + O(h^2).$$

□

**5.1. Numerical Solution of the Fractional Relaxation Equation.** The fractional relaxation equation (2) is an ordinary fractional differential equation with constant coefficients. The exact solution of the fractional relaxation equation is determined with the Laplace transform method [14]. Numerical solutions of the relaxation equation are discussed in [19-21]. In this section we compare the numerical solutions of the equation

$$y^{(\alpha)} + y = F(t), \quad (9)$$

for approximations (1) and (4) of the Caputo derivative. When the solution  $y(t)$  of (9) is a continuously differentiable function, the initial condition  $y(0)$  is determined from the function  $F(t)$  by  $y(0) = F(0)$ . Let

$$F(t) = 1 - 4t + 5t^2 - \frac{4}{\Gamma(2-\alpha)}t^{1-\alpha} + \frac{10}{\Gamma(3-\alpha)}t^{2-\alpha}.$$

Equation (9) has the solution

$$y(t) = 1 - 4t + 5t^2,$$

and the initial value  $y(0) = 1$ . Now we determine a second order numerical solution of (9) on the interval  $[0, 1]$ , using approximations (4) and (8) for the Caputo derivative.

Let  $h = 1/N$ , where  $N$  is a positive integer, and  $y_n = y(x_n) = y(nh)$ . In Lemma 11, we showed that (8)

$$\frac{y(h) - y(0)}{\Gamma(2-\alpha)h^\alpha} = y^{(\alpha)}(h) + O(h^{2-\alpha}). \quad (10)$$

Approximate the Caputo derivative  $y^{(\alpha)}(h)$  in equation (9)

$$\frac{y(h) - y(0)}{\Gamma(2-\alpha)h^\alpha} + y(h) = F(h) + O(h^{2-\alpha}),$$

$$y_1(1 + \Gamma(2-\alpha)h^\alpha) = y_0 + \Gamma(2-\alpha)h^\alpha F_1 + O(h^2).$$

Let  $\{\tilde{y}_k\}_{k=0}^N$  be an approximation for the exact solution  $y_k$  at the points  $x_k = kh$ . Set  $\tilde{y}_0 = y(0) = 1$ . The value of  $\tilde{y}_1$  is computed from the above approximation with accuracy  $O(h^2)$

$$\tilde{y}_1 = \frac{\tilde{y}_0 + \Gamma(2-\alpha)h^\alpha F_1}{1 + \Gamma(2-\alpha)h^\alpha}.$$

The numbers  $\tilde{y}_n$ , for  $n \geq 2$ , are computed from equation (9) by approximating the Caputo derivative  $y_n^{(\alpha)}$  with (4).

$$\frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \delta_k^{(\alpha)} y_{n-k} + y_n = F_n + O(h^2),$$

$$y_n \left( \delta_0^{(\alpha)} + \Gamma(2-\alpha)h^\alpha \right) = \Gamma(2-\alpha)h^\alpha F_n - \sum_{k=1}^n \delta_k^{(\alpha)} y_{n-k} + O(h^{2+\alpha}).$$

The numerical solution  $\{\tilde{y}_k\}_{k=0}^N$ , for  $2 \leq n \leq N$ , is computed explicitly with

$$\tilde{y}_n = \frac{1}{\delta_0^{(\alpha)} + \Gamma(2-\alpha)h^\alpha} \left( \Gamma(2-\alpha)h^\alpha F_n - \sum_{k=1}^n \delta_k^{(\alpha)} \tilde{y}_{n-k} \right). \quad (11)$$

Similarly, we obtain an explicit formula for the numerical solution  $\{\tilde{y}_k\}_{k=0}^N$  of equation (9), by approximating the Caputo derivative  $y_n^{(\alpha)}$  with (1)

$$\tilde{y}_n = \frac{1}{1 + \Gamma(2 - \alpha)h^\alpha} \left( \Gamma(2 - \alpha)h^\alpha F_n - \sum_{k=1}^n \sigma_k^{(\alpha)} \tilde{y}_{n-k} \right). \tag{12}$$

Numerical solution (11) converges faster to the solution of the fractional relaxation equation, because it has a second order accuracy  $O(h^2)$ , and the accuracy of numerical solution (12) is  $O(h^{2-\alpha})$ .

