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# ON NUMERICAL APPROXIMATION OF SECOND-ORDER FRACTIONAL DIFFERENTIAL EQUATIONS IN THE FRAME OF THE CAPUTO FRACTIONAL DERIVATIVE

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Abstract. Numerical rules to approximate the Caputo fractional derivative and the Riemann-Liouville integral operator given in [25] are used to deduce a numerical method to approximate the solution of arbitrary Second-Order Fractional Differential Equations with constant coefficients in the frame of the Caputo fractional derivative.

Consistency of the method is proved and we illustrate its applicability and convergence with numerical examples.

## 1. Introduction

Fractional Differential Equations (shortly, FDEs) are involved in many mathematical modelings such as dynamic of viscoelastic material [1, 17], economics [2, 15], continuum and statistical mechanics [21], solid mechanics [30], electrochemistry [28], biology [6] and acoustics [7] just to mention a few examples.

In this context, the search for numerical methods that approximate the solution of FDEs has grown in recent years. In fact, there are many and diverse numerical methods proposed for different classes of FDEs (see, for instance, [5, 8, 9, 10, 14, 16, 18, 19, 20, 31]), however, most of them deal with solutions of single term or multi-order FDEs. In particular, as far as we know, FDEs where iterated derivatives are also involved have not been widely considered. Indeed, the bibliography on the matter is scarce even in the case of Second-Order Fractional Differential Equations (shortly, SOFDEs), i.e. FDEs where a fractional derivative and its iterated derivative are involved.

In [12, 13] general methods, based on the variation of parameters and on the Homotopy Perturbation Method respectively, have been presented to solve SOFDEs where the fractional derivative is described in the conformable sense. On the other hand, in [27] the generalized Taylor's formula was used in order to describe the solution of a concrete SOFDE in the frame of the Caputo fractional derivative.

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In this work, we present a numerical scheme to approximate the solution of arbitrary SOFDEs with constant coefficients and where the fractional derivative is described in the Caputo sense. Essentially, the proposed method is based on rewriting the Fractional Differential Equation as an Integro-Differential Equation and, in a discretization of the domain, using numerical rules to approximate the fractional derivative and the Riemann-Liouville integral operator.

Regarding the numerical rules, we consider the Modified Trapezoidal Rule (MTR) and the Caputo Fractional Derivative Rule (CFDR) introduced in [25, 26]. The MTR is a generalization of the classical trapezoidal rule used to approximate the Riemann-Liouville integral operator of fractional order for a given function by a weighted sum of function values at specified points. On the other hand, the CFDR is an algorithm to approximate the Caputo fractional derivative for a given function by a weighted sum of function and its ordinary derivatives values at specified points.

By approximating the ordinary derivative of a function by a weighted sum of suitable evaluations (classical finite-difference scheme), we achieve that the method uses only function values at specific points. In this sense, the proposed approach can be regarded as a finite-difference type scheme. Furthermore, the method is reduced to solving a linear algebraic system and, since the associated matrix is a lower triangular one, its implementation is extremely simple.

The organization of the paper is as follows: In Section 2, we introduce basic definitions and notations and give a brief overview of the Modified Trapezoidal Rule and the Caputo Fractional Derivative Rule. In Section 3, the rewritting of the Fractional Differential Equation as an Integro-Differential Equation is presented and the development of the method is given, we show that such method is consistent and we also partially study the approximation error. In Section 4, some numerical examples are presented with the aim to illustrate the applicability and the convergence of the method. Finally, conclusions and additional comments will be given in Section 5.

## 2. The numerical rules

Let $0 < s < 1$. We recall that the Riemann-Liouville integral operator of $u$ of order $s$ is defined as

$$I_0^s u(x) = \frac{1}{\Gamma(s)} \int_0^x (x-t)^{s-1} u(t)\, dt \quad (x \geq 0). \tag{1}$$

Details and properties of the operator $I_0^s$ can be found in [4, 22]. The Caputo fractional derivative of $u$ of order $s$ can be defined by $I_0^{1-s}$ as follows [4, 11]

$$D_0^s u = I_0^{1-s} u',$$

where $u'$ denotes the ordinary derivative of $u$, i.e.

$$D_0^s u(x) = \frac{1}{\Gamma(1-s)} \int_0^x \frac{u'(t)}{(x-t)^s}\, dt \quad (x \geq 0). \tag{2}$$

The operators $I_0^s$ and $D_0^s$ are also related in the following ways

$$D_0^s I_0^s u = u \tag{3}$$

and

$$I_0^s D_0^s u(x) = u(x) - u(0) \tag{4}$$

(see, for instance, Theorems 3.7 and 3.8 in [4] respectively).

