Numerical methods for differential equations with non integer order derivatives

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ABSTRACT

We consider a time-fractional diffusion equation problem with a Caputo time derivative of order $\alpha \in]0,1[$. We present the existence and uniqueness results for this problem. We study the type of solutions with a singularity near the origin in time using two types of meshes in time (a uniform and a non-uniform). We approximate the solution of the problem using the L1 approximation for the fractional derivative with respect to time and the finite difference formula for the second derivative with respect to space. Since the uniform mesh does not perform well for solutions with singularities we focus on the non-uniform mesh. We prove the stability and convergence of the numerical scheme. We conclude that the optimal convergence is achieved with a proper choice of the grading exponent defining the non-uniform (graded) mesh, taking into account the behaviour of solution and we present several examples to support this conclusion. We apply the methods to a real world problem (the fractional cable equation applied to Neurophysiology) and present some numerical results that confirm the theoretical previsions for the time-fractional diffusion equation problem.

1. Introduction

Fractional calculus is an area of mathematics that recently became the research topic of many investigators, not only mathematicians but also researchers of other fields as physicists and engineers, although this is not a recent area. When we use the word "fractional", we mean non-integer order, that is, we do not restrict the order of the differential and integral operators to be integers, but we allow them to be real (or even complex) numbers.

Many famous mathematicians, such as Grünwald, Letnikov, Riemann, Liouville, Caputo and others have dealt with these same questions. If you are familiar with this area then you know that some of these mathematicians came up with different definitions of fractional differentiation operator.

We will discuss an application of this branch of mathematics when we introduce the time-fractional cable equation in Neurophysiology. We will compare an approximate solution of the problem of two cases, a integer order time derivative cable problem and a fractional order time derivative cable problem. We present these two approaches because in the article [2], the authors say that the fractional version describes better the approximate solution than the usual cable equation.

1.1. The beginning of Fractional Calculus

Before we briefly introduce the theory of Fractional Calculus, we present the "history" of this area of mathematics. It can be traced back to the seventeenth century when Leibniz introduced the notation of nth derivative of a function f, $\frac{d^n}{dx^n}f(x)$, L'Hôpital raised the question "what if n is 1/2?" to Leibniz in a letter sent from the first to the second dated September 30th, 1695. Leibniz's response: "An apparent paradox, from which one day useful consequences will be drawn". This question raised by LHôpital marks the birth of Fractional Calculus.

Nowadays, several defintions (not always equivalent) of fractional derivatives and integrals exist defined by some researchers. For our problem in study, the Caputo derivative is used following the article in [2].

The mathematical and numerical treatment of fractional-order problems is substantially different than the integer-order ones, as it can be seen in the forthcoming sections.

1.2. Fractional derivatives

Before we define the fractional derivative, we introduce two important functions. The function $\Gamma : [0,\infty[\to \mathbb{R}$, defined by

$$\Gamma(\alpha) = \int_0^\infty t^{\alpha-1} \exp(-t)dt \tag{1}$$

is the Euler's Gamma function for $\alpha \in]0,1[$. Note that for the a given integer number, n we have $\Gamma(n) = (n-1)!$. In the following definition, we present a generalization of the Mittag-Leffler function.

Definition 1. [3] Let $\gamma, \beta > 0$. The function $E_{\gamma,\beta}$ defined by

$$E_{\gamma,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\gamma+\beta)} \tag{2}$$

whenever the series converges is called the two-parameter Mittag-Leffler funtion with parameters γ and β.

We start with the definition of the fractional Riemann-Liouville integral:

$$J_a^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1} f(t)dt, \tag{3}$$

where $0 \leq a < x < b$ and α is a real positive number.

The Riemann-Liouville fractional differential derivative of order α of a function f, $D_a^\alpha f$, is defined as

$$D_a^\alpha f := D^\beta J_a^{\beta-\alpha} f, \tag{4}$$

where $\beta = \lceil\alpha\rceil$ and D^β is the classical (integer-order) derivative.We define this according to [3].

The Caputo differential operator of order $\alpha > 0$, ${}^C D_a^\alpha f$, is defined in the following way:

$$ {}^C D_a^\alpha f = D_a^\alpha [f - T_{\beta-1}[f;a]] \tag{5} $$

for functions f such that $D_a^\alpha[f - T_{\beta-1}[f;a]]$ exists [3], where $T_{\beta-1}[f;a]$ represents the Taylor polynomial of degree $\beta - 1$ of the function f, centered at a. We studied Caputo's derivative because it is one of the most appropriated definitions for the type of problems in Neurophysiology that we are going to study.

Theorem 2. *[4] Let $x > 0$, $\alpha \in \mathbb{R}$, $\beta - 1 < \alpha < \beta \in \mathbb{N}$. Then the following relation between the Riemann-Liouville* (4) *and Caputo* (5) *operators holds*

$$ {}^C D_a^\alpha f(x) = D^\alpha f(x) - \sum_{k=0}^{\beta-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} f^{(k)}(a). \tag{6} $$

We will consider the case $a = 0$, and we will be particularly interested in the case where $0 < \alpha < 1$.

Since we are going to deal with a two-dimensional problem whose solution is $u(t,x)$, with a Caputo derivative in time, whenever we use the notation $\frac{\partial^\alpha u(t,x)}{\partial t^\alpha}$, we mean the fractional Caputo derivative of $u(t,x)$ of order α, with respect to the variable t:

$$ \frac{\partial^\alpha u(t,x)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial u(s,x)}{\partial s} ds, \quad t > 0, \quad \alpha \in]0,1[. \tag{7} $$

2. L1 Method

2.1. Introduction to the L1 Method

The L1 method, or L1 scheme, is one of the most popular methods to dicretize Caputo an Riemann-Liouville fractional derivatives and for solving fractional diffusion problems.

It was initially developed by Kai Diethelm in [5] with the name Diethelm's fractional backward difference formula instead of L1 method or L1 scheme. The purpose was to develop a scheme to approximate the solution of a Caputo fractional differential equation. At that time, 1997, there were not that many numerical algorithms, able to approximate fractional derivatives, for which an error analysis was available. In our case, we will use it to approximate the solution of a problem for a partial differential equation and latter on use it in a problem in Neurophysiology.

Fractional Calculus has several applications; more and more numerical methods are being developed in this field, with high precision, fast convergence and inexpensive when implemented in some programming language. We mention the books [6] [7], containing a good amount of numerical methods for partial differential equations including the L1 method.

We will only study and implement the $L1$ method for the time fractional derivative. This method is used for values of $0 < \alpha < 1$, which is the case of our problem under study. As a first approach we discretize the solution in a uniform mesh, then we move to a non-uniform mesh.

2.2. How we obtain the L1 Method

Let $t_i = i\tau$, $i = 0, 1, ..., N$ be the points of a uniform mesh where τ is the space between two consecutive points. Taking into consideration the Caputo definition we get the equivalent

$$ \begin{aligned} \frac{d^\alpha u(t)}{dt^\alpha}\Big|_{t=t_i} &= \frac{1}{\Gamma(1-\alpha)} \int_{t_0}^{t_i} (t_i - s)^{-\alpha} \frac{du(s)}{ds} ds \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \int_{t_k}^{t_{k+1}} (t_i - s)^{-\alpha} \frac{du(s)}{ds} ds \end{aligned} \tag{8} $$

In each interval of partition $[t_k, t_{k+1}]$, for each $k = 1, ..., N-1$, $u(s) \approx u^I(s)$, $s \in [t_k, t_{k+1}]$ where $u^I(s)$ is the interpolating polynomial of u in nodes t_k and t_{k+1}. Hence, we have

$$ \frac{d^\alpha u(t)}{dt^\alpha}\Big|_{t=t_i} = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \int_{t_k}^{t_{k+1}} (t_i - s)^{-\alpha} (u^I(s))' ds \tag{9} $$

$$ = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \int_{t_k}^{t_{k+1}} (t_i - s)^{-\alpha} \frac{u(t_{k+1}) - u(t_k)}{t_{k+1} - t_k} ds + R_1(\tau) \tag{10} $$

Neglecting $R_1(\tau)$ we can approximate the Caputo's derivative by

$$ \frac{d^\alpha u(t)}{dt^\alpha}\Big|_{t=t_i} \approx \sum_{k=0}^{i-1} b_{i-k-1}(u(t_{k+1}) - u(t_k)) \tag{11} $$

where the coefficients b_k are given by

$$ b_k = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} [(k+1)^{1-\alpha} - k^{1-\alpha}], \quad k = 0, 1, ..., i-1. \tag{12} $$

Since we also will deal with non-uniform meshes, we define $t_i = T(i/N)^r$ as the points of this non-uniform (graded), for $i = 0, ..., N$ and $r \geq 1$. The length of the intervals in this non-uniform partition is variable $\tau_i = t_{i+1} - t_i$ where $i = 0, ..., N-1$. r is called the grading exponent and it should be noticed that when $r = 1$, this graded mesh reduces to a uniform mesh. When $r > 1$, the grid-points are more densely placed near the origin, which is a potential singularity.