FIGURE 2. Graph of the exact solution of equation (9) and numerical solutions (11)-black, and (12)-red, for  $h = 0.1$  and  $\alpha = 0.8$ .

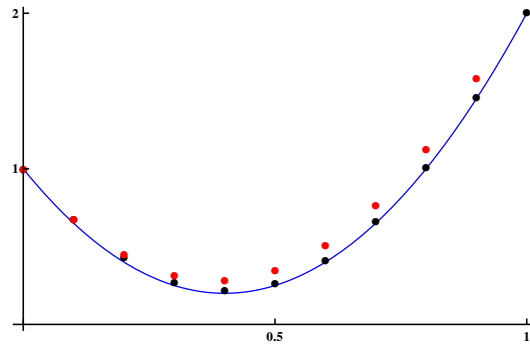


TABLE 4. Maximum error and order of numerical solutions (12) and (11) for equation (9) on the interval  $[0, 1]$ , when  $\alpha = 0.8$ .

$h$	<i>Error</i>	<i>Order</i>	$h$	<i>Error</i>	<i>Order</i>
0.05	0.0628014	1.17381	0.05	0.0081544	1.85708
0.025	0.0275997	1.19262	0.025	0.0021629	1.91461
0.0125	0.0120751	1.19262	0.0125	0.0005599	1.94979
0.00625	0.0052704	1.19603	0.00625	0.0001428	1.97076
0.003125	0.0022975	1.19785	0.003125	0.0000361	1.98307

**5.2. Numerical Solution of the Fractional Subdiffusion Equation.** The time-fractional fractional subdiffusion equation is obtained from the heat transfer equation by replacing the time derivative with a fractional derivative of order  $\alpha$ , where  $0 < \alpha < 1$

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2} + F(x, t), \tag{13}$$

with initial and boundary conditions

$$u(x, 0) = u_0(x), \quad u(0, t) = u_L(t), \quad u(1, t) = u_R(t).$$

Numerical solutions of the fractional subdiffusion equation are discussed in [19, 21, 24, 34]. In this section we determine the numerical solutions (15) and (16) for the

fractional subdiffusion equation obtained by approximating the Caputo derivative with (1) and (4) on the region

$$(x, t) \in [0, 1] \times [0, 1].$$

Let  $h = 1/N, \tau = 1/M$ , where  $M$  and  $N$  are positive integers, and  $\mathcal{G}$  be a grid on the square  $[0, 1] \times [0, 1]$

$$\mathcal{G} = \{(nh, m\tau) \mid 1 \leq n \leq N, 1 \leq m \leq M\}.$$

Denote by  $u_n^m$  and  $F_n^m$  the values of the functions  $u(x, t)$  and  $F(x, t)$  on  $\mathcal{G}$

$$u_n^m = u(nh, m\tau), \quad F_n^m = F(nh, m\tau).$$

By approximating the values of the Caputo derivative in the time direction at the points  $(nh, \tau)$  using (10) and using a central difference approximation for the second derivative in the space direction we obtain

$$\frac{u_n^1 - u_n^0}{\tau^\alpha \Gamma(2 - \alpha)} = \frac{u_{n-1}^1 - 2u_n^1 + u_{n+1}^1}{h^2} + F(nh, \tau) + O(h^2 + \tau^{2-\alpha}).$$

Let

$$\eta = \Gamma(2 - \alpha) \frac{\tau^\alpha}{h^2}.$$

The solution of the fractional subdiffusion equation satisfies

$$-\eta u_{n-1}^1 + (1 + 2\eta)u_n^1 - \eta u_{n+1}^1 = u_n^0 + \Gamma(2 - \alpha)\tau^\alpha F(nh, \tau) + O(\tau^\alpha h^2 + \tau^2).$$