In what follows we will give a brief overview of the Modified Trapezoidal Rule and the Caputo Fractional Derivative Rule that allow us to approximate the operator $I_0^s$ and the operator $D_0^s$, respectively, at the nodes of a uniform partition of a certain interval $[0, a]$ (see [25, 26] for more details). In order to keep our explanation as simple as possible, we are going to consider $a = 1$, i.e. the interval considered will be $[0, 1]$.

Let $n \geq 1$. Suppose that the interval $[0, 1]$ is subdivided into subintervals $[x_k, x_{k+1}]$ of equal width $h = \frac{1}{n}$ by using the nodes $x_k = kh$, for $k = 0, 1, \ldots, n$.

For any $k = 0, 1, \ldots, n$, we use $u_k$ to denote the function value $u(x_k)$ and define

$$U_k = \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_k \end{bmatrix}.$$

**Modified Trapezoidal Rule.** For any $k = 1, \ldots, n$, the value $I_0^s u(x_k)$ can be approximated [25, 26] by the quantity $T_k(U_k, h, s)$ given by

$$T_k(U_k, h, s) = \frac{h^s}{\Gamma(s+2)} \left[ \alpha_k u_0 + \sum_{i=1}^{k} \delta_{ki} u_i \right] \tag{5}$$

with

$$\alpha_k = (k-1)^{s+1} - (k-s-1)k^s$$

and

$$\delta_{ki} = \begin{cases} (k-i+1)^{s+1} - 2(k-i)^{s+1} + (k-i-1)^{s+1} & i < k \\ 1 & i = k \end{cases}.$$

From [25, Theorem 2] we know that, for any $k = 1, \ldots, n$,

$$I_0^s u(x_k) = T_k(U_k, h, s) + E_k^I; \tag{6}$$

and, if $u \in C^2[0, 1]$, there is a positive constant $C_I$ depending only on $s$ such that

$$|E_k^I| \leq C_I h^2 \|u\|_{2,\infty}. \tag{7}$$

**Caputo Fractional Derivative Rule.** For $k = 1, \ldots, n$, the Caputo fractional derivative at $x_k$, $D_0^s u(x_k)$, can be approximated [25, 26] by the value $C_k(u, h, s)$ given by

$$C_k(u, h, s) = \frac{h^{1-s}}{\Gamma(3-s)} \left[ a_k u'(0) + \sum_{i=1}^{k} d_{ki} u'(x_i) \right] \tag{8}$$

with

$$a_k = (k-1)^{2-s} - (k+s-2)k^{1-s}$$

and

$$d_{ki} = \begin{cases} (k-i+1)^{2-s} - 2(k-i)^{2-s} + (k-i-1)^{2-s} & i < k \\ 1 & i = k \end{cases}.$$

Indeed, from [25, Theorem 3] we know that, for any $k = 1, \ldots, n$,

$$D_0^s u(x_k) = C_k(u, h, s) + E_k^C \tag{9}$$

where

$$|E_k^C| \leq C_s' h^2 \|u\|_{3,\infty} \qquad (u \in C^3[0,1]) \tag{10}$$

with $C_s'$ a positive constant depending only on $s$.

We use (8) to obtain a rule to approximate the Caputo fractional derivative by using only evaluations of the function. Indeed, from the Taylor expansion of first order of $u$ we deduce the following identities

$$u'(0) = \frac{u_1 - u_0}{h} - \frac{h}{2}u''(\xi_0), \tag{11}$$

$$u'(x_k) = \frac{u_k - u_{k-1}}{h} + \frac{h}{2}u''(\xi_k), \quad 1 \leq k \leq n, \tag{12}$$

with $\xi_0 \in (0, x_1)$ and $\xi_k \in (x_{k-1}, x_k)$ for any $k = 1, 2, \ldots, n$.