For the non-uniform mesh, we define the Caputo fractional partial derivative following the same idea as before for $0 < \alpha < 1$ and using the same partition and the interpolating polynomial of u. The result is the following

$$ \frac{d^\alpha u(t)}{dt^\alpha}\Big|_{t=t_i} \approx \sum_{k=0}^{i-1} b_{k+1}^i (u(t_{k+1}) - u(t_k)), \tag{13} $$

but now considering the coefficients b_{k+1}^i given by

$$ b_{k+1}^i = \frac{(t_i - t_k)^{1-\alpha} - (t_i - t_{k+1})^{1-\alpha}}{\Gamma(2-\alpha)\tau_k}, \quad k = 0, 1, ..., i-1. \tag{14} $$

To simplify further approaches we will consider some notations. Let's assume $\delta_t^\alpha u^i$ as the approximated derivative of the L1 method in (11) or in (13) for each $i = 1, ..., N$. Let's also consider $\frac{d^\alpha}{dt^\alpha} u(t_i)$ as the derivative of order α of the exact solution defined in (7). From the article [8] we introduce the following Lemma and Corollary and we will only apply it to the one-dimentional case. In the two-dimensional case the application is analogous.

Let's consider the following notation for the next problem and Lemma.

$$ \delta_t^\alpha u^i := \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^{i} \delta_t u^j \int_{t_{j-1}}^{t_j} (t_i - s)^{-\alpha} ds, \quad \delta_t u^j := \frac{u^j - u^{j-1}}{t_j - t_{j-1}} $$

(15)

for $i = 1, ..., N$. Let's assume the following type of fractional derivative problems with the discretization that we mentioned before:

$$\begin{cases} \frac{d^\alpha}{ds^\alpha} u(t) = f(t) \ \ for \ \ t \in]0, T], \\ u(0) = u_0 \end{cases} \tag{16}$$

and

$$\begin{cases} \delta_t^\alpha u^i = f(t_i) \ \ for \ \ i =, ..., N \\ u(0) = u_0 \end{cases} \tag{17}$$

Lemma 1. *Assuming that*

$$S^i = \delta_t^\alpha u^i - \frac{d^\alpha}{ds^\alpha} u(s_i), \tag{18}$$

then

$$|S^n| \leq C_1 t_n^{-\alpha} \{ \frac{\tau_1}{t_n} \phi^1 + \max_{i=2,...,n} \phi^i \} \tag{19}$$

(where

$$\phi^1 = \tau_1^\alpha \sup_{s \in]0, t_1[} (s^{1-\alpha} |\delta_t^\alpha u^1 - \frac{d^\alpha}{ds^\alpha} u(s)|), \tag{20}$$

$$\phi^i = \tau_i^{2-\alpha} t_i^\alpha \sup_{s \in]t_{i-1}, t_i[} | \frac{d^2}{ds^2} u(s)| \tag{21}$$

for $i \geq 2$ and C_1 is a real constant). Taking into consideration the previous assumptions and the fact that $\frac{\tau_1}{t_n} < 1$, we get that

$$|S^n| \leq t_n^{-\alpha} \max_{k=1,...,n} \phi^k. \tag{22}$$

Corollary 2. *[8] Under the conditions of the previous Lemma and assuming that $|\frac{d^l u}{dt}(t)| \leq C_1(1 + t^{\alpha - l})$ with $t \in]0, T]$ and $l = 1, 2$. Then $|u(t_i) - u^i| \leq C_1 N^{-min\{\alpha r, 2-\alpha\}}$ for $i = 1, ..., N$.*

In the following, we generalize this corollary for less singular solutions.

Corollary 3. *Under the conditions of last Lemma, suppose that*

$$|\frac{d^l u}{dt}(t)| \leq C(1 + t^{\beta - l}) \ \ for \ \ l = 1, 2 \ \ and \ \ t \in [0, T], \tag{23}$$

$\beta \geq \alpha$. Then

$$|u(t_n) - u^n| \leq C N^{-min\{\beta r, 2-\alpha\}} \ \ for \ \ n = 1, 2, ..., N. \tag{24}$$

In the cases where (23) and (24) holds the optimal convergence order, $2 - \alpha$ is achieved by choosing $r = \frac{2-\alpha}{\beta}$. The L1 method for initial value problems of the type (2.10) can be easily extended to the case of partial differential equations, where the time derivative is of fractional order and the space derivative is of integer one. Such problems will be considered in the next section.

For illustration, we consider the following initial-value problem for a fractional order equation example.

Example 1.

$$\begin{cases} ({}^C D^\alpha u)(t) = u(t) + \frac{1}{\Gamma(5/2-\alpha)} \frac{3\sqrt{\pi} t^{3/2-\alpha}}{4} - t^{3/2}, \ \ 0 < t < T \\ u(0) = 0 \end{cases} \tag{25}$$

The exact solution of the problem (25) is $u(t) = t^{3/2}$.

At each point of the non-uniform mesh we will replace the fractional derivative by its approximation (13). Disregarding the errors of this approximation, we obtain a system of algebraic equations, from which the approximate values of the solution at points t_i are calculated, with $i = 0, 1, ..., N$ which we denote by u_i.

To compare the numerical results with the exact solution we use the following examples and compare the norm of the maximum of its absolute error. We use the notations:

$$\epsilon_N = \max_{1 \leq i \leq N} |u(t_i) - u^i| \ \ for \ \ i \in 0, 1, ...N \ \ and \ \ \alpha \in]0, 1[. \tag{26}$$

We estimate the convergence order of the L1 Method using the following formula:

$$p = \frac{ln(\frac{\epsilon_N}{\epsilon_{2N}})}{ln(2)} \tag{27}$$

α	0.25		0.5		0.75	
N	ϵ_N	p	ϵ_N	p	ϵ_N	p
10	0.021009		0.03843		0.07240	
20	0.006977	1.590	0.01456	1.400	0.03162	1.195
40	0.002261	1.626	0.005426	1.424	0.01374	1.203
80	0.000718	1.654	0.001993	1.445	0.005923	1.214
160	0.000225	1.676	0.000724	1.461	0.00254	1.224
320	0.0000696	1.692	0.0002608	1.473	0.00108	1.231

Table 1. Table with the errors (26) obtained by each spacing and the respective experimental order of the method for problem (25) using a uniform mesh.

r	$\frac{2-\alpha}{\beta} \approx 1.167$		$\frac{2-\alpha}{\alpha} = 7$		$\frac{2(2-\alpha)}{\alpha} = 14$	
N	ϵ_N	p	ϵ_N	p	ϵ_N	p
64	0.000898		0.006002		0.01697	
128	0.0002795	1.684	0.00195	1.623	0.00563	1.591
256	0.0000862	1.697	0.000622	1.647	0.00183	1.620

Table 2. Table with the errors (26) and the respective experimental order of the method for problem (25) and $\alpha = 0.25$.

r	$\frac{2-\alpha}{\beta} = 1$		$\frac{2-\alpha}{\alpha} = 3$		$\frac{2(2-\alpha)}{\alpha} = 6$	
N	ϵ_N	p	ϵ_N	p	ϵ_N	p
64	0.002755		0.004151		0.00952	
128	0.001004	1.456	0.001508	1.461	0.00350	1.445
256	0.0003638	1.469	0.0005435	1.472	0.001273	1.459

Table 3. Table with the errors (26) and the respective experimental order of the method for problem (25) and $\alpha = 0.5$.