Let  $U_n^m$  be the numerical solution of the fractional subdiffusion equation on the grid  $\mathcal{G}$ . The numbers  $U_n^m$  are approximations for the values of the solution  $u_n^m = u(nh, m\tau)$ . The numbers  $U_n^0$  are computed from the initial condition  $U_n^0 = u_0(nh)$ . The numbers  $U_n^1$  are approximations for the solution of (13) at time  $t = \tau$ . We compute the numbers  $U_n^1$  implicitly from the equations

$$-\eta U_{n-1}^1 + (1 + 2\eta)U_n^1 - \eta U_{n+1}^1 = U_n^0 + \Gamma(2 - \alpha)\tau^\alpha F_n^1,$$

where the values of  $U_0^1$  and  $U_N^1$  are determined from the boundary conditions

$$U_0^1 = u_L(\tau), \quad U_N^1 = u_R(\tau).$$

The numbers  $U_n^1$  are computed with the linear system ( $k = 2, \dots, N - 2$ )

$$\begin{cases} (1 + 2\eta)U_1^1 - \eta U_2^1 = u_0(h) + \eta u_L(\tau) + \Gamma(2 - \alpha)\tau^\alpha F_1^1 \\ -\eta U_{k-1}^1 + (1 + 2\eta)U_k^1 - \eta U_{k+1}^1 = u_0(kh) + \Gamma(2 - \alpha)\tau^\alpha F_k^1 \\ -\eta U_{N-2}^1 + (1 + 2\eta)U_{N-1}^1 = u_0((N - 1)h) + \eta u_R(\tau) + \Gamma(2 - \alpha)\tau^\alpha F_{N-1}^1. \end{cases}$$

Let  $K$  be a tridiagonal matrix of dimension  $N - 1$  with values  $1 + 2\eta$  on the main diagonal, and  $-\eta$  on the diagonals above and below the main diagonal.

$$K_5 = \begin{pmatrix} 1 + 2\eta & -\eta & 0 & 0 & 0 \\ -\eta & 1 + 2\eta & -\eta & 0 & 0 \\ 0 & -\eta & 1 + 2\eta & -\eta & 0 \\ 0 & 0 & -\eta & 1 + 2\eta & -\eta \\ 0 & 0 & 0 & -\eta & 1 + 2\eta \end{pmatrix}$$

and  $U^m = (U_1^m, U_2^m, \dots, U_{N-1}^m)$ . The vector  $U^1$  is solution of the linear system

$$KU^1 = R_1 + \eta R_2, \tag{14}$$

where  $R_1$  and  $R_2$  are the column vectors

$$R_1 = [u_0(kh) + \Gamma(2 - \alpha)\tau^\alpha F_n^1]_{n=1}^{N-1},$$



$$R_2 = [u_L(\tau), 0, \dots, 0, u_R(\tau)]^T.$$

We determined a second order approximation  $U^1$  for the solution of the fractional subdiffusion equation, on the first layer of  $\mathcal{G}$ , as a solution of the linear system (14). When  $m \geq 2$  we discretize the Caputo derivative with equation (13) with the second order approximation (4)

$$\frac{1}{\tau^\alpha \Gamma(2-\alpha)} \sum_{k=0}^m \delta_k^{(\alpha)} u_n^{m-k} = \frac{u_{n-1}^m - 2u_n^m + u_{n+1}^m}{h^2} + F(nh, m\tau) + O(h^2 + \tau^2).$$

The values of the numerical solution  $U_n^m$  are determined from the equations

$$-\eta U_{n-1}^m + (\delta_0^{(\alpha)} + 2\eta)U_n^m - \eta U_{n+1}^m = - \sum_{k=1}^m \delta_k^{(\alpha)} U_n^{m-k} + \Gamma(2-\alpha)\tau^\alpha F_n^m,$$

and the boundary conditions

$$U_0^m = u_L(m\tau), \quad U_N^m = u_R(m\tau).$$

The vector  $U^m$  is a solution of the linear system

$$(K - \zeta(a-1)I)U^m = R_1 + \eta R_2, \quad (15)$$

where  $R_1$  and  $R_2$  are the column vectors

$$R_1 = \left[ - \sum_{k=1}^m \delta_k^{(\alpha)} U_n^{m-k} + \Gamma(2-\alpha)\tau^\alpha F_n^m \right]_{n=1}^{N-1},$$