Now, combining (11)-(12) with (8), for any $k = 1, 2, \ldots, n$, we obtain

$$C_k(u,h,s) = \frac{h^{-s}}{\Gamma(3-s)}\left[a_k(u_1 - u_0) + \sum_{i=1}^{k} d_{ki}(u_i - u_{i-1})\right] + R_k(u,h,s) \tag{13}$$

where

$$R_k(u,h,s) = \frac{h^{2-s}}{2\Gamma(3-s)}\left[-a_k u''(\xi_0) + \sum_{i=1}^{k} d_{ki}u''(\xi_i)\right]. \tag{14}$$

For any $k = 1, 2, \ldots, n$ we define

$$C_k^*(U_k,h,s) = \frac{h^{-s}}{\Gamma(3-s)}\left[(a_k + d_{k1})(u_1 - u_0) + \sum_{i=2}^{k} d_{ki}(u_i - u_{i-1})\right]; \tag{15}$$

therefore

$$C_k(u,h,s) = C_k^*(U_k,h,s) + R_k(u,h,s).$$

As expected, the Caputo fractional derivative of $u$ at $x_k$, $D_0^s u(x_k)$, can be approximated by the value $C_k^*(U_k,h,s)$. Indeed, from (9) we get

$$D_0^s u(x_k) = C_k^*(U_k,h,s) + E_k^D \tag{16}$$

with

$$E_k^D = E_k^C + R_k(u,h,s), \tag{17}$$

and, as we see in Lemma 1, the absolut value of the error $E_k^D$ is $O(h)$.

**Lemma 1.** *Let $E_k^D$ be as in (17), with $1 \leq k \leq n$, and let $C_s'$ be the constant involved in (10). Then*

$$|E_k^D| \leq C_s' h^2 \|u\|_{3,\infty} + \frac{2-s}{2\Gamma(3-s)} h \|u\|_{2,\infty} \qquad (u \in C^3[0,1]). \tag{18}$$

*Proof.* From the triangular inequality applied to (14), and taking into account that the quantities $a_k, \alpha_k, d_{ki}$ and $\delta_{ki}$ are non-negative, we have

$$|R_k(u,h,s)| \leq \frac{h^{2-s}}{2\Gamma(3-s)}\left(a_k + \sum_{i=1}^{k} d_{ki}\right)\|u\|_{2,\infty}.$$

Now, since $a_k + \sum_{i=1}^{k} d_{ki} = (2-s)k^{1-s}$ and $k^{1-s} \leq h^{s-1}$, it follows that

$$|R_k(u,h,s)| \leq \frac{2-s}{2\Gamma(3-s)} h \|u\|_{2,\infty}. \tag{19}$$

Finally, applying the triangular inequality to (17) and taking into account (10) and (19), (18) follows easily. □

## 3. Numerical method

In this section we introduce the Second-Order Fractional Differential Equations that we study and develop a numerical method to approximate their solutions which is based on the numerical rules seen in the previous section.

3.1. **Second-Order Fractional Differential Equations.** Let $D_0^s u$ be the Caputo fractional derivative of $u$ of order $s$ defined by (2). We use $D_0^{2\,s} u$ to denote the sequential or iterated derivative of order $s$ of $u$, i.e.

$$D_0^{2\,s} u = D_0^s \, D_0^s u.$$

In general, $D_0^{2\,s} u$ is not equivalent to the derivative of order $2s$ of $u$, $D_0^{2s} u$. Iterated derivatives play a fundamental role, for instance, in generalized Taylor's formula [27].

In this work, we consider SOFDEs of the following type

$$D_0^{2\,s} u(x) = p D_0^s u(x) + q u(x) + r(x) \quad \text{in } (0,1), \tag{20}$$

where $p, q$ are arbitrary constants and $r$ is a bounded function on $(0,1)$; subject to the initial value conditions

$$u(0) = \beta_0, \quad D_0^s u(0) = \beta_1 \tag{21}$$

with $\beta_0$ and $\beta_1$ arbitrary escalars.

A direct modification of the arguments that we will use can be established in order to consider the interval $(0,a)$, instead of $(0,1)$, with $a$ an arbitrary positive constant. As we have already clarified, the choice $a = 1$ responds only to keeping our exposition as clear as possible.

3.2. **Integro-Differential Equation.** In this section we present an alternative formulation of the Second-Order Fractional Differential Equation (20)-(21) as an Integro-Differential Equation. We use this alternative formulation to guarantee existence and uniqueness of a solution to the problem (20)-(21) and, in Section 3.3, to establish a numerical method that allows us to approximate it.

After applying the integral operator $I_0^s$ to (20) and taking into account the identity (4), together with the initial value conditions (21), we obtain

$$D_0^s u(x) - \beta_1 = p(u(x) - \beta_0) + q I_0^s u(x) + I_0^s r(x). \tag{22}$$

Then, assuming the existence of a solution $u$ of (20)-(21), it follows that $u$ solves the following Integro-Differential Equation

$$\begin{cases} D_0^s u(x) = p u(x) + q I_0^s u(x) + \tilde{r}(x) & \text{in } (0,1), \\ u(0) = \beta_0, \end{cases} \tag{23}$$

with $\tilde{r}(x) = I_0^s r(x) + \beta_1 - \beta_0 p$.