Looking at Table 1 we notice that the experimental order of the method is is slowly increasing to $p \approx 2 - \alpha$ but when we look at the Tables 2, 3 and 4 we see that using a non uniform mesh gets the expected experimental order,$p \approx 2 - \alpha$ much faster when using the optimal grading exponent,$r = \frac{2-\alpha}{\beta}$ and $r = \frac{2-\alpha}{\alpha}$.

Since this problem follows the conditions 23 and 24, we can conclude the following inequality:

$$\epsilon_N \leq C N^{-min\{\beta r, 2-\alpha\}}. \tag{28}$$

r	$\frac{2-\alpha}{\beta}\approx 0.8$		$\frac{2-\alpha}{\alpha}\approx 1.7$		$\frac{2(2-\alpha)}{\alpha}\approx 3.3$	
N	ϵ_N	p	ϵ_N	p	ϵ_N	p
64	0.01038		0.006800		0.01099	
128	0.004609	1.171	0.002874	1.243	0.00465	1.240
256	0.002029	1.184	0.001213	1.245	0.00197	1.243

Table 4. Table with the errors and the respective experimental order of the method for problem (25) and $\alpha = 0.75$.

Next, we consider an example with a stronger singularity at $t = 0$.

Example 2.

$$\begin{cases} ({}^C D^\alpha u)(t) = u(t) + \frac{3t^{3/4-\alpha}\Gamma(3/4)}{4\Gamma(7/4-\alpha)} - t^{3/4}, & 0 < t < T \\ u(0) = 0 \end{cases} \tag{29}$$

The exact solution of the problem (29) is $u(t) = t^{3/4}$.

r	1		$\frac{2-\alpha}{\beta} = 2.33$		$\frac{2-\alpha}{\alpha} = 7$	
N	ϵ_N	p	ϵ_N	p	ϵ_N	p
64	0.003069		0.0007522		0.002588	
128	0.001695	0.856	0.0002337	1.623	0.000826	1.648
256	0.0009516	0.834	0.0000720	1.698	0.000260	1.667

Table 5. Table with the errors (26) and the respective experimental order of the method for problem (49) and $\alpha = 0.25$.

r	1		$\frac{2-\alpha}{\beta} = 2$		$\frac{2-\alpha}{\alpha} = 3$	
N	ϵ_N	p	ϵ_N	p	ϵ_N	p
64	0.007221		0.002056		0.002340	
128	0.003239	1.157	0.000738	1.478	0.000841	1.476
256	0.001677	0.949	0.0002636	1.485	0.0003011	1.482

Table 6. Table with the errors (26) and the respective experimental order of the method for problem (29) and $\alpha = 0.5$.

r	1		$\frac{2-\alpha}{\beta} = \frac{2-\alpha}{\alpha} \approx 1.67$	
N	ϵ_N	p	ϵ_N	p
64	0.01948		0.00759	
128	0.01029	0.9194	0.003321	1.194
256	0.005386	0.9353	0.00144	1.210

Table 7. Table with the errors (26) and the respective experimental order of the method for problem (29) and $\alpha = 0.75$.

We see, from the results in Tables 5, 6 and 7 that the optimal convergence order is not achieved in the case where $r = 1$ (uniform mesh). It is attained for both cases, $r = (2-\alpha)/\beta$ and $r = (2-\alpha)/\alpha$ where $r = (2-\alpha)/\beta$ is slightly better than $r = (2-\alpha)/\alpha$. Nevertheless, with $r = 1$, we observe an increasing of the absolute error when compared with the ones obtained with $r = (2-\alpha)/\beta$ and $r = (2-\alpha)/\alpha$.

3. Diffusion equations with non-integer order partial derivatives in time

In this section we will determine numerically the solution of partial problems of the type:

$$\begin{cases} \frac{\partial^\alpha u(t,x)}{\partial t^\alpha} = \frac{\partial^2 u(t,x)}{\partial x^2} - u(t,x) + v(t,x), & t \in (0,T), \quad x \in (0,L) \\ u(0,x) = g(x), & x \in (0,L) \\ u(t,0) = u_0(t), & t \in (0,T) \\ u(t,L) = u_L(t), & t \in (0,T) \end{cases} \tag{30}$$

where $\frac{\partial^\alpha u(t,x)}{\partial t^\alpha}$ is the Caputo derivative of order α, $0 < \alpha < 1$ of the function u with respect to the variable t (see (7)) and where we assume that all the involved functions, $v(t,x)$, $g(x)$, $u_0(t)$ and $u_L(t)$ are continuous in their respective domains. The problem (30) is the one that we are going to approximate using the L1 formula for time discretization and a finite difference formula for space discretization that we will present next using two different time meshes, a uniform and a non-uniform/graded one.

3.1. Finite difference scheme

The initial-boundary value problem (30) has a second partial order derivative which we are going to approximate by a second order finite difference formula, while the time-fractional derivative will be discretized using the $L1$ approximation formula. We choose this scheme because it is quite popular when dealing with this kind of problems and it was used in [9] and [8].

Namely:

$$\frac{d^2 u(t_i, x_j)}{dx^2} = \frac{u(t_i, x_{j+1}) - 2u(t_i, x_j) + u(t_i, x_{j-1})}{h^2} + R_2^{(i,j)}(h) \tag{31}$$

where $t_i = i\tau$ or $t_i = i\tau_i$, depending if the mesh is uniform or not, and $x_j = jh$ are the space discretization points. Here $i = 0, 1, ..., N$ and $j = 0, 1, ..., M$ and h and τ or τ_i correspond to the length of the sub-intervals of the interval $[0, L]$ and $[0, T]$, respectively.

Neglecting the error $R_2^{(i,j)}(h)$ we can approximate the second order space derivative as

$$\frac{d^2 u(t_i, x_j)}{dx^2} \approx \frac{u(t_i, x_{j+1}) - 2u(t_i, x_j) + u(t_i, x_{j-1})}{h^2}, \quad j = 1, ..., M-1. \tag{32}$$

We can observe that (32) introduces an error $R_2^{(i,j)}(h)$ such that, if the solution is sufficiently regular with respect to x, the approximation of the second partial derivative in space, it is of the order of $O(h^2)$.

3.2. Problem analysis

Tthis type of problem has a unique solution under certain conditions presented in detail in [1]. Some results on the continuous dependence of the solution on the given data of the problem are also available, as well as some regularity properties of the solution of this kind of problems.

Let the fractional power $\mathcal{L}^\gamma$ of the operator $\mathcal{L}$ be defined for each $\gamma \in \mathbb{R}$ in the domain

$$D(\mathcal{L}^\gamma) = \{u \in L_2[0,L] : \sum_{i=1}^{\infty} \lambda_i^{2\gamma} |(u, \psi_i)|^2 < \infty\} \tag{33}$$

where $\{(\lambda_i, \psi_i) : i = 1, 2, ...\}$ are the eigenvalues and eigenfunctions of the Sturm-Liouville two-point boundary value problem

$$\mathcal{L}\psi_i := -\psi_i'' + \psi_i = \lambda_i \psi_i \quad in \quad]0, L[, \quad \psi_i(0) = \psi_i(L) = 0, \tag{34}$$

and the eigenfunctions are normalised by requiring $\|\psi_i\|_2 = 1$ for all i and $\lambda_i > 0$ for all i as well.

