University of Chester
Department of Mathematics

Numerical Solution of Fractional Differential Equations and their Application to Physics and Engineering

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Abstract

This dissertation presents new numerical methods for the solution of fractional differential equations of single and distributed order that find application in the different fields of physics and engineering.

We start by presenting the relationship between fractional derivatives and processes like anomalous diffusion, and, we then develop new numerical methods for the solution of the time-fractional diffusion equations.

The first numerical method is developed for the solution of the fractional diffusion equations with Neumann boundary conditions and the diffusivity parameter depending on the space variable. The method is based on finite differences, and, we prove its convergence (convergence order of $O(\Delta x^2 + \Delta t^{2-\alpha})$, $0 < \alpha < 1$) and stability. We also present a brief description of the application of such boundary conditions and fractional model to real world problems (heat flux in human skin). A discussion on the common substitution of the classical derivative by a fractional derivative is also performed, using as an example the temperature equation.

Numerical methods for the solution of fractional differential equations are more difficult to develop when compared to the classical integer-order case, and, this is due to potential singularities of the solution and to the nonlocal properties of the fractional differential operators that lead to numerical methods that are computationally demanding .

We then study a more complex type of equations: distributed order fractional differential equations where we intend to overcome the second problem on the numerical approximation of fractional differential equations mentioned above. These equations allow the modeling of more complex anomalous diffusion processes, and can be viewed as a continuous sum of weighted fractional derivatives. Since the numerical solution of distributed order fractional differential equations based on finite differences is very time consuming, we develop a new numerical method for the solution of the distributed order fractional differential equations based on Chebyshev polynomials and present for the first time a detailed study on the convergence of the method.

The third numerical method proposed in this thesis aims to overcome both problems on the numerical approximation of fractional differential equations. We start by solving the problem of potential singularities in the solution by presenting a method based on a non-polynomial approximation of the solution. We use the method of lines for the numerical approximation of the fractional diffusion equation, by proceeding in two separate steps: first, spatial derivatives are approximated using finite differences; second, the resulting system of semi-discrete ordinary differential equations in the initial value variable is integrated in time with a non-polynomial collocation method. This numerical method is further improved by considering graded meshes and an hybrid approximation of the solution by considering a non-polynomial approximation in the first subinterval which contains the origin in time (the point where the solution may be singular) and a polynomial approximation in the remaining intervals. This way we obtain a method that allows a faster numerical solution of fractional differential equations (than the method obtained with nonpolynomial approximation) and also takes into account the potential singularity of the solution.

The thesis ends with the main conclusions and a discussion on the main topics presented along the text, together with a proposal of future work.

Declaration

The material being presented for examination is my own work and has not been submitted for an award of this or another HEI except in minor particulars which are explicitly noted in the body of the thesis. Where research pertaining to the thesis was undertaken collaboratively, the nature and extent of my individual contribution has been made explicit.

Signed: .....

Date: .....

The list of published or submitted papers related to Fractional Calculus during the execution of the working plan that gave rise to this dissertation is given below.

Articles

- L.L. Ferrás, N.J. Ford, M.L. Morgado, M. Rebelo, High order methods for the time-fractional diffusion equation. To be submitted (2018);
- M.L. Morgado, M. Rebelo, L.L. Ferrás, N.J. Ford, Numerical solution for diffusion equations with distributed order in time using a Chebyshev collocation method. Applied Numerical Mathematics 114 (2017) 108-123;
- L.L. Ferrás, N.J. Ford, M.L. Morgado, J.M. Nóbrega, M. Rebelo, Fractional Pennes' bioheat equation: theoretical and numerical studies. Fractional Calculus and Applied Analysis 18 (2015) 1080-1106.

Book Chapters

- L.L. Ferrás, N.J. Ford, M.L. Morgado, M. Rebelo, A Hybrid Numerical Scheme for Fractional-Order Systems. To appear in Volume 505 of the Lecture Notes in Electrical Engineering series (2018);
- L.L. Ferrás, N.J. Ford, M.L. Morgado, M. Rebelo, A Numerical Method for the Solution of the Time-Fractional Diffusion Equation. B. Murgante et al. (Eds.): ICCSA 2014, Part I, Lecture Notes in Computer Science 8579 (2014) 117–131;

Conference Proceedings

- L.L. Ferrás, N.J. Ford, M.L. Morgado, J.M. Nóbrega, M. Rebelo, Fractional Bioheat Equation. 15th International Conference on Computational and Mathematical Methods in Science and Engineering (CMMSE 2015) ISBN: 978-84-617-2230-3;

- L.L. Ferrás, M.L. Morgado, M. Rebelo, Comparison of different numerical methods for the solution of the time-fractional reaction-diffusion equation with variable diffusion coefficient. 15th International Conference on Computational and Mathematical Methods in Science and Engineering (CMMSE 2015) ISBN: 978-84-617-2230-3;

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Conference Abstracts

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Posters

- M. Rebelo, M.L. Morgado, L.L. Ferrás, N.J. Ford, A spectral collocation method for the diffusion equation with distributed order in time, IWANASP (2015) Lagos, Portugal;

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Introduction 1

1.1 The (brief) History of Fractional Calculus

The concept of a derivative in the sense of a tangent line is a very old one, and can be traced back to 300 BC, but, the modern development of calculus is usually credited to Sir Isaac Newton (1642-1727) and Gotfried Wihelm Leibniz (1646-1716) for their new notations, new approaches to differentiation and derivatives, and most important, the fundamental theorem of calculus relating differentiation and integration [1].

FIGURE 1.1: Newton and Leibniz

Newton was an English mathematician, astronomer, and physicist that laid the foundations of classical mechanics. He also formulated the laws of motion and universal gravitation. Gottfried Wilhelm (von) Leibniz was a German polymath and philosopher who occupies a prominent place in the history of mathematics and the history of philosophy, having developed differential and integral calculus independently of Isaac Newton [2; 3].

Regarding fractional differential calculus, it is wrong to think that this is a recent subject. For instance, the symbol $d^n y/dx^n$ was first proposed by Leibniz, and, in 1695 L'Hôpital asked Leibniz the meaning of $d^n y/dx^n$ if $n = 1/2$; that is " what if n is fractional?". Leibniz responded with the following [1]:

> "...Although infinite series and geometry are distant relations, infinite series admits only the use of exponents that are positive and negative integers and does not, as yet, know the use of fractional exponents..."

He continues with:

> "This is an apparent paradox from which, one day, useful consequences will be drawn."

This letter can be understood as the beginning of fractional differential calculus, and, the name *fractional* comes from the L'Hôpital question regardind the fraction $1/2$ (although the

order of differentiation may be a real or a complex number). From this letter, we learn that the traditional (integer-order) and the fractional differential calculus were born almost at the same time.

Figure 1.2: L'Hôpital

Marquis de l'Hôpital was a French mathematician, being well known for the l'Hôpital's rule for calculating limits involving indeterminate forms $0/0$ and ∞/∞. He published a treatise on the infinitesimal calculus, entitled Analyse des Infiniment Petits pour l'Intelligence des Lignes Courbes. This book was a first systematic exposition of differential calculus. The book's publication is controversial because l'Hôpital made a proposal to Johann Bernoulli: in exchange for an annual payment of 300 Francs, Bernoulli would inform L'Hôpital of his latest mathematical discoveries [2; 3].

Besides the 1695 letter, other letters were written regarding this subject. In 1697, Leibniz sent letters to J. Wallis and J. Bernoulli, and, he mentioned the possible approach to fractional-order differentiation in that sense, that for non-integer values of n the definition could be the following, $\frac{d^n e^{ax}}{dx^n} = a^n e^{ax}$.

In 1716 Leibniz died, but, the urge to understand the derivatives of fractional order increased, and several other authors devoted their time to the subject. The well known Leonard Euler also contributed to the understanding and generalization of fractional differential calculus. He generalized the notion of factorial $n!$ to non-integer values, latter called gamma function ($\Gamma(.)$) by Adrien-Marie Legendre around 1811,

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} \mathrm{d}t \tag{1.1}$$

with $Re(z) > 0$.