Moreover, as we claim, (23) is equivalent to (20)-(21). Indeed, taking into account the identity (3), after applying the differential operator $D_0^s$ to the first line in (23) we get

$$\begin{aligned} D_0^{2\,s}u(x) &= pD_0^s u(x) + qD_0^s I_0^s u(x) + D_0^s \tilde{r}(x) \\ &= pD_0^s u(x) + qu(x) + D_0^s(I_0^s r(x) + \beta_1 - \beta_0 p) \\ &= pD_0^s u(x) + qu(x) + r(x) + D_0^s(\beta_1 - \beta_0 p). \end{aligned}$$

Since $\beta_1 - \beta_0 p$ is a constant term it follows that $D_0^s(\beta_1 - \beta_0 p) = 0$ and equation (20) is obtained. On the other hand, the initial value condition on $D_0^s u$ in (21) follows from a direct evaluation in (23).

As we have just seen, problems (20)-(21) and (23) are equivalent in the sense that the solution of one of them is also the solution of the other. However, up to now there is no guarantee that any of these problems will actually support a solution.

The existence and uniqueness of local solution can be easily obtained thanks to known results. Indeed, observe that (23) can be written as follows

$$D_0^s u(x) = f(x,u) + \int_0^x K(x,t,u(t))dt, \qquad u(0) = \beta_0$$

where

$$f(x,u) = p(u(x) - \beta_0) + \beta_1 \quad \text{and} \quad K(x,t,u(t)) = \frac{1}{\Gamma(s)}(qu(t) + r(t))(x-t)^{s-1}.$$

Then, a direct application of Theorem 1 in [23] allows to conclude the existence of a local solution of this Integro-Differential Equation and, therefore, a local solution of the SOFDE (20)-(21). On the other hand, Theorem 3.1 in [24] is also directly applicable where the function $\phi$ involved in the statement of such theorem can be taken as $\phi(y) = |p|y$ with $p$ as the same constant in the expression of $f$. Then, invoking such a theorem, the local uniqueness of solution is guaranteed.

3.3. **The numerical method.** We use the rules $T_k$ and $C_k^*$ introduced in Section 2 to present a numerical approximation scheme for the problem (23) (resp. (20)-(21)). Indeed, suppose that the interval $[0,1]$ is subdivided into subintervals $[x_k, x_{k+1}]$ of equal width $h = \frac{1}{n}$ by using the nodes $x_k = kh$, for $k = 0, 1, \ldots, n$.

For any $k \geq 1$, after evaluating the first line of (23) at $x_k$, we obtain

$$D_0^s u(x_k) = pu_k + qI_0^s u(x_k) + \tilde{r}_k \tag{24}$$

where $\tilde{r}_k = \tilde{r}(x_k)$. Then, thanks to (6) and (16) we get

$$C_k^*(U_k, h, s) + E_k^D = pu_k + q(T_k(U_k, h, s) + E_k^I) + \tilde{r}_k,$$

or, equivalently,

$$C_k^*(U_k, h, s) = pu_k + qT_k(U_k, h, s) + \tilde{r}_k + qE_k^I - E_k^D. \tag{25}$$

Collecting all these equations, we obtain the linear system

$$MU = B + E \tag{26}$$

where $M$ is the lower triangular matrix

$$M = \begin{bmatrix} m_{11} & 0 & 0 & 0 & \cdots & 0 \\ m_{21} & m_{22} & 0 & 0 & \cdots & 0 \\ m_{31} & m_{32} & m_{33} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 0 \\ m_{n1} & m_{n2} & m_{n3} & m_{n4} & \cdots & m_{nn} \end{bmatrix} \tag{27}$$

with

$$m_{11} = \frac{2-s}{\Gamma(3-s)} - h^s \left( p + \frac{qh^s}{\Gamma(s+2)} \right), \tag{28}$$

$$m_{ii} = \frac{1}{\Gamma(3-s)} - h^s \left( p + \frac{qh^s}{\Gamma(s+2)} \right), \quad 2 \le i \le n, \tag{29}$$

$$m_{i1} = \frac{a_i + d_{i1} - d_{i2}}{\Gamma(3-s)} - \frac{\delta_{i1} q h^{2s}}{\Gamma(s+2)}, \quad 2 \le i \le n, \tag{30}$$

$$m_{ij} = \frac{d_{ij} - d_{i\,j+1}}{\Gamma(3-s)} - \frac{\delta_{ij} q h^{2s}}{\Gamma(s+2)}, \quad 3 \le i \le n,\ 2 \le j \le i-1, \tag{31}$$