The problem (30) has the solution:

$$u(t, x) = \sum_{j=1}^{\infty}[(g(x), \psi_j)E_{\alpha,1}(-\lambda_j t^\alpha) + J_j(t)]\psi_j(x), \tag{35}$$

where

$$J_j(t) = \int_{s=0}^{t} s^{\alpha-1}E_{\alpha,\alpha}(-\lambda_j s^\alpha)v_j(t - s)ds \tag{36}$$

with

$$v_j(t) = (v(\cdot, t), \psi_j(\cdot)) \tag{37}$$

and the Mittag-Leffler function is given by (2). Since the analytical solution involves a Mittag-Leffler function, which is a series, it is not always practical to compute it using (34), so we will solve it numerically using the previous methods.

The following theorem establishes some smoothness properties of the solution of (30).

Theorem 1. *[9] Assume that $g \in D(\mathcal{L}^{5/2})$, $v(t,\cdot) \in D(\mathcal{L}^{5/2})$, $\frac{\partial v}{\partial t}(t, \cdot)$ and $\frac{\partial^2 v}{\partial t^2}(t, \cdot)$ are in $D(\mathcal{L}^{1/2})$ for each $t \in]0, T]$ with*

$$\|v(t, \cdot)\|_{\mathcal{L}^{5/2}} + \|\frac{\partial v}{\partial t}(t, \cdot)\|_{\mathcal{L}^{1/2}} + t^\alpha\|\frac{\partial^2 v}{\partial t^2}(t, \cdot)\|_{\mathcal{L}^{1/2}} \leq C_1$$

for all $t \in]0, T]$ and some constant $0 < \alpha < 1$, where C_1 is a constant independent of t. Then the problem (30) has a unique solution and there exists a constant C such that

$$|\frac{\partial^k u}{\partial x^k}(t, x)| \leq C \quad for \quad k = 0, 1, 2, 3, 4, \tag{38}$$

$$|\frac{\partial^l u}{\partial t^l}(t, x)| \leq C(1 + t^{\alpha-l}) \quad for \quad l = 0, 1, 2, \tag{39}$$

for all $(t, x) \in]0, T] \times [0, L]$.

As we can conclude, from (39), we can expect the solution of such problems to be singular at $t = 0$, in the sense that the first and second time partial derivatives may not be continuous at that point.

3.3. Numerical methods

3.3.1. Using a uniform mesh

Let $t_i = i\tau$, $i = 0, 1, ..., N$, the points of a uniform mesh. Using the formula (32) to approximate the second derivative in order to x, at each point x_j, $j = 1, ..., M - 1$ and the formula (11) to approximate the Caputo derivative in order to t, at each point t_i, $i = 1, ..., N$. For $i = 1$ and $j = 1, ..., M - 1$ we have the following:

$$\begin{aligned}\sum_{k=0}^{0} b_{1-k-1}(u(t_1, x_j) - u(t_0, x_j)) + R_1^{(1,j)}(\tau) = \\ \frac{u(t_1, x_{j+1}) - 2u(t_1, x_j) + u(t_1, x_{j-1})}{h^2} - \\ u(t_1, x_j) + v(t_i, x_j) + R_2^{(1,j)}(h) \Leftrightarrow \\ u(t_1, x_j)(h^2 b_0 + 2 + h^2) - u(t_1, x_{j+1}) - \\ u(t_1, x_{j-1}) + R_1^{(1,j)}(\tau) = \\ h^2 b_0 u(t_0, x_j) + v(t_i, x_j)h^2 + R_2^{(1,j)}(h)\end{aligned} \tag{40}$$

The linear system (40) can be written in the form:

$$\begin{cases} u(t_1, x_1)(h^2 b_0 + 2 + h^2)- \\ u(t_1, x_2) - u_0(t_1) + R_1^{(1,1)}(\tau) = \\ h^2 b_0 u(t_0, x_1) + v(t_1, x_1)h^2 + R_2^{(1,1)}(h) \\ u(t_1, x_2)(h^2 b_0 + 2 + h^2)- \\ u(t_1, x_3) - u(t_1, x_1) + R_1^{(1,2)}(\tau) = \\ h^2 b_0 u(t_0, x_2) + v(t_1, x_2)h^2 + R_2^{(1,2)}(h) \\ \vdots \\ u(t_1, x_{M-1})(h^2 b_0 + 2 + h^2)- \\ u_L(t_1) - u(t_1, x_{M-2}) + R_1^{(1,M-1)}(\tau) = \\ h^2 b_0 u(t_0, x_{M-1}) + v(t_1, x_{M-1})h^2 + R_2^{(1,M-1)}(h) \end{cases} \tag{41}$$

Writing the system (41) in the matrix form, substituting some known values for the boundary conditions, $u(t_i, x_0) = u_0(t_i)$ and $u(t_i, x_M) = u_L(t_i)$ and neglecting the errors $R_1^{(i,j)}(\tau)$ and $R_2^{(i,j)}(h)$, we obtain

$$\begin{bmatrix} h^2b_0+2+h^2 & -1 & 0 & ... & 0 \\ -1 & h^2b_0+2+h^2 & -1 & ... & 0 \\ \vdots & & & & \\ 0 & 0 & ... & -1 & h^2b_0+2+h^2 \end{bmatrix}\begin{bmatrix} u(t_1,x_1) \\ u(t_1,x_2) \\ \vdots \\ u(t_1,x_{M-1}) \end{bmatrix}$$

$$= h^2 b_0 \begin{bmatrix} u(t_0,x_1) \\ u(t_0,x_2) \\ \vdots \\ u(t_0,x_{M-1}) \end{bmatrix} + h^2 \begin{bmatrix} v(t_1,x_1) \\ v(t_1,x_2) \\ \vdots \\ v(t_1,x_{m-1}) \end{bmatrix} + \begin{bmatrix} u_0(t_1) \\ 0 \\ \vdots \\ 0 \\ u_L(t_1) \end{bmatrix} \tag{42}$$

The system (42) defines the approximate solution u_j^1, $j = 0, ..., M$ such that $u_j^1 \approx u(t_1, x_j)$.

$$\begin{bmatrix} h^2b_0+2+h^2 & -1 & 0 & ... & 0 \\ -1 & h^2b_0+2+h^2 & -1 & ... & 0 \\ \vdots & & & & \\ 0 & 0 & ... & -1 & h^2b_0+2+h^2 \end{bmatrix}\begin{bmatrix} u_1^1 \\ u_2^1 \\ \vdots \\ u_{M-1}^1 \end{bmatrix} =$$

$$= h^2 b_0 \begin{bmatrix} u_1^0 \\ u_2^0 \\ \vdots \\ u_{M-1}^0 \end{bmatrix} + h^2 \begin{bmatrix} v_1^1 \\ v_2^1 \\ \vdots \\ v_{M-1}^1 \end{bmatrix} + \begin{bmatrix} u_0^1 \\ 0 \\ \vdots \\ u_M^1 \end{bmatrix} \tag{43}$$

Following the same logic for $i = 1$ we get the following system for $i = 2, ..., N$ in the matrix form:

$$\begin{bmatrix} h^2b_0+2+h^2 & -1 & 0 & ... & 0 \\ -1 & h^2b_0+2+h^2 & -1 & ... & 0 \\ \vdots & & & & \\ 0 & 0 & ... & -1 & h^2b_0+2+h^2 \end{bmatrix}\begin{bmatrix} u_1^i \\ u_2^i \\ \vdots \\ u_{M-1}^i \end{bmatrix} =$$

$$= h^2 b_0 \begin{bmatrix} u_1^{i-1} \\ u_2^{i-1} \\ \vdots \\ u_{M-1}^{i-1} \end{bmatrix} - h^2 \begin{bmatrix} \sum_{k=0}^{i-2} b_{i-k-1}(u_1^{k+1} - u_1^k) \\ \sum_{k=0}^{i-2} b_{i-k-1}(u_2^{k+1} - u_2^k) \\ \vdots \\ \sum_{k=0}^{i-2} b_{i-k-1}(u_{M-1}^{k+1} - u_{M-1}^k) \end{bmatrix} + h^2 \begin{bmatrix} v_1^i \\ v_2^i \\ \vdots \\ v_{M-1}^i \end{bmatrix} + \begin{bmatrix} u_0^i \\ 0 \\ \vdots \\ u_M^i \end{bmatrix}, \tag{44}$$

for $i = 3, ..., N$ and where b_j are defined by (12).