Figure 1.3: Euler and Legendre

Leonhard Euler was a Swiss mathematician, physicist, astronomer, logician and engineer. He was one of the most eminent mathematicians of the 18th century, and is held to be one of the greatest in history. He is also widely considered to be the most prolific mathematician of all time. Adrien-Marie Legendre was a French mathematician. He is well-known for the Legendre polynomials and Legendre transformation. Curiosity: for two centuries, until the recent discovery of the error in 2005, books, paintings and articles have incorrectly shown a side-view portrait of the obscure French politician Louis Legendre (1752–1797) as that of the mathematician Legendre [2; 3].

Another important discovery was the Beta function in 1730 (also called the Euler integral of the first kind), denoted by $B(a,b)$ due to Jacques Binet (1786-1856),

$$B(a,b) = \int_0^1 x^{a-1} (1-x)^{b-1} \, \mathrm{d}x, \; Re(a) > 0, \; Re(b) > 0. \tag{1.2}$$

Between 1810 and 1819, the French mathematician Sylvestre François Lacroix (1765-1843) adopted Euler's derivation for his successful textbook Traite du Calcul Diferentiel et du Calcul Integral [4]. Using the gamma function, Lacroix showed that the derivative of x^m, $\frac{d^n x^m}{dx^n} = m\,(m-1)\,....\,(m-n+1)\,x^{m-n}$ could be generalized for arbitrary fractional α and β by simply writting the derivative with the help of gamma function:

$$\frac{d^\alpha x^\beta}{dx^\alpha} = \frac{\Gamma\,(\beta+1)}{\Gamma\,(\beta-\alpha+1)} x^{\beta-\alpha} \tag{1.3}$$

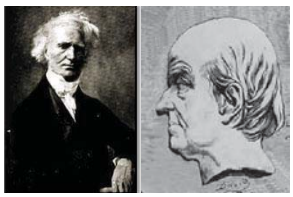


FIGURE 1.4: Binet and Lacroix

Jacques Philippe Marie Binet was a French mathematician, physicist and astronomer. He made significant contributions to number theory, and the mathematical foundations of matrix algebra. He is also recognized as the first to describe the rule for multiplying matrices in 1812. He was a professor of mechanics at the Ecole Polytechnique, succeeding Poisson in 1815. Sylvestre François Lacroix was a French mathematician. Lacroix's path to mathematics started with the novel Robinson Crusoe. That gave him an interest in sailing and thus navigation too. At that point geometry captured his interest and the rest of mathematics followed [2; 3].

Later, Joseph Fourier (1768-1830) gave the first step to the generalization of the notion of differentiation for arbitrary functions with his 1822 book, Theorie Analytique de la Chaleur [5]. He obtained the following integral representation of a function $f\,(x)$,

$$f\,(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} f\,(z)\,\mathrm{d}z \int_{-\infty}^{+\infty} \cos t\,(x-z)\,\mathrm{d}t \tag{1.4}$$

and noted that,

$$\frac{d^n f\,(x)}{dx^n} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} f\,(z)\,\mathrm{d}z \int_{-\infty}^{+\infty} t^n \cos\left(tx - tz + \frac{n\pi}{2}\right) \mathrm{d}t \tag{1.5}$$

This formula could serve as a definition of the n-th order derivative for non-integer n.

Until 1822, the only interest on fractional differential calculus was merely to set the basis of this field, and, there were no attempts to describe physical phenomena with this type of more generalized derivatives.

In 1823, Niels Henrik Abel [6] applied the fractional differential calculus in the solution of the tautochrone problem (to find the curve for which the time taken by an object sliding without friction in uniform gravity to its lowest point is independent of its starting point).

Figure 1.5: Fourier and Abel

Jean-Baptiste Joseph Fourier was a French mathematician and physicist and best known for initiating the investigation of Fourier series. He took a prominent part in promoting the French Revolution, serving on the local Revolutionary Committee. He was imprisoned briefly in 1795. He succeeded Joseph-Louis Lagrange at the École Polytechnique. Niels Henrik Abel was a Norwegian mathematician. His most famous single result is the first complete proof demonstrating the impossibility of solving the general quintic equation in radicals. Abel made his discoveries while living in poverty and died at the age of 26 [2; 3].

Later (1832), Liouville (possibly inspired by the solution given by Abel [7]) presented two different definitions for the fractional derivatives [8]. The first definition is based on a series that depends on the order of differentiation to be convergent. Liouville second definition of fractional derivative applies to functions of the form x^{-a} with $a > 0$. He considered the integral $\int_0^\infty u^{a-1}e^{-xu}\mathrm{d}u$, and by performing the transformation $u = \frac{t}{x}$ we have that $du = \frac{1}{x}dx$ and $\int_0^\infty u^{a-1}e^{-xu}\mathrm{d}u = x^{-a}\int_0^\infty t^{a-1}e^{-t}\mathrm{d}t = x^{-a}\Gamma(a)$,

$$x^{-a} = \frac{1}{\Gamma(a)}\int_0^\infty u^{a-1}e^{-xu}\mathrm{d}u. \tag{1.6}$$

By applying the derivative operator on both side of the equation [9], a fractional order derivative is obtained for the function x^{-a},

$$\frac{d^\alpha(x^{-a})}{dx^\alpha} = \frac{(-1)^\alpha\Gamma(a+\alpha)}{\Gamma(a)}x^{-\alpha-a} \tag{1.7}$$

This derivative is of no use for functions other than rational.

There is a main difference between the definition provided by Lacroix and the definition by Liouville (Eq. 1.7). The first one gives a nonzero value for the fractional derivative of a constant, while the second one gives zero. This lead to a great discussion in the 19th century, regarding whose definition was the correct one.

Following the timeline, Riemann was the next well known mathematician to present a definition for the fractional derivative. His idea is shared with Liouville, since Liouville has probably influenced Riemann, with his memoirs.

Figure 1.6: Riemann and Liouville

Bernhard Riemann was a German mathematician who made contributions to analysis, number theory, and differential geometry. In the field of real analysis, he is mostly known for the first rigorous formulation of the integral, the Riemann integral. In 1859, following Lejeune Dirichlet's death, he was promoted to head the mathematics department at Göttingen. He was also the first to suggest using dimensions higher than merely three or four in order to describe physical reality. Joseph Liouville was a French mathematician. He was appointed as professor at the École Polytechnique in 1838. He worked in a number of different fields in mathematics, including number theory, complex analysis, differential geometry and topology, mathematical physics and astronomy. He is remembered particularly for Liouville's theorem [2; 3].

Based on the fact that $\left\{1, x, x^2, ..., x^{n-1}\right\}$ is a fundamental solution set of the homogeneous equation, $\frac{d^n y(x)}{dx^n} = 0$, Riemann tried to find the solution $y(x)$ of $\frac{d^n y(x)}{dx^n} = f(x)$ with $d \leq x \leq e$ and $f(x)$ a continuous function on this interval. At that time, Riemann obtained some inconsistencies in his results.

Note that by setting the boundary conditions $y^{(k)}(a) = 0$ with $0 \leq k \leq n-1$, $a \in (d,\, e)$, the solution obtained is unique and given by,

$$y(x) = \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} f(t)\, \mathrm{d}t \tag{1.8}$$

By naturally extending this equation from integer n to non-integer order α we have the Riemann-Liouville definition of fractional order integral,

$$y = {}_a J_x{}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1} f(t)\, \mathrm{d}t \tag{1.9}$$

with $\alpha \geq 0$. The symbol ${}_a J_x^{\alpha}$ denotes the integration of arbitrary order along the x axis, with a and x the limits of integration.

The corresponding derivative is calculated using Lagrange's rule for differential operators. Computing the n-th order derivative over the integral of order $(n-\alpha)$, the α order derivative is obtained (n is the nearest integer bigger than α),

$${}_a D_x^{\alpha} f(x) = \frac{d^n}{dx^n}\, {}_a J_x^{(n-\alpha)} f(x) \tag{1.10}$$

Note that the original definition provided by Riemann and Liouville was not (exactly) the one given by Eq. 1.9 (see [7], [10]). When $a = 0$ we have Riemann's definition and when $a = -\infty$ Liouville definition is equivalent to Eq. 1.9. Also, it is important to note that Eq. 1.9 verifies some important properties expected from an operator of this kind [7].

Before the Riemann-Liouville formula was achieved, there were some important works that need to be stated. First, the work of Cauchy, that defined the Cauchy's differentiation formula [11],

$$D^n f(z) = \frac{n!}{2\pi i} \int_{\gamma} \frac{f(t)}{(t-z)^{n+1}} \mathrm{d}t \tag{1.11}$$

with D^n the n-th derivative operator and γ a closed contour on which $f(z)$ is analytic.