and

$$U = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}, \qquad B = \begin{bmatrix} \tilde{r}_1 h^s + \beta_0 \left( \dfrac{a_1 + d_{11}}{\Gamma(3-s)} + \dfrac{\alpha_1 q h^{2s}}{\Gamma(s+2)} \right) \\ \tilde{r}_2 h^s + \beta_0 \left( \dfrac{a_2 + d_{21}}{\Gamma(3-s)} + \dfrac{\alpha_2 q h^{2s}}{\Gamma(s+2)} \right) \\ \vdots \\ \tilde{r}_n h^s + \beta_0 \left( \dfrac{a_n + d_{n1}}{\Gamma(3-s)} + \dfrac{\alpha_n q h^{2s}}{\Gamma(s+2)} \right) \end{bmatrix}, \qquad E = \begin{bmatrix} qE_1^I - E_1^D \\ \vdots \\ qE_n^I - E_n^D \end{bmatrix}.$$

**Lemma 2.** *With the previous notations*

$$\|E\|_\infty \le h \left( \frac{2-s}{2\Gamma(3-s)} + |q| C_I h \right) \|u\|_{2,\infty} + C'_s h^2 \|u\|_{3,\infty} \qquad (u \in C^3[0,1]).$$

*Proof.* It is an immediate consequence of the triangular inequality, equation (7) and Lemma 1. □

For a sufficiently regular function $u$, Lemma 2 implies that $\|E\|_\infty \to 0$ as $h \to 0$. This fact suggests that the solution $\hat{U} = \begin{bmatrix} \hat{u}_1 \\ \vdots \\ \hat{u}_n \end{bmatrix}$ of the linear system

$$M\hat{U} = B \tag{32}$$

seems to be a reasonable approximation of $U$ (which satisfies (26)).

In concrete, the proposed method to approximate the solution of the discrete system (26) associated to the Integro-Differential Equation (23) (resp. the SOFDE (20)-(21)) consists to find the vector $\hat{U}$ satisfying the linear algebraic system (32).

3.4. **On the approximation error $\|U-\hat{U}\|_\infty$.** As we have pointed out, the proposed method becomes relevant when $h$ is small. Observe that, under this assumption, the following additional requirement can be regarded as *virtual*: there exists a constant $\xi_0$ such that

$$(H) \quad \frac{1}{\Gamma(3-s)} - h^s\left(p+\frac{qh^s}{\Gamma(s+2)}\right) \geq \xi_0 > 0.$$

In the sequel, we assume that condition $(H)$ is satisfied.

Since $0<s<1$, we get

$$\frac{2-s}{\Gamma(3-s)} = \frac{1-s}{\Gamma(3-s)} + \frac{1}{\Gamma(3-s)} \geq \frac{1}{\Gamma(3-s)};$$

therefore,

$$\frac{2-s}{\Gamma(3-s)} - h^s\left(p+\frac{qh^s}{\Gamma(s+2)}\right) \geq \xi_0 > 0.$$

Then, taking into account (28) and (29), we deduce that the lower triangular matrix $M$ introduced in (27) is non-singular.

On the other hand, substracting (32) to (26) we obtain

$$M(U-\hat{U}) = E$$

and then

$$U-\hat{U} = M^{-1}E.$$

Therefore, the approximation error can be estimated in the usual way

$$\|U-\hat{U}\|_\infty \leq \|M^{-1}\|_\infty \|E\|_\infty. \tag{33}$$

However, although the proposed method is consistent (c.f. Lemma 2), numerical examples suggest that it is not stable in the usual sense since there does not seem to be a uniform constant $C$ verifying

$$\|M^{-1}\|_\infty \leq C.$$

In consequence, it is not possible to obtain an explicit estimate of the approximation error; however, in the following section we illustrate the convergence of the method with numerical examples even for less regular functions than required in Lemma 2.

## 4. Numerical examples

In this section we present some examples with the aim to illustrate the applicability and the convergence of the numerical method (32) to approximate the solution of SOFDEs with constant coefficients. To this end, we have implemented in `Octave` codes such method to the problems (34), (35), (36) and (37) listed below.

**Example 1.** *Let $0<s<1$. Consider the following Second-Order Fractional Differential Equation*

$$\begin{cases} D_0^{2\,s}u(x) = D_0^s u(x) + u(x) - 1 \quad \textit{in } (0,1), \\ u(0)=1, \quad D_0^s u(0) = 0. \end{cases} \tag{34}$$

A simple inspection shows that $u(x) = 1$ is the exact solution of the problem (34).