Lemma 2. *Since the matrix on the left side of* (44) *is of strictly dominant diagonal because the coefficients $b_k > 0$, for each $k = 1, ..., i$, the system* (44) *turns out to have a unique solution.*

The formula (44) is used to implement the algorithm to obtain an approximation of the exact solution of (30).

3.3.2. Numerical results and discussion

To analyse the results obtained by the algorithm we are going to define the absolute error as follows:

$$\epsilon(t_i) = \max_{i=1,...,M} |u(t_i, x_j) - u_j^i| \quad (45)$$

$$\epsilon(x_j) = \max_{j=1,...,N} |u(t_i, x_j) - u_j^i| \quad (46)$$

where $u(t_i, x_j)$ is the exact solution at the point (t_i, x_j) and u_j^i is the solution obtained by the algorithm implemented at these points. We are dealing with two variables (t, x) and the solution is a function in time (t) and in space (x). For each of these variables we have a different spacing, τ (time spacing) and h (space step). Therefore, the error will depend on these two spacings.

To test the order of convergence of the method with respect to t and x, for each example we use the following absolute errors definitions:

$$k_1 = \frac{ln(\frac{\epsilon_{N,M}}{\epsilon_{2N,M}})}{ln(2)} \quad (47) \qquad k_2 = \frac{ln(\frac{\epsilon_{N,M}}{\epsilon_{N,2M}})}{ln(2)}. \quad (48)$$

Example 3.

$$\begin{cases} \frac{\partial^\alpha u(t,x)}{\partial t^\alpha} = \frac{\partial^2 u(t,x)}{\partial x^2} - u(t,x) + v(t,x), t \in [0,1], x \in [0,1] \\ u(0,x) = 0, x \in [0,1] \\ u(t,0) = 0, t \in [0,1] \\ u(t,1) = 0, t \in [0,1] \end{cases} \quad (49)$$

The function $u(t, x) = t^{3/2} sin(\pi x)$ is the exact solution to this problem and $v(t, x) = \frac{3\sqrt{\pi} t^{3/2-\alpha} sin(\pi x)}{4\Gamma(5/2-\alpha)} + t^{3/2} sin(\pi x) + \pi^2 sin(\pi x) t^{3/2}$. We will present the results for $\alpha = 0.5$, $\alpha = 0.25$ and $\alpha = 0.75$ with the same spacing values as in the previous example. In Table 8 we present the experimental orders of the discretization method with respect to time, obtained using the estimate (47). The same is achieved in Table 9 for the experimental orders of discretization method with respect to space, obtained using the estimate (48).

α	0.25		0.5		0.75	
N	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1
10	0.0003743		0.001391		0.003573	
20	0.000153	1.291	0.000631	1.141	0.00170	1.069
40	0.0000623	1.297	0.000279	1.178	0.0008378	1.025
80	0.0000252	1.304	0.0001198	1.219	0.000391	1.100
160	0.0000102	1.312	0.00004996	1.262	0.000178	1.137

Table 8. Table with the errors obtained for a fixed value of $M = 1000$ and several values of N and the respective experimental order of the method for problem 49.

α	0.25		0.5		0.75	
M	$\epsilon_{N,M}$	k_2	$\epsilon_{N,M}$	k_2	$\epsilon_{N,M}$	k_2
5	0.02599		0.02561		0.02528	
10	0.006762	1.943	0.006666	1.977	0.006587	1.940
20	0.001686	2.004	0.001663	2.003	0.001651	1.996
40	0.0004214	2.001	0.0004167	1.997	0.0004205	1.973

Table 9. Table with the errors obtained for a fixed value of $N = 500$ and several values of M and the respective experimental order of the method for problem 49.

Example 4.

$$\begin{cases} \frac{\partial^\alpha u(t,x)}{\partial t^\alpha} = \frac{\partial^2 u(t,x)}{\partial x^2} - u(t,x) + v(t,x), t \in [0,1], x \in [0,1] \\ u(0,x) = 0, x \in [0,1] \\ u(t,0) = 0, t \in [0,1] \\ u(t,1) = 0, t \in [0,1] \end{cases} \quad (50)$$

The function $u(t, x) = t^{1/2} sin(\pi x)$ is the exact solution to this problem and $v(t, x) = \frac{\sqrt{\pi} t^{1/2-\alpha} sin(\pi x)}{2\Gamma(3/2-\alpha)} + t^{1/2} sin(\pi x) + \pi^2 sin(\pi x) t^{1/2}$. We will present the experimental orders of the discretization method with respect to time, obtained using the estimate (47) for $\alpha = 0.5$, $\alpha = 0.25$ and $\alpha = 0.75$ with the same spacing values as in the previous example.

α	0.25		0.5		0.75	
N	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1
10	0.00485		0.01677		0.03958	
20	0.0039	0.291	0.0152	0.141	0.0377	0.069
40	0.00322	0.297	0.01344	0.178	0.03363	0.166
80	0.00261	0.304	0.01155	0.219	0.02815	0.257
160	0.002104	0.312	0.009631	0.262	0.02234	0.333

Table 10. Table with the errors obtained for a fixed value of $M = 1000$ and several values of N and the respective experimental order of the method for problem 50.

Assuming that the solution of the problem (30) satisfies the conditions $u(t, \cdot) \in C^4([0, L])$ (for any $t \in [0, T]$ and $u(t, \cdot) \in C^2([0, T])$, for any $x \in [0, L]$ (see (38) and (39)), the error of the method has an upper bound and it is mentioned in [9]. More precisely, the error satisfies:

$$\epsilon_{N,M} \leq C_1 \tau^{k_1} + C_2 h^{k_2} \quad (51)$$

for some constant C_1 and C_2.

In (51), C_1 and C_2 are real constants that do not depend on h or τ, k_1 is the order of convergence with respect to time and k_2 is the order of convergence with respect to space discretization. k_1 and k_2 are independent where the former is related to the method that was previously used to approximate the non-integer derivative with respect to time and the second is related to the method we use to approximate the second derivative with respect to x.

In problem (49) , the solution does not belong to the $C^\infty([0, T])$ (see [9]), since the second derivative does not admit values in $t = 0$. Due to this singularity, the convergence order of the method is lower than in the case of regular solutions. With respect to problem (50), where even the first derivative is unbounded at t=0, we have obtained very low estimates for the convergence order with respect to time.

With respect to the space derivative discretization, since the solution is regular, that is, the spatial partial derivative is of order $C^\infty([0, L])$ in problem (49) and therefore, the convergence order k_2 is not influenced (k_2 is close to 2 as can be seen in Table 9).

For sufficiently smooth solutions, the inequality (51) looks like this:

$$\epsilon_{N,M} \leq C_1 \tau^{2-\alpha} + C_2 h^2 \tag{52}$$

wich is equivalent to the following Since we can not obtain this estimate for non-regular solutions using a uniform mesh, we will try a different non-uniform mesh to see if we can obtain a better order of convergence and consequently, better results.