In 1892 Hadamard, [12] proposed another definition for the fractional integral and also for the fractional derivative. For more on this subject, the following works are advised [13; 14; 15].

In 1917, Weyl [16] proposed another interesting definition, similar to the Riemann-Liouville definition, but with different terminals of integration and different kernel function $(t-x)^{\alpha-1}$.

Figure 1.7: Cauchy and Hadamard

Baron Augustin-Louis Cauchy was a French mathematician who made pioneering contributions to analysis. He stated and proved the theorems of calculus rigorously. He wrote approximately eight hundred research articles and five complete textbooks. He worked as a engineer but always tried to become a pure mathematician. In 1815 he became a professor at École Polytechnique. Jacques Hadamard was also a French mathematician. He made contributions in number theory, complex function theory, differential geometry and partial differential equations [2; 3].

Grünwald (1867 [17]) and Post (1930 [18]) presented the idea of fractional derivative as the limit of a sum, using the classical definitions of a derivative (this concept was also introduced by by Aleksey Vasilievich Letnikov). In 1927, Marchaud [19] formulated an equivalent fractional derivative of arbitrary order. The equivalence was shown by Samko et al. [13] (see [20] for a detailed explanation).

It should be mentioned that in 1903 the Mittag-Leffler function was presented to the world [21], and it plays an important role in fractional calculus. We can say that the Mittag-Leffler function stands for fractional differential equations as the exponential function stands for classical differential equations (The Mittag-Leffler function is a generalization of the exponential function). The Mittag-Leffler function with one parameter α is given by:

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)},\ z \in \mathbb{C},\ Re(\alpha) > 0 \tag{1.12}$$

and the version with two parameters (α and β) is given by:

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)},\ \alpha > 0,\ \beta > 0. \tag{1.13}$$

In 1940, Erdélyi [22] and Kober [23] presented what we call now the Erdélyi–Kober fractional integral. This operator generalizes the Riemann fractional integral and the Weyl integral.

Later, Riesz also proposed a new fractional integral [24]. His integral was successfully used in Potential theory.

Figure 1.8: Caputo

Michele Caputo started his academic life as an assistant Professor of Mathematics at the University of Ferrara, in 1950. He contributed with many papers on the fields of Geophysics, Geodesy, Rheology, Seismology, Fractional calculus, Applied mathematics and Finance. He is best known in the world of fractional calculus for his definition of fractional derivative, and, he is still active.

There is another option for computing fractional derivatives, the Caputo fractional derivative. It was introduced by M. Caputo in 1967 [25] (several other authors presented the idea, but, such derivative is associated with M. Caputo because he was among the first to use this

operator in applications, and to study some of its properties). In contrast to the Riemann-Liouville fractional derivative, when solving differential equations using Caputo's definition, it is not necessary to define the fractional order initial conditions (usually not known and with no physical meaning).

The Caputo fractional derivative is obtained by computing an ordinary derivative followed by the fractional integral, whereas the Riemann-Liouville is obtained in reverse order (more on this will be shown later). Under certain conditions it can be show that all these definitions are equivalent.

Several other definitions and new studies exist in the literature. In 1928 Hardy and Littlewood [26] presented a monograph where they gave a systematic treatment of certain theorems based on the properties of the Riemann-Liouville integrals and derivatives of arbitrary order of functions of certain standard classes, in particular the Lebesgue classes L^p, the Lipschitz classes $Lip\,(k)$ and more general classes of functions which satisfy integrated Lipschitz conditions. In 1932 they extended their early paper to the complex field [27]. In 1927, Davis [28] presented a paper where he shows the benefits from using fractional calculus for certain functional equations. In 1938, Love and Young [29] developed the fractional version of the integration by parts, using the Riemann- Liouville and Weyl integrals. The formulas were given for the Lebesgue, Riemann-Stieltjes, and generalized Stieltjes integrals. In 1967 Love [30] devised explicit solutions for two integral equations, and also devised necessary and sufficient conditions for existence, and sufficient for uniqueness, of solutions. Later, in 1971, Love [31] extended the properties of the fractional calculus of real order to the complex order. Pitcher and Sewell [32] (1938) proved some theorems on the existence and uniqueness of solutions of the differential equation ${}_aD_x^{\alpha}y = \varphi\,(x,y)$, $\alpha > 0$, where $\varphi\,(x,y)$ is a known function, $y\,(x)$ is an unknown function, and ${}_aD_x^{\alpha}y$ is the Riemann-Liouville generalized derivative. In 1945 Zygmund [33] presented a theorem on the fractional derivatives and in 1965 Stein and Zygmund [34] published a paper on the necessary and sufficient conditions for a function to have a fractional derivative. In 1968 Welland published two papers on this subject, in one paper, Welland [35] studied the fractional differentiation for functions with lacunary Fourier series (lacunary series is an analytic function that cannot be analytically continued anywhere outside the radius of convergence), and, on the other paper he presented an extension of the fractional derivative for functions of several variables [36]. In 1972 Prabhakar [37] studied integral equations with the kernels containing a confluent hypergeometric function in two variables, by using fractional integration. In 1973, Saxena and Kumbhat, introduced two new fractional integration operators associated with the H-function of two variables.

In 1974 the first conference on fractional calculus was held at New Haven. Since then, the number of papers and books on the subject has increased significantly. Some important papers are the ones by Campos (1984)[38], where a generalization of both the Cauchy and Weyl integrals was devised, and, the rules of association and commutation for the derivatives of complex orders were proved, and the papers by Debnath and Grum (1988) [39; 40] where they studied the concepts and properties of derivintegrals of arbitrary order (real or complex), demonstrated the relation between the Cauchy formula for repeated integrals and the Riemann-Liouville integral of integer order, and developed a systematic method of evaluation of the derivintegrals of the important transcendental and special functions.

Regarding the existence, uniqueness, smoothness and stability of ordinary fractional differential equations of the Caputo type, it is worth mentioning that Kai Diethelm and Neville J. Ford were the first to study this subject, providing relevant results for the scientific

community, and, that they also developed several numerical methods that are still regularly used in the numerical solution of fractional differential equations [41; 42; 43; 44; 45; 46; 47; 48; 49; 50; 51; 52; 53; 54; 55].

More information on this subject can be found in the paper by Machado et al. [56] entitled Recent history of fractional calculus, where a survey of the literature is presented.

Nowadays it is still impossible to say that one definition is better than the other one (although it is fair to say that the Caputo definition is often used for the application of fractional calculus to physics).

Perhaps the various definitions are particular cases of a more general theory, yet to come.

A question that we should ask ourselves is:

"Why study fractional differential calculus, if we cannot find a unique definition for the fractional derivative?"

There are at least two reasons. First, we already found application of this theory to different fields of physics and engineering. Note that the real breakthrough is to prove and deduce that a model with a fractional derivative is *more correct* than the integer order one. For more on fractional calculus applications see [57], [58], [59], [20].

Second, in the beginning of times there were only natural numbers, and nowadays, we do not have a gap between number 3 and number 4, because, real numbers exist. The main difference is that we need the real numbers in our daily lives, while, we still do not need fractional derivatives to *survive*.

In short, fractional differential and integral calculus is still under strong development and prone to modifications. It is not a consensual field of mathematics.

1.2 Fractional Derivatives

What is the best definition of fractional derivative?

"I would say it depends on who asks!" *Prof. Neville Ford (2015)*

1.2.1 Introduction

We now present the basic theory on fractional derivatives and integrals, allowing this thesis to become self-contained. We start by presenting the mathematical preliminaries that will be useful when presenting the main results on fractional derivatives, numerical analysis, solvability, convergence and stability. Based on the quotation by Prof. Neville Ford, we then present the main definitions of fractional derivatives that are the Riemann-Liouville and the Caputo. Since the Grünwald–Letnikov definition evolves from the classical finite difference approximation, special attention is also given to this definition.

1.2.2 Mathematical Preliminaries

The results that are about to be presented, heavily rely on the exposition by Kai Diethelm [60], Samko, Kilbas and Marichev [61] and Podlubny [20].