On the other hand, although the implementation of the method is immediate, we point out that the parameters involved in this case are

$$p = 1 = q = \beta_0 \qquad \text{and} \qquad \beta_1 = 0,$$

while the function $\tilde{r}$ involved in the construction of matrix $B$ is given by

$$\tilde{r}(x) = -1 - \frac{x^s}{s\Gamma(s)}.$$

In Table 1 we compile some results obtained for the approximation error $\|\widehat{U} - U\|_\infty$, where $\widehat{U}$ is the numerical solution given by (32) and $U$ is the vector containig 1 in each entry, when $s$ assumes the values 0.9, 0.5 and 0.1 respectively. We have also compiled the values of $\|M^{-1}\|_\infty$ with the intention of illustrating that this quantity seems not to be uniformly bounded (c.f. Section 3.4). Moreover, it is observed that $\|M^{-1}\|_\infty$ grows when $n$ does and this growth seems to depend strongly on $s$. Despite the increase in the value of $\|M^{-1}\|_\infty$, the approximation error is significantly small, which is in accordance with (33) and Lemma 2.

| $n$ | $h$ | $\|\widehat{U} - U\|_\infty$ | | | $\|M^{-1}\|_\infty$ | | |
|---|---|---|---|---|---|---|---|
| | | $s = 0.9$ | $s = 0.5$ | $s = 0.1$ | $s = 0.9$ | $s = 0.5$ | $s = 0.1$ |
| 10 | 0.1 | 1.110 e-015 | 9.103 e-015 | 1.332 e-015 | 22.305 | 62.003 | 3.674 |
| 25 | 0.04 | 4.329 e-015 | 2.664 e-015 | 9.325 e-015 | 46.970 | 73.731 | 7.653 |
| 50 | 0.02 | 1.776 e-014 | 2.220 e-015 | 2.264 e-014 | 85.612 | 95.829 | 21.875 |
| 100 | 0.01 | 3.619 e-014 | 4.107 e-015 | 6.183 e-014 | 158.042 | 129.355 | 73.486 |

TABLE 1. Approximation errors for problem (34) and values of $\|M^{-1}\|_\infty$.

**Example 2.** *Consider the following Second-Order Fractional Differential Equation*

$$\begin{cases} D_0^{2\,\frac{1}{2}} u(x) = u(x) + 2x - x^2 \quad \textit{in } (0,1), \\ u(0) = 0, \quad D_0^{\frac{1}{2}} u(0) = 0. \end{cases} \tag{35}$$

In this case, we clearly have $s = \frac{1}{2}$. On the other hand, the exact solution of (35) is $u(x) = x^2$ and, although the implementation of the method (32) does not present any difficulty, it seems pertinent to point out that the function $\tilde{r}$ is given by

$$\tilde{r}(x) = \frac{8x^{3/2}}{3\sqrt{\pi}} \left(1 - \frac{2}{5}x\right)$$

while the rest of the parameters are

$$p = 0 = \beta_0 = \beta_1 \qquad \text{and} \qquad q = 1.$$

In Table 2 we compile the obtained results for the approximation error $\|\widehat{U} - U\|_\infty$, where $\widehat{U}$ is the numerical solution given by (32) and $U$ is the vector that contains the evaluations of the function $u$ at the corresponding nodes. We have also compiled the values of $\|M^{-1}\|_\infty$ for the different values of $n$ considered.

It is observed that as $h = n^{-1}$ decreases, the approximation error also decreases; in this sense our method seems asymptotically convergent. Moreover, although

in this case $\|M^{-1}\|_\infty$ is not uniformly bounded either, the order of the values it assumes for $n \geq 100$ is considerably less than the order of $h^{-1} = n$. The fact that $\|M^{-1}\|_\infty$ does not increase significantly when $h$ decreases allows to explain, taking into account (33) and Lemma 2, that the order in the approximation error is similar to the order of $h$.

| $n$ | $h$ | $\|\widehat{U} - U\|_\infty$ | $\|M^{-1}\|_\infty$ |
|---|---|---|---|
| 50 | 0.02 | 3.433 e-002 | 16.82 |
| 100 | 0.01 | 1.717 e-002 | 23.69 |
| 250 | 0.004 | 6.871 e-003 | 37.15 |
| 500 | 0.002 | 3.436 e-003 | 52.23 |
| 1000 | 0.001 | 1.718 e-003 | 73.50 |
| 2000 | 0.0005 | 8.591 e-004 | 103.55 |
| 5000 | 0.0002 | 3.436 e-004 | 163.12 |

TABLE 2. Approximation errors for problem (35) and values of $\|M^{-1}\|_\infty$.