$$R_2 = [u_L(m\tau), 0, \dots, 0, u_R(m\tau)]^T.$$

The numerical solution  $\{U^2, \dots, U^M\}$ , using approximation (4) for the Caputo derivative, is computed with linear systems (15). Similarly we determine the numerical solution  $\{V^2, \dots, V^M\}$  for approximation (1) with linear system (16) and first layer  $V^1 = U^1$ . The numerical solution  $V^m$  is computed with the linear system

$$KV^m = R_1 + \eta R_2 \quad (16)$$

where  $R_1$  and  $R_2$  are the vectors

$$R_1 = \left[ - \sum_{k=1}^m \sigma_k^{(\alpha)} V_n^{m-k} + \Gamma(2-\alpha)\tau^\alpha F_n^m \right]_{n=1}^{N-1},$$

$$R_2 = [u_L(m\tau), 0, \dots, 0, u_R(m\tau)]^T.$$

Numerical solution (15) has accuracy  $O(h^2)$  and the accuracy of (16) is  $O(h^{2-\alpha})$ . When

$$F(x, t) = 2(1-3x)(5t^2 - 4t + 1) + x^2(1-x) \left( \frac{10t^{2-\alpha}}{\Gamma(3-\alpha)} - \frac{4t^{1-\alpha}}{\Gamma(2-\alpha)} \right),$$

the fractional sub-diffusion equation

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2} + F(x, t), \quad (x, t) \in [0, 1] \times [0, 1] \quad (17)$$

with initial and boundary conditions

$$u(x, 0) = x^2(1-x), \quad u(0, t) = u(1, t) = 0,$$

has solution

$$u(x, t) = x^2(1-x)(1-4t+5t^2).$$

The maximal error and numerical order of numerical solutions (16) and (15) for  $\tau = h$  and  $\tau = h/2$  at time  $t = 1$  for the fractional subdiffusion equation (17) are given in Table 5 and Table 6.

TABLE 5. Maximum error and order of numerical solutions (16) and (15) for equation (17) when  $\alpha = 0.6$  and  $\tau = h$ , at time  $t = 1$ .

$h$ ( $\tau = h$ )	<i>Error</i>	<i>Order</i>	$\tau$ ( $\tau = h$ )	<i>Error</i>	<i>Order</i>
0.05	0.00051794	1.37686	0.05	0.00001170	1.93892
0.025	0.00019766	1.38974	0.025	$2.99 \times 10^{-6}$	1.96593
0.0125	0.00007530	1.39222	0.0125	$7.62 \times 10^{-7}$	1.97559
0.00625	0.00002864	1.39467	0.00625	$1.93 \times 10^{-7}$	1.98175
0.003125	0.00001087	1.39657	0.003125	$4.87 \times 10^{-8}$	1.98648

In numerical solutions (15) and (16), we use (10) to obtain a second order approximation for the solution of the fractional subdiffusion equation on the first layer of  $\mathcal{G}$ . Another way to determine a second order approximation for the solution at time  $t = \tau$  is to compute the partial derivative  $u_t(x, t)$  at time  $t = 0$  and approximate the solution  $u(x, \tau)$  with a second order Taylor expansion. The function  $u(x, t)$  satisfies

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2} + F(x, t).$$

Apply fractional differentiation of order  $1 - a$

$$\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial^2 u(x, t)}{\partial x^2} + \frac{\partial^{1-\alpha} F(x, t)}{\partial t^{1-\alpha}},$$

$$u_t(x, t) = \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial^2 u(x, t)}{\partial x^2} + \frac{\partial^{1-\alpha} F(x, t)}{\partial t^{1-\alpha}}.$$

Set  $t = 0$

$$u_t(x, 0) = \left. \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial^2 u(x, t)}{\partial x^2} \right|_{t=0} + \left. \frac{\partial^{1-\alpha} F(x, t)}{\partial t^{1-\alpha}} \right|_{t=0}.$$

When the solution  $u(x, t)$  is a sufficiently smooth function

$$\left. \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial^2 u(x, t)}{\partial x^2} \right|_{t=0} = 0,$$

we obtain

$$u_t(x, 0) = \left. \frac{\partial^{1-\alpha} F(x, t)}{\partial t^{1-\alpha}} \right|_{t=0}.$$