1.2.2.1 Basic Concepts

Definition 1.2.1 ***Riemann Integrable Functions:*** *Let f be a bounded function defined on a closed interval $[a, b]$. We say that f is Riemann integrable on $[a, b]$ if the infimum of upper sums through all partitions of $[a, b]$ is equal to the supremum of all lower sums through all partitions of $[a, b]$.*

Lemma 1.2.1 *If f is continuous on $[a, b]$, then f is Riemann-integrable on $[a, b]$.*

We now present the Fundamental Theorem of Calculus, that will be later generalized to Lebesgue spaces.

Theorem 1.2.1 ***Fundamental Theorem of Calculus:*** *Let $f : [a, b] \to \mathbb{R}$ be a continuous function, and let $F : [a, b] \to \mathbb{R}$ be defined by*

$$F(x) = \int_a^x f(t)dt. \tag{1.14}$$

Then, F is differentiable and

$$F' = \frac{dF}{dt} = f. \tag{1.15}$$

In order to write in a more compact way some of the results to come, we now define the following differential and integral operators.

Definition 1.2.2 ***Derivative and Integral Operators:*** *We denote by D the differential operator that maps a function f into its derivative $Df(x) = f'(x)$ and by J_a the integral operator that maps a funtion $f(x)$ into its primitive (whenever the integration can be performed on the compact interval $[a,\, b]$):*

$$J_a f(x) = \int_a^x f(t)dt,\ x \in [a,\, b] \tag{1.16}$$

These operators can be generalized to perform n-fold iterates:

$$D^n f(x) = \frac{d}{dt}...\frac{d}{dt}\frac{df}{dt} = D^1 D^{n-1} f(x), \tag{1.17}$$

$$J_a^n f(x) = \int_a^x ... \int_a^x \int_a^x f(t)dt = J_a^1 J_a^{n-1} f(x). \tag{1.18}$$

Lemma 1.2.2 ***n-fold Integration:*** *Let f be Riemann integrable on $[a,\, b]$. Then, for $a \leq x \leq b$ and $n \in \mathbb{N}$, we have*

$$J_a^n f(x) = \frac{1}{(n-1)!}\int_a^x (x-t)^{n-1} f(t)dt \tag{1.19}$$

Lemma 1.2.3 ***n-fold Integration:*** *Let $m,\ n \in \mathbb{N}$, with $m > n$, and let f be a function with a continuous n^{th} derivative on the interval $[a,\, b]$. Then,*

$$D^n f = D^m J_a^{n-n} f. \tag{1.20}$$

The previous two lemmata together with the Gamma function defined before, set the basis for the defining fractional derivatives of the Riemann-Liouville and Caputo type.

Let us now define some spaces that will be useful along the thesis.

Definition 1.2.3 ***Space L_p:*** *Let $\Omega = [a,\, b]$, $-\infty \leq a < b \leq \infty$. L_p represents the set of all Lebesgue measurable functions $f(x) : \Omega \to \mathbb{R}$ for which $\int_a^b |f(t)|^p\, dt < \infty$ $(1 \leq p < \infty)$.*

Definition 1.2.4 ***Space L_∞:*** *Let $\Omega = [a,\, b]$, $-\infty \leq a < b \leq \infty$. L_∞ consists of all measurable functions $f(x) : \Omega \to \mathbb{R}$ that are almost everywhere bounded, that is, $\exists c \in \mathbb{R}$: $\mu(\{|f| > c\}) = 0$, where μ is the Lebesgue measure.*

Definition 1.2.5 ***L_p Norms:*** *We set the norm*

$$\|f\|_p = \left(\int_a^b |f(t)|^p\, dt\right)^{1/p}, \tag{1.21}$$

and its extension to $p = \infty$,

$$\|f\|_\infty = ess\ \sup |f(t)| \tag{1.22}$$

where $ess\sup$ *is the essencial supreme, the proper generalization to measurable functions of the maximum (the values of a function on a set of measure zero don't affect the essential supremum).*

Definition 1.2.6 C^m ***Spaces:*** *Let* $f : [a, b] \to \mathbb{R}$ *and* $m \in \mathbb{N}_0 = \{0, 1, 2, ...\}$*, the space* C^m *is the set of functions* f *with a continuous* m^{th} *derivative (*$f \in C^0$ *means that the function is continuous).*

Theorem 1.2.2 ***Fundamental Theorem in Lebesgue Spaces:*** *Let* $f \in L_1[a, b]$*. Then,* $J_a f$ *is differentiable almost everywhere in* $[a, b]$ *and* $DJ_a f = f$ *also holds almost everywhere on* $[a, b]$*.*

Definition 1.2.7 ***Absolutely Continuous Function:*** *A function* $f(x)$ *is called absolutely continuous on an interval* Ω*, if for any* $\varepsilon > 0$ *there exists a* $\delta > 0$ *such that for any finite set of pairwise non-intersecting intervals* $[a_k, b_k] \subset \Omega$*,* $k = 1, 2, ..., n$*, such that* $\sum_{k=1}^{n}(b_k - a_k) < \delta$*, the inequality* $\sum_{k=1}^{n} |f(b_k) - f(a_k)| < \varepsilon$ *holds. The space of these functions is denoted by* $A(\Omega)$*.*

Definition 1.2.8 A^n ***Space:*** *Consider the finite interval* $\Omega = [a, b]$*. It is known that the space* $A(\Omega)$ *coincides with the space of primitives of Lebesgue summable functions, that is:*

$$f(x) \in A(\Omega) \Leftrightarrow f(x) = c + \int_a^x \psi(t)dt, \ \psi(t) \in L_1(\Omega) \tag{1.23}$$

Therefore, for an absolutely continuous function f *we have that* $\psi(t) = f'(t)$ *and* $c = f(a)$*. Let* $n \in \mathbb{N} = \{0, 1, 2, ...\}$*, and,* $A^n(\Omega)$ *denote the set of functions with an absolutely continuous* $(n-1)st$ *derivative, i.e. the functions* f *for which there exists (almost everywhere) a function* $g \in L_1(\Omega)$ *such that*

$$f^{(n-1)}(x) = f^{(n-1)}(a) + \int_a^x g(t)dt. \tag{1.24}$$

Lemma 1.2.4 *The space* $A^n(\Omega)$ *consists only of functions* $f(x)$ *that can be represented in the form:*

$$f(x) = \frac{1}{(n-1)!}\int_a^x (x-t)^{n-1}\psi(t)dt + \sum_{k=0}^{n-1} c_k(x-a)^k \tag{1.25}$$

with $\psi(t) \in L_1(\Omega)$ *and* c_k *arbitrary constants (*$k = 0, 1, ..., n-1$*). Moreover, we have that* $\psi(t) = f^{(n)}(t)$ *and* $c_k = \frac{f^{(k)}(a)}{k!}$*.*

1.2.2.2 Riemann-Liouville Integral

We start by presenting the definition of the Riemann-Liouville Integral:

Definition 1.2.9 ***Riemann-Liouville Fractional Integral*** *Let* $n \in \mathbb{R}_+$ *and* J_a^n *be the operator defined on* $L_1[a, b]$ *by*

$$J_a^n f(x) = \frac{1}{\Gamma(n)} \int_a^x (x-t)^{n-1} f(t) dt, \ x \in [a, b]. \tag{1.26}$$

Then J_a^n is called the Riemann-Liouville fractional integral operator of order n.

This generalization of Lemma 1.2.2 appears naturally, considering the fact that $\Gamma(n) = (n-1)!$.

Since $\lim_{n \to 0} J_a^n f(x) = f(x)$ we set $J_a^0 := I$, where I is the identity operator.

We will now present an important property, that will allow the definition of fractional derivatives of the Riemann-Liouville and Caputo type.

Theorem 1.2.3 *Let $\alpha, \beta \in [0, \infty)$ and $f \in L_1[a, b]$, then,*

$$J_a^\alpha J_a^\beta f = J_a^{\alpha+\beta} f \tag{1.27}$$

holds almost everywhere on $[a, b]$. Note that if $f \in C[a, b]$ or $\alpha + \beta \geq 1$ this identity holds everywhere on $[a, b]$. An important consequence of this results is the commutative property

$$J_a^\alpha J_a^\beta f = J_a^\beta J_a^a f \tag{1.28}$$

1.2.3 The Different Definitions of Fractional Derivative

1.2.3.1 Riemann-Liouville Fractional Derivative

It was shown before how the definition of the Riemann-Liouville fractional integral could be obtained from Lemma 1.2.2 and the preperties of the Γ function. Now, in order to obtain a proper definition for the Riemann-Liouville fractional derivative we will make use of a generalization of Lemma 1.2.3 (stating that for $m > n$ (integers) and $f \in C^n[a, b]$, $D^n f = D^m J_a^{m-n} f$).