In the previous examples, the solution function is regular enough to foresee, thanks to the Lemma 2 and a not very significant growth of $\|M^{-1}\|_\infty$, that the method will converge by virtue of what was seen in Section 3.4.

In what follows we present two examples in which the regularity of the solution function is considerably less than what is required in the Lemma 2 and, however, the proposed method is also asymptotically convergent.

**Example 3.** *Let $0 < s < 1$. Consider the following Second-Order Fractional Differential Equation*

$$\begin{cases} D_0^{2\,s} u(x) = D_0^s u(x) - \Gamma(s+1) \quad \text{in } (0,1), \\ u(0) = 0, \quad D_0^s u(0) = \Gamma(s+1). \end{cases} \tag{36}$$

A direct verification allows us to conclude that $u(x) = x^s$ is the exact solution of the problem (36). In this case, the parameters involved in the construction of matrices $M$ and $B$ in (32) are

$$p = 1,\ q = 0 = \beta_0,\ \beta_1 = \Gamma(s+1) \ \text{ and } \ \tilde{r}(x) = -\frac{\Gamma(s+1)x^s}{s\Gamma(s)}.$$

In Table 3 we list the values of the error approximation $\|\widehat{U} - U\|_\infty$, where $U$ is the vector containig the evaluations of $u$ at the nodes $x_i = i/n$, $i = 0, \ldots, n$ for the considered values of $n$, and $\widehat{U}$ is the obtained solution according to (32).

For each $s$ considered in Table 3 it is observed that as $h$ decreases, the approximation error $\|\widehat{U} - U\|_\infty$ also decreases; in this sense our method seems asymptotically convergent. On the other hand, note that the closer $s$ is to 1, the better the convergence speed. This fact, among other issues, may possibly be linked to an improvement in the regularity of the solution function.

Although we have only tabulated results for values of $s$ in the range $[0.5, 1)$, a similar behavior is observed when $s$ is less than 0.5. However, convergence becomes considerably slower in these cases, that is, a large number of nodes must be considered to obtain an acceptable error. Furthermore, the closer $s$ is to 0, the slower the convergence becomes.

| $n$ | $h$ | $\|\widehat{U}-U\|_\infty$ | | | | |
|---|---|---|---|---|---|---|
| | | $s=0.95$ | $s=0.9$ | $s=0.8$ | $s=0.6$ | $s=0.5$ |
| 10 | 0.1 | 2.617 e-002 | 5.455 e-002 | 1.219 e-001 | 3.459 e-001 | 5.590 e-001 |
| 50 | 0.02 | 7.412 e-003 | 1.616 e-002 | 3.985 e-002 | 1.413 e-001 | 2.564 e-001 |
| 100 | 0.01 | 4.254 e-003 | 9.460 e-003 | 2.436 e-002 | 9.595 e-002 | 1.846 e-001 |
| 250 | 0.004 | 2.012 e-003 | 4.593 e-003 | 1.255 e-002 | 5.706 e-002 | 1.191 e-001 |
| 500 | 0.002 | 1.130 e-003 | 2.632 e-003 | 7.533 e-003 | 3.830 e-002 | 8.524 e-002 |
| 1000 | 0.001 | 6.298 e-004 | 1.496 e-003 | 4.490 e-003 | 2.561 e-002 | 6.080 e-002 |

TABLE 3. Approximation errors for problem (36).

**Example 4.** *Let $0 < s < 1$. Consider the following Second-Order Fractional Differential Equation*

$$\begin{cases} D_0^{2s}u(x) = -D_0^s u(x) + 2u(x) \quad \textit{in } (0,1) \\ u(0) = 1, \quad D_0^s u(0) = 1. \end{cases} \tag{37}$$

The exact solution of this problem is $u(x) = E_s(x^s)$ where $E_s$ denotes the Mittag-Leffler function

$$E_s(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(sk+1)}$$

(details can be found in [27, Example 4]). By virtue of the exact solution, a similar behavior to that described in Example 3 is expected.