3.4. Using a non-uniform mesh

We are considering a time non-uniform mesh (graded mesh) where $t_i = T(i/N)^r$ for $i = 0, ..., N$ and $r \geq 1$. This mesh will produce more subintervals close to the singularity, $t = 0$. The distances between one point and the next one is $\tau_i = t_{i+1} - t_i$ where $i = 0, ..., N-1$. Following the same idea as the previous section to obtain (44), we present the following matrix form equations but now considering (14) instead of (12).

$$\begin{bmatrix} h^2 b_i^i + 2 + h^2 & -1 & 0 & ... & 0 \\ -1 & h^2 b_i^i + 2 + h^2 & -1 & ... & 0 \\ \vdots & & & & \\ 0 & 0 & ... & -1 & h^2 b_i^i + 2 + h^2 \end{bmatrix} \begin{bmatrix} u_1^i \\ u_2^i \\ \vdots \\ u_{M-1}^i \end{bmatrix} =$$

$$h^2 b_i^i \begin{bmatrix} u_1^{i-1} \\ u_2^{i-1} \\ \vdots \\ u_{M-1}^{i-1} \end{bmatrix} - h^2 \begin{bmatrix} \sum_{k=0}^{i-2} b_{k+1}^i (u_1^{k+1} - u_1^k) \\ \sum_{k=0}^{i-2} b_{k+1}^i (u_2^{k+1} - u_2^k) \\ \vdots \\ \sum_{k=0}^{i-2} b_{k+1}^i (u_{M-1}^{k+1} - u_{M-1}^k) \end{bmatrix} + h^2 \begin{bmatrix} v_1^i \\ v_2^i \\ \vdots \\ v_{M-1}^i \end{bmatrix} + \begin{bmatrix} u_0^i \\ 0 \\ \vdots \\ u_M^i \end{bmatrix} \tag{53}$$

The right hand side matrix in (53) is strictly dominant diagonal with the coefficients $b_i^i > 0$ for each $i = 1, ..., N$ (see Lemma 2), so we prove that the system (53) turns out to have a unique solution.

Lemma 3. *The coefficients b_i^i, $i = 1, 2, ...N$, defined in* (14)*, satisfy*

1. $b_i^i > 0$, $i = 1, 2, ..., N$
2. $b_i^i > b_{i+1}^{i+1}$, $i = 1, 2, ..., N-1$
3. $b_{k+1}^i > 0$, *with* $k = 1, 2, ..., i-2$ *and* $i = 1, 2, ...N$
4. $b_{k+1}^{i+1} > b_k^{i+1}$, $k = 1, ..., i$ *and* $i = 1, ..., N$
5. $b_1^i \geq b_1^l$, $1 \leq j \leq l$ *and* $l = 1, ..., N$
6. $t_j^\alpha b_1^j \geq t_l^\alpha b_1^l$, $1 \leq j \leq l$, $l = 1, ..., N$ *and* $\alpha \in]0, 1[$.

We prove in [1] that the numerical scheme (53) is unconditionally stable and convergent.

3.4.1. Numerical results and discussion

Proven the stability and the convergence of the method we can apply it to problems as (30).

We are going to start with the example from [9]. The authors mentioned that the optimal convergence order is recovered by choosing $r = (2-\alpha)/\alpha$ for the examples with nonsmooth solutions.

The optimal grading exponent is chosen on the assumption that the solution meets the conditions (38) and (39). The example that the authors presents in their article satisfies exactly these conditions, that is, the order of the derivative in time is α and the singularity in the solution is in the term t^α. Thus, the optimal grading exponent is $r = (2-\alpha)/\alpha$ which will allow us to achieve the optimal convergence order $2-\alpha$.

For the examples where the solution is equal/similar to the problem (55) we will obtain the experimental order $2-\alpha$ by choosing $r = (2-\alpha)/\beta$. We want to show that the numerical results are in agreement with the conditions (23) and (24).

Example 5.

$$\begin{cases} \frac{\partial^\alpha u(t,x)}{\partial t^\alpha} = \frac{\partial^2 u(t,x)}{\partial x^2} + v(t,x), t \in [0,1], x \in]0, \pi[\\ u(0,x) = 0, x \in]0, \pi[\\ u(t,0) = 0, t \in [0,1] \\ u(t,\pi) = 0, t \in [0,1] \end{cases} \tag{54}$$

The function $u(t,x) = (t^\alpha + t^3) sin(x)$ is the exact solution to this problem and $v(t,x) = (t^\alpha + t^3) sin(x) + (\frac{-6t^{3-\alpha}}{-6+11\alpha-6\alpha^2+\alpha^3} + \alpha\pi csc(\alpha\pi) sin(x))/\Gamma(1-\alpha)$ is the function chosen in agreement with the exact solution. The experimental orders of the method for $\alpha = 0.8$, $\alpha = 0.6$ and $\alpha = 0.4$ with different values of N and M are presented in Tables 11, 12 and 13.

r	1		$\frac{2-\alpha}{2\alpha} = 0.75$		$\frac{2-\alpha}{\alpha} = 1.5$		$\frac{2(2-\alpha)}{\alpha} = 3$	
$N = M$	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1
64	0.0053		0.011		0.0080		0.0167	
128	0.0032	0.75	0.0075	0.56	0.0035	1.20	0.007	1.18
256	0.0019	0.77	0.0050	0.57	0.0015	1.20	0.0033	1.19

Table 11. Table with the errors and the respective experimental order of the method for problem (54) and $\alpha = 0.8$.

r	1		$\frac{2-\alpha}{2\alpha} \approx 1.167$		$\frac{2-\alpha}{\alpha} \approx 2.33$		$\frac{2(2-\alpha)}{\alpha} \approx 4.667$	
$N = M$	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1
64	0.0159		0.0108		0.0051		0.0111	
128	0.0108	0.57	0.0067	0.67	0.0019	1.37	0.0044	1.34
256	0.007	0.58	0.0042	0.641	0.0008	1.38	0.0017	1.36

Table 12. Table with the errors and the respective experimental order of the method for problem (54) and $\alpha = 0.6$.

r	1		$\frac{2-\alpha}{2\alpha} = 2$		$\frac{2-\alpha}{\alpha} = 4$		$\frac{2(2-\alpha)}{\alpha} = 8$	
$N = M$	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1
64	0.0336		0.0072		0.0041		0.0107	
128	0.0264	0.35	0.0042	0.7808	0.0014	1.51	0.0039	1.44
256	0.0206	0.36	0.0024	0.79	0.0005	1.54	0.0014	1.49

Table 13. Table with the errors and the respective experimental order of the method for problem (54) and $\alpha = 0.4$.

Next, we consider an example with a less singular solution than the previous ones.

Example 6.

$$\begin{cases} \frac{\partial^\alpha u(t,x)}{\partial t^\alpha} = \frac{\partial^2 u(t,x)}{\partial x^2} + v(t,x), t \in [0,1], x \in]0, \pi[\\ u(0,x) = 0, x \in]0, \pi[\\ u(t,0) = 0, t \in [0,1] \\ u(t,\pi) = 0, t \in [0,1] \end{cases} \tag{55}$$

The function $u(t,x) = (t^{3/2} + t^3) sin(x)$ is the exact solution to this problem and $v(t,x) = -(t^{3/2} + t^3) sin(x) + t^{-\alpha}(\frac{1.32934t^{1.5}}{\Gamma(2.5-\alpha)} + \frac{6t^3}{\Gamma(4-\alpha)}) sin(x)$ is the function chosen in agreement with the exact solution. The experimental orders of the method for $\alpha = 0.8$, $\alpha = 0.6$ and $\alpha = 0.4$with different values of N and M are presented in the following Tables.

r	1		$\frac{2-\alpha}{\beta}=0.8$		$\frac{2-\alpha}{\alpha}=1.5$		$\frac{2(2-\alpha)}{\alpha}=3$	
$N=M$	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1
64	0.0081		0.0074		0.0110		0.0219	
128	0.0035	1.200	0.0032	1.19	0.0048	1.19	0.0097	1.18
256	0.0015	1.20	0.0032	1.19	0.0021	1.20	0.0043	1.19

Table 14. Table with the errors and the respective experimental order of the method for problem (55) and $\alpha = 0.8$.

r	1		$\frac{2-\alpha}{\beta}\approx 0.933$		$\frac{2-\alpha}{\alpha}\approx 2.33$		$\frac{2(2-\alpha)}{\alpha}\approx 4.667$	
$N=M$	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1
64	0.0027		0.0026		0.0067		0.0157	
128	0.0010	1.41	0.0010	1.41	0.0026	1.37	0.0062	1.34
256	0.00038	1.41	0.000361	1.41	0.00099	1.38	0.0024	1.36

Table 15. Table with the errors and the respective experimental order of the method for problem (55) and $\alpha = 0.6$.

r	1		$\frac{2-\alpha}{\beta}\approx 1.067$		$\frac{2-\alpha}{\alpha}=4$		$\frac{2(2-\alpha)}{\alpha}=8$	
$N=M$	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1	$\epsilon_{N,M}$	k_1
64	0.00091		0.0010		0.00516		0.01345	
128	0.0003	1.63	0.00031	1.63	0.0018	1.52	0.0049	1.46
256	0.00009	1.62	0.000101	1.62	0.00062	1.54	0.0017	1.50

Table 16. Table with the errors and the respective experimental order of the method for problem (55) and $\alpha = 0.4$.