The case when n is not an integer does not pose any problem since the integral can be easily evaluated through Eq. 1.26. The main difference is that the derivative on the left-hand-side ($D^n f$) may now depend on the constant a ($D_a^n f$) and therefore we have the following theorem:

Theorem 1.2.4 *Let $\alpha \in \mathbb{R}_+$ and $m \in \mathbb{N}$ with $m > \alpha$, then*

$$D_a^\alpha = D^m J_a^{m-\alpha} \tag{1.29}$$

By looking at the Fundamental Theorem of Calculus, it is obvious why in the case $m, n \in \mathbb{N}$ the derivative does not depend on a.

We still have another problem, that is, what value should we use for m. Note that the only restriction is $m > \alpha$. A possible solution is to assume that m is the smallest integer that is bigger than α.

Definition 1.2.10 *Riemann-Liouville Fractional Derivative: Let $\alpha \in \mathbb{R}_+$ and $m = \lceil \alpha \rceil$. The Riemann-Liouville fractional derivative of order α (${}_a^R D_t^\alpha f$) is given by*

$$ {}_a^R D_x^\alpha f(x) = D^m J_a^{m-\alpha} f(x) = \frac{D^m}{\Gamma(m-\alpha)} \int_a^x (x-t)^{m-\alpha-1} f(t) dt. \tag{1.30} $$

For $n = 0$ we have ${}_a^R D_t^0 := I$.

The following Lemma provides a useful way to calculate the Riemann-Liouville fractional derivative.

Lemma 1.2.5 *Assume that $f \in A^1([a,\, b])$ and that $0 < \alpha < 1$, then ${}_a^R D_x^\alpha f(x)$ exists almost everywhere in $[a,\, b]$, ${}_a^R D_x^\alpha f \in L_p([a,\, b])$ ($1 \leq p < 1/\alpha$) and*

$$ {}_a^R D_x^\alpha f(x) = \frac{1}{\Gamma(1-\alpha)} \left(\frac{f(a)}{(x-a)^\alpha} + \int_a^x (x-t)^{-\alpha} f'(t) dt \right). \tag{1.31} $$

In order to gain some insight into this fractional derivative let us assume that $f(x) = 1$ is a constant function and that $a = 0$ and $\alpha = 1/2$. Then, using Eq. 1.31 we instantaneously obtain the result ${}_0^R D_x^{0.5} f((x) = \frac{1}{\Gamma(0.5)\sqrt{x}}$. We would expect the derivative to be zero (assuming the generalized derivative follows our common sense on derivatives).

Another important thing on Riemann-Liouville fractional derivatives is the fact that the initial conditions for a fractional differential equation are given by fractional order derivatives. For example, if we are solving a problem (single term fractional differential equations) with velocity, the use of the Riemann-Liouville derivative operator forces these initial conditions to be non integer order derivatives, making it difficult to perform a physical interpretation (for example, aceleration is the first derivative of velocity)

In order to better understand this idea, we will now provide an example. The Laplace transform is given by:

Definition 1.2.11 *Laplace Transform: The Laplace transform of a function $f(t)$, defined for all real numbers $t \geq 0$, is the function $F(s)$ (a unilateral transform) defined by*

$$ F(s) = \int_0^\infty f(t) e^{-st} dt, \tag{1.32} $$

where s is a complex number.

It is often used to solve applied problems involving fractional derivatives. The Laplace transform of the Riemann-Liouville fractional derivative is given by:

$$ \int_0^\infty \{ {}_0^R D_x^\alpha f(t) \} e^{-st} dt = s^\alpha F(s) - \sum_{k=0}^{m-1} \left[{}_0^R D_x^{\alpha-k-1} f(t) \right]_{t=0}, \; m-1 \leq \alpha \leq m \tag{1.33} $$

and therefore, we need to provide $\left[{}_0^R D_x^{\alpha-k-1} f(t) \right]_{t=0}$, which, based on our common sense, is difficult to do.

A solution to these *problems* seems to be the fractional derivative definition proposed by M. Caputo (as presented next).

1.2.3.2 Caputo Fractional Derivative

Definition 1.2.12 *Caputo Fractional Derivative: Let* $\alpha \in \mathbb{R}_+$, $m = \lceil \alpha \rceil$ *and* $D^m f(t) \in L_1([a,\, b])$. *The Caputo fractional derivative of order* α ($_a^C D_t^\alpha f$) *is given by*

$$ {}_a^C D_x^\alpha f(x) = J_a^{m-\alpha} D^m f(x) = \frac{1}{\Gamma(m-\alpha)} \int_a^x (x-t)^{m-\alpha-1} D^m f(t) dt. \tag{1.34} $$

Note the resemblance with the Riemann-Liouville fractional derivative. The difference is that we have exchanged the order of integration and differentiation. The following theorem establishes the relationship between the two definitions.

Theorem 1.2.5 *Let* $\alpha \in \mathbb{R}_+$, $m = \lceil \alpha \rceil$ *and* $f \in A^n([a,\, b])$ *the following relationship is verified almost everywhere*

$$ {}_a^C D_x^\alpha f(x) = {}_a^R D_x^\alpha [f(x) - T_{m-1}[f(x), a]] \tag{1.35} $$

$T_{m-1}[f(x), a]$ *is the Taylor expansion of* f *centered at* a,

$$ T_{m-1}[f(x), a] = \sum_{k=0}^{m-1} \frac{f^{(k)}(a)}{k!} (x-a)^k. \tag{1.36} $$

Note that we now have that the Caputo fractional derivative of a constant is zero. This happens because in this case we first perform a differentiation. Also, the Laplace transform of the Caputo fractional derivative is given by:

$$ \int_0^\infty \{ {}_0^R D_x^\alpha f(t) \} e^{-st} dt = s^\alpha F(s) - \sum_{k=0}^{m-1} p^{\alpha-k-1} f^{(k)}(0),\ m-1 \leq \alpha \leq m \tag{1.37} $$

and therefore, the initial conditions are classical derivatives (it becomes easier to assign physical boundary conditions).

1.2.3.3 Grünwald–Letnikov

Another important definition is the one provided by Grünwald and Letnikov. It is well known that a classical derivative can be approximated as a limit of difference quotients. For example,

$$ f'(t) = D^1 f(t) = \lim_{h \to 0} \frac{f(t) - f(t-h)}{h} \tag{1.38} $$

We know that:

$$\begin{aligned}
\nabla_h^1 f(t) = &\quad f(t) - f(t-h) \\
\nabla_h^2 f(t) = &\quad \nabla_h^1 f(t) - \nabla_h^1 f(t-h) = f(t) - 2f(t-h) + f(t+2h) \\
&\quad \vdots \qquad\qquad \vdots \\
\nabla_h^n f(t) = &\quad \sum_{k=0}^{n} (-1)^k \binom{n}{k} f(t-kh).
\end{aligned} \tag{1.39}$$

Therefore, we can state the following:

Theorem 1.2.6 *Let $n \in \mathbb{N}$, $f \in C^n([a,\, b])$ and $a < t \leq b$, then:*

$$D^n f(t) = \lim_{h \to 0} \frac{\nabla_h^n f(t)}{h^n} \tag{1.40}$$

Grünwald and Letnikov, performed a generalization of this result to non-integer n values, leading to the following definitions of fractional derivative:

Definition 1.2.13 *Let $\alpha \in \mathbb{R}_+$, $f(t) \in C^{\lceil \alpha \rceil}([a,\, b])$ and $h_N^\alpha = (t-a)/N$. The Grünwald–Letnikov fractional derivative of order α (${}_a^{GL}D_t^\alpha f$) is given by*

$${}_a^{GL}D_t^\alpha f(x) = \lim_{N \to \infty} \frac{\nabla_{h_N}^\alpha f(t)}{h_N^\alpha}. \tag{1.41}$$

with

$$\nabla_h^\alpha f(t) = \quad \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} f(t-kh). \tag{1.42}$$

Note that

$$\binom{\alpha}{k} = \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)}. \tag{1.43}$$

1.2.3.4 Conclusions

We have resumed the basic theory that allows the understanding of fractional derivatives. We also presented the definitions of fractional derivatives of Riemann-Liouville and Caputo (the two definitions that are most widely used). The Grünwald–Letnikov fractional derivative is also presented due to its straight relationship with the common finite difference approximation of the classical derivatives. Several definitions for fractional derivatives and integrals can be found in the literature, for more on this please consult [61]. Since the Caputo fractional derivative is the one that is often used to model real world phenomena, only this definition will be considered along the thesis.