The values of the solution at time  $t = \tau$  are approximated using the second order Taylor expansion

$$u(x, \tau) = u(x, 0) + \tau u_t(x, 0) + O(\tau^2)$$

In the fractional subdiffusion equation (17)

$$F(x, t) = 2(1 - 3x)(5t^2 - 4t + 1) + x^2(1 - x) \left( \frac{10t^{2-\alpha}}{\Gamma(3 - \alpha)} - \frac{4t^{1-\alpha}}{\Gamma(2 - \alpha)} \right),$$

$$\frac{\partial^{1-\alpha} F(x, t)}{\partial t^{1-\alpha}} = 2(1 - 3x) \left( \frac{10t^{1+\alpha}}{\Gamma(2 + \alpha)} - \frac{4t^\alpha}{\Gamma(1 + \alpha)} \right) + x^2(1 - x)(10t - 4).$$

TABLE 6. Maximum error and order of numerical solutions (16) and (15) for equation (17) when  $\alpha = 0.4$  and  $\tau = 0.5h$ , at time  $t = 1$ .

$h$ ( $h = 2\tau$ )	<i>Error</i>	<i>Order</i>	$h$ ( $h = 2\tau$ )	<i>Error</i>	<i>Order</i>
0.05	0.00006172	1.56262	0.025	$4.41 \times 10^{-6}$	1.98507
0.025	0.00002069	1.57697	0.0125	$1.11 \times 10^{-6}$	1.99521
0.0125	$6.91 \times 10^{-6}$	1.58139	0.00625	$2.78 \times 10^{-7}$	1.99589
0.00625	$2.30 \times 10^{-6}$	1.58597	0.00625	$6.95 \times 10^{-8}$	1.99701
0.003125	$7.65 \times 10^{-7}$	1.58946	0.003125	$1.74 \times 10^{-8}$	1.99811

The partial derivative  $u_t(x, t)$  at time  $t = 0$  has values

$$u_t(x, 0) = \left. \frac{\partial^{1-\alpha} F(x, t)}{\partial t^{1-\alpha}} \right|_{t=0} = -4x^2(1 - x).$$

Then

$$u(x, \tau) = u(x, 0) + \tau u_t(x, 0) + O(\tau^2)$$

$$u(x, \tau) = x^2(1 - x) - 4\tau x^2(1 - x) = x^2(1 - x)(1 - 4\tau) + O(\tau^2)$$

We obtain the second order approximation for the solution of equation (17) on the first layer on the grid  $\mathcal{G}$ .

$$U_n^1 = (nh)^2(1 - nh)(1 - 4\tau), \quad (n = 1, 2, \dots, N - 1) \tag{18}$$

TABLE 7. Maximum error and order of numerical solutions (15) and (16) with approximation (18) for the solution of equation (17) on the first layer of  $\mathcal{G}$ , at time  $t = 1$  when  $\alpha = 0.6$  and  $\tau = h$ .

$h$ ( $\tau = h$ )	<i>Error</i>	<i>Order</i>	$\tau$ ( $\tau = h$ )	<i>Error</i>	<i>Order</i>
0.05	0.00051282	1.35060	0.05	0.00001730	2.28453
0.025	0.00019690	1.38100	0.025	$3.85 \times 10^{-6}$	2.16657
0.0125	0.00007518	1.38896	0.0125	$9.02 \times 10^{-7}$	2.09523
0.00625	0.00002862	1.39337	0.00625	$2.17 \times 10^{-7}$	2.05667
0.003125	0.00001088	1.39601	0.003125	$5.29 \times 10^{-8}$	2.03510

## 6. CONCLUSION

In section 4 we compared the numerical solutions of the ordinary fractional relaxation equation and the partial fractional subdiffusion equation using approximations (1) and (4) for the Caputo derivative. The higher accuracy of approximation (4) results in a noticeable improvement in the performance of the numerical solutions. Numerical experiments suggest that the numerical solutions converge to the exact solutions of the fractional relaxation and subdiffusion equations for all  $\alpha$  between 0 and 1. We are going to work on a proof for the convergence of the numerical solutions discussed in section 4.

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