In order to construct the matrices $M$ and $B$ involved in (32), we point out that the parameters to consider in this case are

$$p = -1,\ q = 2,\ \beta_0 = 1 = \beta_1 \ \text{ and } \ \tilde{r}(x) = 0.$$

We have used the MATLAB routine [29] for evaluating the Mittag-Leffler function at the nodes of the uniform mesh of step $h = 1/n$ for the values of $n$ and $s$ listed in Table 4 with accuracy $10^{-6}$, indeed, we use $\bar{U}$ to denote the vector containing such values. That is, if $U$ is the vector that contains the exact evaluations of $u$, then $\|\bar{U} - U\|_\infty$ is $O(10^{-6})$.

| $n$ | $h$ | $\|\widehat{U}-\bar{U}\|_\infty$ | | | | |
|---|---|---|---|---|---|---|
| | | $s=0.95$ | $s=0.9$ | $s=0.8$ | $s=0.6$ | $s=0.5$ |
| 10 | 0.1 | 7.332 e-002 | 7.051 e-002 | 6.309 e-002 | 5.134 e-002 | 9.168 e-002 |
| 50 | 0.02 | 1.365 e-002 | 1.207 e-002 | 7.263 e-003 | 2.614 e-002 | 6.630 e-002 |
| 100 | 0.01 | 6.615 e-003 | 5.526 e-003 | 4.915 e-003 | 2.157 e-002 | 5.667 e-002 |
| 250 | 0.004 | 2.529 e-003 | 1.907 e-003 | 2.785 e-003 | 1.614 e-002 | 4.148 e-002 |
| 500 | 0.002 | 1.218 e-003 | 8.264 e-004 | 1.765 e-003 | 1.204 e-002 | 3.138 e-002 |
| 1000 | 0.001 | 5.848 e-004 | 3.517 e-004 | 1.099 e-003 | 8.662 e-003 | 2.323 e-002 |

TABLE 4. Approximation errors for problem (37)

In Table 4 we compile the values of $\|\widehat{U}-\bar{U}\|_\infty$ computed for the indicated choices of $n$ and $s$ where $\widehat{U}$ is the obtained solution of (32).

Now, from the triangular inequality we get

$$\|\widehat{U} - U\|_\infty \leq \|\widehat{U} - \bar{U}\|_\infty + \|\bar{U} - U\|_\infty \lesssim \|\widehat{U} - \bar{U}\|_\infty + 10^{-6}$$

and, since $\|\widehat{U} - \bar{U}\|_\infty > 10^{-6}$ in the studied cases (see Table 4), we conclude that the approximation error $\|\widehat{U} - U\|_\infty$ is conditionated by $\|\widehat{U} - \bar{U}\|_\infty$.

We can observe (c.f. Table 4) that as $h$ decreases, so does the quantity $\|\widehat{U} - \bar{U}\|_\infty$ and, therefore, the approximation error $\|\widehat{U} - U\|_\infty$ also decreases. This suggest that the method is asymptotically convergent.

On the other hand, we have only tabulated results for values of $s$ in the interval $[0.5, 1)$ since for values in the range $(0, 0.5)$ a slow convergence is observed. Finally, also in accordance with Example 3, a better performance is observed when the value of $s$ is close to 1.

## 5. Conclusions and final comments

In this work, we present a consistent numerical method to approximate the solution of arbitrary Second-Order Fractional Differential Equations with constant coefficients in the frame of the Caputo fractional derivative. Such approximation scheme is reduced to solving a linear algebraic system which is extremely simple since the associated matrix is a lower triangular one.

Numerical examples are explored in order to illustrate the applicability of the method. An asymptotic convergence is observed in each case and, when the solution function is enough regular and the method is close to being stable, the order in the approximation error is the expected one according to (33) and Lemma 2. However, the method seems to be asymptotically convergent even when the solution funcion is less regular than required in Lemma 2. An improvement in the speed of convergence is observed when the fractional order $s$ is close to 1, which is in accordance with the aforementioned.

Both the formulation of the numerical method that we did and the examples that we explore are based on explicitly knowing the function $\tilde{r}$ introduced in (23), or at least the values $\tilde{r}_k$ it assumes in each node $x_k$ (recall that the values $\tilde{r}_k$ are used to define the matrix $B$ involved in (32)). However, this may not occur, i.e. it may happen that the exact values $\tilde{r}_k$ are not known. In this case, since $\tilde{r}$ is defined as the sum of the constant term $\beta_1 - \beta_0 p$ and the term $I_0^s r$, the Modified Trapezoid Rule can be used to approximate the latter and, therefore, to obtain an approximation of $\tilde{r}_k$ for each $k$.

No additional complexity appears in the case that evaluations of $\tilde{r}$ should be approximated; however, we prefer to present our explanation the way we did it in order to keep it as clear as possible.

Finally, due the equivalence exhibited in Section 3.2 between the SOFDE (20)-(21) and the Integro-Differential Equation (23), many of the numerical methods available to approximate the latter can be applied to the former. As part of our future work we propose to explore this line.

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