As it happens with classical derivatives, fractional derivatives also find application in modeling real world phenomena. Therefore, in the next Section we establish a relationship between fractional derivatives and the diffusion process (the spreading of *something* more widely), providing in this way a realistic sense of application of such operators. The reason for choosing this physical process lies on the fact that several works can be found in the literature on this topic, and, this is one of the most common transport phenomenon found in our daily lives (oxygen in the lungs diffuses from the alveolar air space into the blood circulating around the lungs; a mug getting hot when a hot liquid is placed in it; perfume diffuses into the air; diffusion of people into other countries, etc).

1.3 Time Fractional Diffusion Equations

1.3.1 Introduction

In this Section we present the basic theory on *normal* and anomalous diffusion. We start by presenting in an axiomatic way the physical process and we finish with a relationship between fractional operators and anomalous diffusion.

1.3.2 Normal Diffusion

Definition 1.3.1 *Diffusion can be seen as a transport phenomena where distribution, mixing or transport of mass/particles occurs without requiring bulk motion (the spreading of something more widely).*

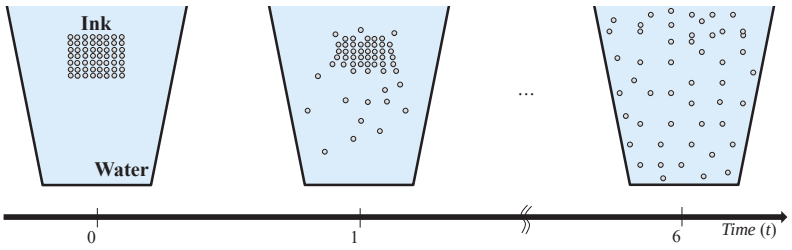


Figure 1.9: Schematic of the diffusion of small particles of ink in water.

By looking at figure 1.9 we see that the particles of ink that were all gathered at one location ($t = 0$), just spread out (in latin *diffundere* means *to spread out*) or diffused through all the domain (note that is just a schematic to help understanding the concept of diffusion and not a real life experiment).
The way these *particles* diffuse in water was an intriguing mystery for a long period of time. In 1827, the botanist Robert Brown observed the jittering (small quick jumpy movements) movement of small particles such as pollen grains, when these were immersed in water (figure 1.11- see also the following video: https://www.youtube.com/watch?v=R5t-oA796to).

Figure 1.10: Robert Brown

Robert Brown was a Scottish botanist and palaeobotanist who made important contributions to botany largely through his pioneering use of the microscope. His discovery of Brownian motion while examining grains of pollen of the plant Clarkia pulchella suspended in water under a microscop, was denied in a brief paper in 1991. Shortly thereafter, in an illustrated presentation, British microscopist Brian J. Ford showed that Brown's original microscope could indeed show Brownian motion.

Nowadays it is well known that this motion (jittery movement) is caused by the rapid movement of water molecules colliding with the pollen grains and insight into this problem was provided by Albert Einstein in 1905, in his work regarding Brownian motion, entitled "On the motion, required by the molecular-kinetic theory of heat, of particles suspended in fluids at rest" [62]. His work served as a definitive confirmation that atoms and molecules actually exist (it is worth mentioning that Louis Bachelier, a student of Henri Poincaré, developed a theory of Brownian motion in his 1900 thesis [63] regarding stock market fluctuation [64]).

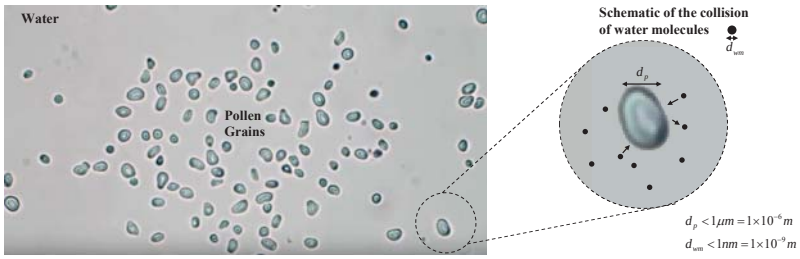
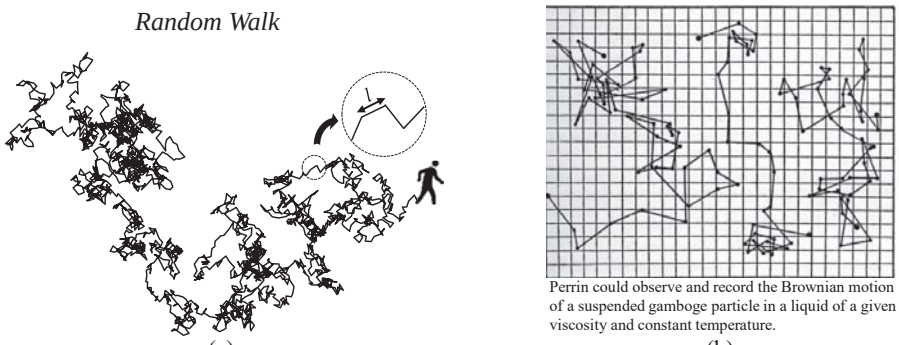


FIGURE 1.11: Pollen grains in water. The inset shows water molecules (black dots) colliding into a pollen grain. This collision promotes the jittering movement of the pollen grains.

There are two ways to introduce the notion of diffusion: either a phenomenological approach starting with Fick's laws of diffusion (Fick set up the diffusion equation in 1855 [65]) where the diffusion flux is proportional to the negative gradient of concentrations (it goes from regions of higher concentration to regions of lower concentration), or a physical and atomistic one, by considering the random walk (Brownian motion) of the diffusing particles.

The random walk theory was popularized by Karl Pearson in his letter to Nature (1905) [66], where he proposed the following problem: a man starts from a point O and walks l yards in a straight line; after this step he turns through a random angle and takes another step of length l (see figure 1.12). He repeats this process n times. What is the probability that after n steps he is at a distance between r and $r + \delta r$ from the original point O? This problem is basically the idea behind Brownian motion.



(a) (b)

Figure 1.12: (a) Example of a Random Walk. (b) Experimental verification of Brownian motion for three particles of gambooge (these results were obtained by Jean Perrin in 1909 [67] and gave him a Nobel Prize in 1926).

We will now derive the diffusion equation by considering the *random walk* of a single ink particle. For that, we will need the following definitions and lemmas:

Definition 1.3.2 ***Random Variable:*** *A random variable $X : \Omega \to E$ is a measurable function from a set of possible outcomes Ω to a measurable space E. Ω is a probability space. Usually X is real-valued (i.e. $E = \mathbb{R}$).*

Definition 1.3.3 ***Expected Value:*** *Let X be a discrete random variable taking values $x_1, x_2, ...$ with probabilities $p_1, p_2, ...$ respectively. Then the $expected\ value$ of this random variable is the infinite sum $\mathbb{E}[X] = \sum_{i=1}^{\infty} x_i\, p_i$ provided that this series converges absolutely. If this series does not converge absolutely, we say that the expected value of X does not exist.*

If the probability distribution of X admits a probability density function $f(x)$ then the expected value can be computed as $\mathbb{E}[X] = \int_{-\infty}^{\infty} x f(x)\, dx$.

Definition 1.3.4 *Random variables are identically distributed if they have the same probability law. They are i.i.d. (independent and identically distributed) if they are also independent.*

Definition 1.3.5 ***Variance and Covariance:*** *The $variance$ (Var) of a random variable X with expected value $\mathbb{E}(X) = \mu_X$ is defined as $Var(X) = \mathbb{E}\left((X - \mu_X)^2\right)$ (The square root of the variance of a random variable is called its standard deviation). The $covariance$ between random variable Y and Z, with expected values μ_Y and μ_z, is defined as $cov(Y, Z) = \mathbb{E}((Y - \mu_y)(Z - \mu_z))$*

Let us derive the diffusion equation by first considering the diffusion of only one particle of ink.