Observing the results that we have obtained by using this non uniform mesh for the L1 method in time, we can conclude two things. The first is that, when we have a uniform mesh in time we have the result in (52) for sufficiently smooth solutions, otherwise the convergence order with respect to time decreases. The second thing is that, when we consider the non uniform mesh, the rate of convergence satisfies the following inequality:

$$\epsilon_{N,M} \leq C_1 N^{-min\{2-\alpha,\alpha r\}} + C_2 h^2 \tag{56}$$

under the conditions (38) and (39) of the Theorem 2.1 from [9]. For the case where the solution is less singular, namely, for solutions satisfying (23) and (24) we have the following

$$\epsilon_{N,M} \leq C_1 N^{-min\{2-\alpha,\beta r\}} + C_2 h^2 \tag{57}$$

and therefore the optimal time convergence order is recovered for non smooth solutions, with a proper choice of the grading exponent.

4. Applications to Neurophysiology

The motivation for this application was the article [2], where the authors propose "an extension of the cable equation by introducing a Caputo time fractional derivative." This equation can be "useful to describe anomalous diffusion phenomena with leakage as signal conduction in spiny dendrites." In this section we are going to analyse this application and its approximate solution obtained by the numerical methods described before using the *Mathematica software*.

Neurophysiology is a scientific field that studies the functioning of the nervous system based on tools like electrophysiological recordings, voltage clamp, extracellular single-unit recording and recording of local field potentials,... This area is related to many others, like electrophysiology, neuroanatomy, mathematical neuroscience, biophysics,...

Our main objective is to model the electrical conduction of non-isopotential excitable cells in the brain. These cells are called neurons. A dendrite looks like branches of a tree around the cell body of the neuron. It is through the dendrites that the neurons receive electrical signals.

4.1. The time fractional cable equation

The cable equation calculates the electric current along neurites. According to [2], the equation "describes the spatial and temporal dependence of transmembrane potential $u(t,x)$ along the axial x direction of a cylindrical nerve cell segment".

The resulting differential equation for the transmembrane potential takes the form of a standard diffusion equation with an extra term to account leakage of ions out of the membrane, which results in a decay of the electric signal in space and in time.

We are dealing with a Cauchy Problem where we see the behaviour of the transmembrane potential when the system is excited at one end. We are going to apply the cable equation to a finite length cable. So, we are considering the spacial rank between $x = 0$ and $x = L$ and time interval $[0, T]$.

When applied to the problem under the consideration, cable equation has the following form [10]:

$$r_m \frac{\partial u_m(t,x)}{\partial t} = \theta^2 \frac{\partial^2 u_m(t,x)}{\partial x^2} - u_m(t,x) + E_m + r_m I_{inj} I(t,x), \tag{58}$$

for $t \in [0, T]$ and $x \in [0, L]$.

In this equation $u_m(t,x)$ is the membrane potential in mV and $I_{inj}(t,x)$ is the injected current in Amperes. The remaining coefficients are constants: r_m is the membrane resistance per unit length of the fibre in Ωcm, $\nu = r_m c_m$ is the membrane time constant and $\theta = (r_m/r_a)^{0.5}$ is the membrane space constant. c_m is capacitance per unit length of cable of diameter d in units of F/cm. r_a is axial resistance per unit length in Ω/cm. E_m is the leakage reversal potential due to different ions in mV and it varies depending on the cell type, but we are going to consider $E_m = 0$ for the simplicity of the problem. In [2], instead of (58), the authors introduce an equation with a non integer order temporal derivative:

$$\frac{\partial^\alpha U(\Upsilon,\chi)}{\partial \Upsilon^\alpha} = \frac{\partial^2 U(\Upsilon,\chi)}{\partial \chi^2} - U(\Upsilon,\chi) + \frac{I(\Upsilon,\chi)}{\theta c_m}, \tag{59}$$

for $\Upsilon \in [0, T]$ and $\chi \in [0, L]$, where $I(\Upsilon,\chi) = \theta \nu I_{inj}(\Upsilon,\chi)$ and $I_{inj}(\Upsilon,\chi)$ is the applied stimulus current density also scaled (per unit length). $c_m = C_m \pi d$ and C_m is the capacitance per unit area in F/cm^2. The diameter of the cable is d and it is in units of μm, θ is the membrane space constant. We also take $\Upsilon = t\nu$ and $\chi = x/\theta$.

Since we take $\alpha \in]0, 1[$, we expect that the solutions of the equation (59) describe better the qualitative behaviour of the membrane potential than the usual approach with $\alpha = 1$. Moreover, by changing α we can fit the numerical results to the experimental ones.

The Caputo's fractional derivative is a non-local operator mentioned by [11] , "it could be also introduced to explain behaviours like multiple timescale dynamics and memory effects, related to the complexity of the medium", as pointed out in [2].

The partial differential equation for a single unbranched cable has a unique solution only if boundary conditions are specified at the endpoints. Since we are going to consider the finite cable equation we define the terminations as $x = 0$ and $x = L$. There are several boundary conditions for the finite cable equation [12] [10] corresponding to different situations. For example, in the killed-end or Dirichlet case the voltage is clamped to zero and the axial current "leaks" out to ground. This is the case that we are going to use because it is in agreement with the problem (30) and it can be simulated using the implementation of the L1 method that we defined in the section 2. This can arise in some preparations such as dissociated cells, and it means that the intracellular and extracellular media are directly connected at the end of the neurite. Thus the membrane potential at the end of the neurite is equal to the extracellular potential:

$$u(0,t) = 0, \quad t > 0 \qquad\qquad u(L,t) = 0, \quad t > 0. \tag{60}$$

The intracellular fluid therefore ends abruptly and abuts the extracellular fluid. If the end at $x = 0$ is killed, then for $x < 0$ the depolarization is zero, as is the resting potential.

The initial data describes the depolarization presented at the beginning of the experiment for all relevant values of x. Thus we have

$$u(x,0) = s(x), \quad 0 \le x \le L. \tag{61}$$

4.2. Numerical results and discussion

In this case, we do not know the exact solution to compare it with the numerical result. For this reason we introduce a new estimate of the convergence order with respect to time and an estimate of the convergence order with respect to space stepsize, h, respectively:

$$k = log_2\left(\frac{|U^N - U^{2N}|}{|U^{2N} - U^{4N}|}\right) \tag{62}$$

$$p = log_2\left(\frac{|U_M - U_{2M}|}{|U_{2M} - U_{4M}|}\right) \tag{63}$$

where U^N stands for the solution of the equation (59) obtained with N steps in time and U_M stands for the numerical solution obtained with M steps in space.

Designation	Value
l	$1000\ \mu m$
d	$2.5\ \mu m$
r_m	$6000\ \Omega cm^2$
r_a	$35.4\ \Omega cm$
C_m	$1\ \mu farad/cm^2$
I_{inj}	$0.5\ nA$
θ	$1029\ \mu m$

Table 17. Parameters of the dendrite used in the *Mathematica* routine taken from the book [13].

$$\begin{cases} \frac{\partial^\alpha U(\Upsilon,\chi)}{\partial \Upsilon^\alpha} = \frac{\partial^2 U(\Upsilon,\chi)}{\partial \chi^2} - U(\Upsilon,\chi) + 300, & \Upsilon \in [0,1], \ \chi \in [0,1] \\ U(0,\chi) = -70x(x-1), & \chi \in]0,1[\\ U(\Upsilon,0) = 0, & \Upsilon \in [0,1] \\ U(\Upsilon,1) = 0, & \Upsilon \in [0,1] \end{cases} \tag{64}$$

In the following table we are going to present the solution of the problem (64) in a single point, $U(\Upsilon_i,\chi_j)$, where $i = N$ and $j = M/2$ because this is where the biggest errors are expected.