Lemma 1.3.1 *If X and Y are independent random variables, then $\mathbb{E}(XY) = \mathbb{E}(X)\mathbb{E}(Y)$ and $Var(X + Y) = Var(X) + Var(Y)$. If $X_1, X_2, ..., X_n$ are i.i.d., each with mean μ and variance σ^2, then $\mathbb{E}(X_1 + \cdots + X_n) = n\mu$, $Var(X_1 + \cdots + X_n) = n\sigma^2$*

Proof 1.3.1 *The proof of this lemma is straightforward.*

In order to derive the diffusion equation, lets first consider the diffusion of only one particle of ink (we will follow the exposition by Cai 2011 [68]).

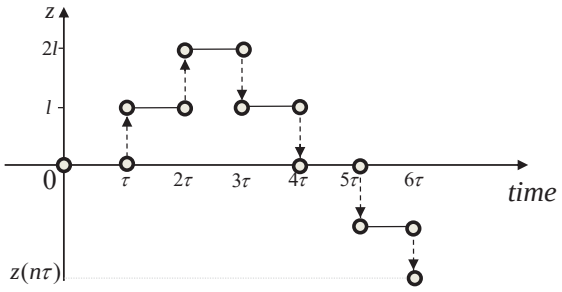


FIGURE 1.13: Random walk of a single particle.

Lemma 1.3.2 ***Random Movement:*** *Let $z(t)$ be the position of one particle of ink ($z(0) = 0$). At each constant time step τ_i $(i = 1, 2, ...)$ the particle can only move/jump to the left or to the right (with the same probability), by a distance of l (see figure 1.13):*

$$z(t+\tau) = \begin{cases} z(t) + l & prob. = 1/2 \\ z(t) - l & prob. = 1/2 \end{cases} \tag{1.44}$$

Therefore we can define the random variable

$$l_i = \begin{cases} +l & prob. = 1/2 \\ -l & prob. = 1/2 \end{cases} \tag{1.45}$$

Since the particles have no memory (the previous step will not affect the next step), the random variables l_i are independent and identically distributed (iid).

Based on this, we have that the average position and the variance of the particle at $t = n\tau$ are $\mathbb{E}(z(t)) = 0$ and $Var(z(t)) = nl^2$, respectively.

Proof 1.3.2 *The position of the particle at $t = n\tau$ is given by $z(t) = z(0) + l_1 + ... + l_n = \sum_{k=1}^{n} l_k$. Therefore, based on the previous Lemma (lemma 1.3.1) we have that $\mathbb{E}(\sum_{k=1}^{n} l_k) = n\mu$ with $\mu = \mathbb{E}(l_i) = (+l)\frac{1}{2} + (-l)\frac{1}{2} = 0$. This means that the average position $\mathbb{E}(z(t)) =< z(t) >= 0$ (in average, the particle is always in the same place). The notation $< . >$ is also very common.*

We know that $Var(z(t)) = Var(\sum_{k=1}^{n} l_k) = \mathbb{E}\left((\sum_{k=1}^{n} l_k - \mathbb{E}(\sum_{k=1}^{n} l_k))^2\right)$. Since $\mathbb{E}(\sum_{k=1}^{n} l_k) = 0$, we have:

$$\begin{aligned} Var(z(t)) = \mathbb{E}\left((\textstyle\sum_{k=1}^{n} l_k)^2\right) &= \mathbb{E}\left((l_1 + ... + l_n)(l_1 + ... + l_n)\right) \\ &= \mathbb{E}\left(l_1 l_1 + ... + l_n l_n + \textstyle\sum_{i \neq j} l_i l_j\right) \\ &= \mathbb{E}\left(l_1 l_1 + ... + l_n l_n\right) + \mathbb{E}\left(\textstyle\sum_{i \neq j} l_i l_j\right) \\ &= \mathbb{E}\left(l_1^2\right) + ... + \mathbb{E}\left(l_n^2\right) + \textstyle\sum_{i \neq j} \mathbb{E}(l_i l_j). \end{aligned} \tag{1.46}$$

We know that

$$l_i^2 = \begin{cases} (+l)^2 & prob. = 1/2 \\ (-l)^2 & prob. = 1/2 \end{cases} \tag{1.47}$$

and that $\mathbb{E}\left(l_i^2\right) = (+l)^2\frac{1}{2} + (-l)^2\frac{1}{2} = l^2$ *and that* $\mathbb{E}(l_i l_j)$ *can be written has* $\mathbb{E}(l_i)\mathbb{E}(l_j) = 0$ *(*l_i *is independent of* l_j*). Therefore we conclude the following:*

$$Var(z(t)) = \mathbb{E}\left((\sum_{k=1}^{n} l_k)^2\right) =< z(t)^2 >= nl^2 \tag{1.48}$$

Remark: This result can be generalized for more particles, and the diffusion equation can be derived in a simple way.

For that, consider that we have an enormous amount of ink particles (continuum hypothesis), in such a way that the density of particles at a point z can be given by the density function ($C(z)$) define by

$$C(z) = \lim_{dz \to 0} \frac{N_{[z,z+dz]}}{dz} \tag{1.49}$$

with $N_{[z,z+dz]}$ the number of particles in the interval $[z, z+dz]$. Note that we assume that even in a small interval $[z, z+dz]$ the number of particles is very large, $N_{[z,z+dz]} \gg 1$, and therefore $C(z)$ can be considered to be smooth. Also, for $dz \to 0$ we have $a \ll dx$.

These are the mathematical assumptions required to derive this *continuum* random walk. In reality (or numerical simulations), dx will never go to 0 and we allways need to define what means *small enough*. For example, if we consider that the ink has a similar composition of water, we have that $1cm^3$ of water has mass $0.997g$, the molar mass of water is $18.02g/mol$ and therefore $18.02g$ contains 6.022×10^{23} molecules. This leads to: $0.997g$ of water ($1cm^3$) contains 3.33×10^{22} molecules, a good approximation to a *continuum*.

Next we derive the diffusion equation by considering a simple 1D discrete case. But before we present the definition of *number density*:

Definition 1.3.6 ***Number Density:*** *Number density is a useful concept for thinking about macroscopic samples in a microscopic way. Number density can be thought of as the number of particles in a particular volume.*

Lemma 1.3.3 *Assume that we managed somehow to obtain the discrete number of particles* N_0*,* N_1*,* N_2 *at a particular location* z_0*,* z_1*,*z_3*, respectively (as shown in figure 1.14). A good approximation for* $C(z) = \lim_{dz \to 0} \frac{N_{[z,z+dz]}}{dz}$ *at* z_i *is* $C(z_i) = \frac{<N_i>}{l}$ *(this is the number density). Note that we use the average* $< N_i >$ *and not the* N_i *because the number of particles is evolving in time at each particular position in space (the ink particles are all performing a random walk). If we consider two distinct time steps/jumps, the step* $(n-1)\tau$ *and the step* $n\tau$*, then we have that the equation governing the evolution of the number density at location* z_1 *is given by,*

$$\frac{\partial C(z_1)}{\partial t} = D\frac{\partial^2 C(z_1)}{\partial x^2} \tag{1.50}$$

with D *the diffusion coefficient.*

Proof 1.3.3 *We know that particles will allways jump a distance $\pm l$, and therefore, the particles that are at $z_1$at instant $(n-1)\tau$ will all jump to a different location (z_0 or z_2) when $t = n\tau$ (see figure 1.14). We can say that the number of particles at location z_1 when $t = n\tau$ is $< N_1^{n\tau} >$, and we also know that these particles came from z_0 and z_2. In average, half of the particles go to the left and the other half goes to the right, therefore:*

$$< N_1^{n\tau} >= \frac{1}{2} < N_0^{(n-1)\tau} > + \frac{1}{2} < N_2^{(n-1)\tau} > \tag{1.51}$$

We are now in position to calculate the derivative in time of $C(z_1)$, that is,

$$\frac{\partial C(z_1)}{\partial t} = \frac{\frac{<N_1^{n\tau}>}{l} - \frac{<N_1^{(n-1)\tau}>}{l}}{\tau} \tag{1.52}$$

Making use of Eq. 1.51 and the fact that $z_0 = z_1 - l$ and $z_2 = z_1 + l$ we have that

$$\begin{array}{rcl} \frac{\partial C(z_1)}{\partial t} & = & \frac{1}{2l\tau}\left[< N_0^{(n-1)\tau} > + < N_2^{(n-1)\tau} > -2 < N_1^{(n-1)\tau} >\right] \\ & = & \frac{1}{2\tau}\left[C(z_0) + C(z_2) - 2C(z_1)\right] \\ & = & \frac{1}{2\tau}\left[C(z_1 + l) - 2C(z_1) + C(z_1 - l)\right] \\ & = & \frac{l^2}{2\tau}\frac{[C(z_1+l)-2C(z_1)+C(z_1-l)]}{l^2} \end{array} \tag{1.53}$$

For really small jumps we can say that:

$$\frac{\partial C(z_1)}{\partial t} = \frac{l^2}{2\tau}\frac{\partial^2 C(z_1)}{\partial x^2} \tag{1.54}$$

Note that we could have taken the limit $l \to 0$ and stated a certain relationship between l and τ so that $\frac{l^2}{2\tau}$ becomes a constant (the relationship between l and τ would involve a certain characteristic velocity of the particles).
Finally, we can say that

$$\frac{\partial C(z_1)}{\partial t} = D\frac{\partial^2 C(z_1)}{\partial x^2} \tag{1.55}$$

with $D = \frac{l^2}{2\tau}$ known as the diffusion coefficient. For a more detailed proof please see the article by Einstein [62].