α	0.2		0.4		0.6		0.8	
N	U^N_M	k	U^N_M	k	U^N_M	k	U^N_M	k
100	345.362		350.825		357.585		365.654	
200	345.375		350.848		357.613		365.68	
400	345.382	1.0051	350.86	1.009	357.627	1.019	365.692	1.04
800	345.386	1.0027	350.866	1.0052	357.634	1.0127	365.698	1.03

Table 18. Solution of the killed end problem with $M = 100$ at the point $(\Upsilon,\chi) = (1,0.5)$, using different uniform meshes in time. k is the estimate of the convergence order with respect to Υ (see 62).

When we calculate the solution using the uniform mesh we obtain a experimental order of $k \approx 1$ (see Table 18), while with the non uniform mesh we get the expected experimental order $k \approx 2-\alpha$ with $\alpha \in]0,1[$ (see Table 19) when using $r = \frac{2-\alpha}{\alpha}$.

α	0.2		0.4		0.6		0.8	
N	U^N_M	k	U^N_M	k	U^N_M	k	U^N_M	k
100	345.44		350.87		357.634		365.681	
200	345.523		350.871		357.638		365.694	
400	345.533	1.82	350.872	1.62	357.64	1.43	365.699	1.19
800	345.513	1.81	350.872	1.61	320.766	1.42	365.702	1.18

Table 19. Solution of the problem killed end problem with $M = 100$ at the point $(\Upsilon,\chi) = (1,0.5)$, using a non uniform mesh in time (see section 2) with $r = \frac{2-\alpha}{\alpha}$. k is the estimate of the convergence order with respect to Υ.

α	0.2		0.4		0.6		0.8	
M	U^N_M	p	U^N_M	p	U^N_M	p	U^N_M	p
100	345.362		350.825		357.585		365.654	
200	345.363		350.826		357.586		365.655	
400	345.364	2.0	350.827	2.0	357.587	2.0	365.655	2.0
800	345.364	2.0	350.827	2.0	357.587	2.0	365.693	2.0

Table 20. Solution of the killed end problem with $N = 100$ at the point $(\Upsilon,\chi) = (0.5,1)$, using a uniform mesh. p is the estimate of the convergence order with respect to χ (see 64).

This was to expect since the solution of problem (65) is not of class C^2 with respect to time.

We can conclude that for the problem (64), the numerical results confirm that the method is convergent and the experimental order is in agreement with the theoretical predictions. In particular, when a graded mesh is used, with the proper value of the grading coefficient, the optimal convergence order $k = 2-\alpha$ is recovered, in spite of the singularity of the problem. This can be easily seen in Table 19 for different values of α.

In Table 20 we calculate the convergence order with respect to h to confirm that the convergence order is $p = 2$.

Besides the problem in (64), we decided to consider the following problem with the first order temporal derivative instead of the fractional one to see the difference between these two approaches.

$$\begin{cases} \frac{\partial U(\Upsilon,\chi)}{\partial \Upsilon} = \frac{\partial^2 U(\Upsilon,\chi)}{\partial \chi^2} - U(\Upsilon,\chi) + 300, & \Upsilon \in [0,1], \ \chi \in [0,1] \\ U(0,\chi) = -70x(x-1), & \chi \in]0,1[\\ U(\Upsilon,0) = 0, & \Upsilon \in [0,1] \\ U(\Upsilon,1) = 0, & \Upsilon \in [0,1] \end{cases} \tag{65}$$

To obtain the numerical results in the case of problem (65), we used the Implicit Euler Method for the time derivative and the central finite difference method for the second order space derivative. This leads us to the following approximation

$$\frac{\partial u(t_i,x_j)}{\partial t} = \frac{u(t_{i+1},x_j) - u(t_i,x_j)}{\tau}, \quad i = 0,...,N-1 \ and \ j = 0,...,M \tag{66}$$

and then we get the following approximation

$$\frac{u(t_{i+1},x_j) - u(t_i,x_j)}{\tau} = \frac{u(t_{i+1},x_{j+1}) - 2u(t_i,x_j) + u(t_i,x_{j-1})}{h^2} - u(t_{i+1},x_j) + v(t_{i+1},x_j), \quad i = 0,...,N \ and \ j = 1,...,M-1 \tag{67}$$

with the initial condition and the boundary conditions defined in (65) we can obtain the solution of the problem.

The graphics of the numerical results obtained by this scheme are plotted in Figures 1 and 2.

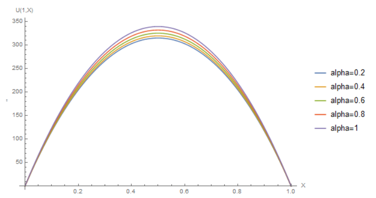

Fig. 1. The membrane potential, $U(1,\chi)$, at the fixed time $\Upsilon = 1$ for different values of $\alpha \in]0,1[$ using a time non uniform mesh (N=400 and M=100). The solution in the case $\alpha = 1$ is also given for comparison.

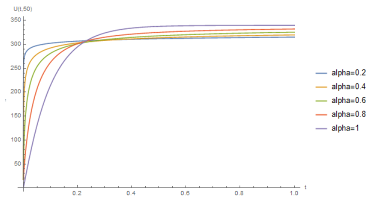

Fig. 2. The membrane potential, $U(\Upsilon, M/2)$, at the fixed point $\chi = M/2$ for different values of $\alpha \in]0,1[$ using a time non uniform mesh (N=400 and M=100). The solution in the case $\alpha = 1$ is also given for comparison.

Looking to the Figures 1 and 2 we can observe that for fixed values of Υ and χ , if Υ is sufficiently high, the values of the solution increase with α, so that the highest values are obtained for $\alpha = 1$.

5. Conclusions

We have confirmed (theoretically and experimentally) that the numerical methods, specially the L1 method is robust and efficient for solving problems of the type (30). We managed to transform the problem (30) into a system of equations and proved that the systems (44) and (53) have a unique solution. We were also able to confirm the theoretical results obtained in [9] and [8] by that an uniform mesh does not perform well in the case of problems with singular solutions, but a graded mesh, with the appropriate grading exponent can give good accuracy. Here we consider a more general class of solutions (see problem (55)) and discuss how to adapt the graded mesh in this case.

When we considered the non-uniform mesh in the first derivative of the solution is singular at the origin, the numerical results satisfied the following error estimate:

$$\epsilon_{N,M} \leq C_1 N^{-min\{2-\alpha,\alpha r\}} + C_2 h^2 \quad (68)$$

under the conditions (38) and (39). Where α is the order of the time derivative ($0 < \alpha < 1$). For the case where the solution satisfies (23) and 24, we have the following result:

$$\epsilon_{N,M} \leq C_1 N^{-min\{2-\alpha,\beta r\}} + C_2 h^2 \quad (69)$$

where $\beta \geq \alpha$ is the the index of regularity of the solution, according to the condition (38). Therefore the optimal time convergence order is recovered for non smooth solutions, with a proper choice of the grading exponent. We managed to prove that the optimal gradient exponent, $r = \frac{2-\alpha}{\alpha}$ or $r = \frac{2-\alpha}{\beta}$ depending the regularity of the solution.

The problems considered have no singularities in x. In the examples where we estimated the convergence order with respect to space we have concluded that $p = 2$, as it was expected.

When we applied the method to the Neurophysiology problem (64), we have obtained the experimental order of convergence $k = 2 - \alpha$ when using a non-uniform mesh, which was in agreement with the results of in section 3. When we used the uniform mesh we obtained a convergence order $k = 1$ with respect to τ and a convergence order $p = 2$ with respect to h.

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