Remark: In the previous proof, we could have taken the limit $l \to 0$ and $\tau \to 0$, while in reality τ and l are finite. This is possible because the differential equation represents a macroscopic view of the microscopic phenomenon with $\tau \ll T$ and $l \ll L$, where T and L are the time of observation and the dimension of the experiment, respectively.

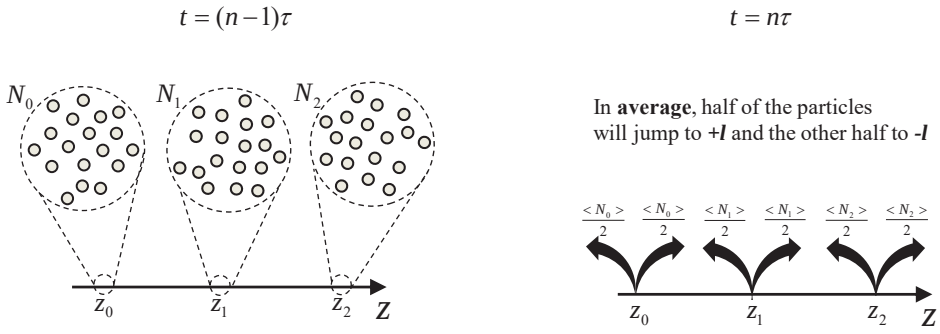


Figure 1.14: Particle jump.

The following Lemma will allow a better understanding of the diffusion equation and the diffusion coefficient.

Lemma 1.3.4 *Consider the diffusion equation* $\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}$ *with* D *constant. Assume we have an infinite domain* $-\infty \leq x \leq +\infty$ *free of substance. For example, water with no ink. At the initial instant* $t = 0$ *we inject a portion of ink that is given by* $C(x,0) = M\delta(x)$ *with* M *the total amount of ink* $\left(M = \int_{-\infty}^{+\infty} C(x,t)dx\ \forall t\right)$ *and* $\delta(x)$ *the Dirac Delta function* ($\delta(x) = 0$ *for* $x = 0$, $\delta(x) = +\infty$ *at* $x = 0$, *and the area under the infinitely tall and infinitely narrow peak is unity). Since that domain is infinite we consider the boundary conditions (the portion of ink will take an infinite time to reach the infinitely far ends of the domain)*

$$\lim_{x\to\pm\infty} C(x,t) = 0 \tag{1.56}$$

Then, the solution to the diffusion equation is given by,

$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \ . \tag{1.57}$$

Proof 1.3.4 *See for example, John Crank - The Mathematics of Diffusion [69].*

Note the resemblance between the solution obtained and the probability density of the normal distribution given in the following definition:

Definition 1.3.7 *In probability theory, the normal (or Gaussian) distribution is a very common continuous probability distribution. The probability density function,* $f(.)$, *is*

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \ . \tag{1.58}$$

with σ^2 *the variance and* μ *the mean or expectation of the distribution.*

The normal diffusion was verified experimentally for example in the works of Kappler in 1931 [70], where he experimentally verifies a Gaussian distribution.

We can say that $C(x,t)$ gives the amount of ink, M, multiplied by the probability of finding ink in the different regions of the domain, along time (basically we have the amount of ink in the different regions of the domain - see figure 1.15). At $t = 0$ it is most likely

to find ink only at the origin with a high concentration, and, for large times, the ink has spread and it is probable to find ink in *all* the domain (the domain is infinite) but with lower concentrations.

Note that by comparing Eqs. 1.57 and 1.58 we observe that the variance is given by: $Var(C(x,t)) = 2Dt$. This is what characterizes the *normal* diffusion. Particles move randomly with a variance that is proportional to time. This is a macroscopic observation (a scale) of the random movement of tiny particles.

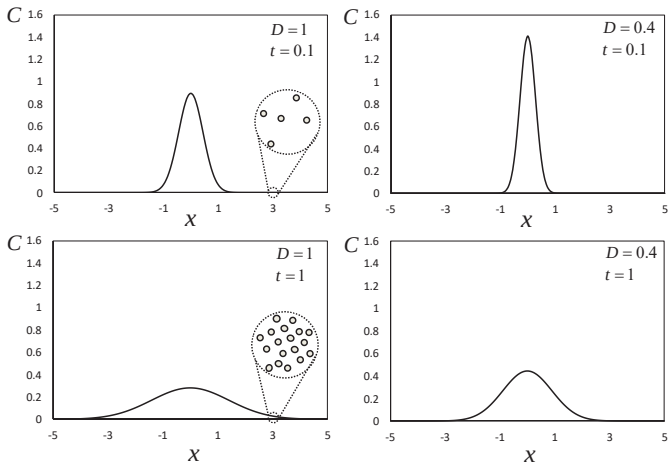


FIGURE 1.15: Evolution of the concentration of ink in time (seconds), for different diffusion coefficients.

Going back to the random walk, remember that the position of a particle at $t = n\tau$ is given by $z(t) = z(0) + l_1 + ... + l_n = \sum_{k=1}^{n} l_k$. Assume that $z(0)$ may not be 0. Then we have:

$$\begin{array}{ll} & z(t) = z(0) + l_1 + ... + l_n = \sum_{k=1}^{n} l_k \\ \Leftrightarrow & \mathbb{E}(z(t) - z(0)) = \mathbb{E}(\sum_{k=1}^{n} l_k) \\ \Leftrightarrow & \mathbb{E}(z(t) - z(0)) = 0 \end{array} \tag{1.59}$$

This means that if we shift our system by $z(0)$ the expected value (mean position of the particle) is zero (the particle goes nowhere). If we calculate the Mean Square Displacement $\mathbb{E}((z(t) - z(0))^2)$ or $< (z(t) - z(0))^2 >$, we have that,

$$\begin{array}{rcl} \mathbb{E}((z(t) - z(0))^2) = & \mathbb{E}\left((\sum_{k=1}^{n} l_k)^2\right) \\ = & nl^2 \\ = & \frac{t}{\tau} l^2 \\ = & 2Dt. \end{array} \tag{1.60}$$

This means that the Mean Square Displacement of a particle is proportional to time (as seen before for the continuous case). Note that for this case, where the probability the particle will jump $+l$ or $-l$ is the same, we have that $z(0) = \mu$ and therefore the Mean Square Displacement can be interpreted as the variance. When we have discrete experimental data,

or discrete data from numerical simulations with particles, the Mean Square Displacement is usually measured by,

$$\frac{1}{N}\sum_{n=1}^{N}(z_n(t)-z_n(0))^2, \tag{1.61}$$

where N is the number of particles to be averaged, $z_n(0)=z_0$ is the reference position of each particle and $z_n(t)$ is the position of each particle at instant t.

Remark: It should be noted that the derivation showed here is not unique. For example, if we consider a particle can still perform jumps $+l$ or $-l$ and that the particles can also stay in the same position, we can still arrive at the diffusion equation. A justification for this is the Central Limit theorem:

Theorem 1.3.1 ***Central Limit Theorem:*** *Let $X_1, X_2, ..., X_n$ be i.i.d. random variables, each with mean μ and variance σ^2, then $S_n = X_1 + \cdots + X_n$ follows a normal distribution with mean $n\mu$ and variance $n\sigma^2$, for large n values.*

This means that no matter the distribution of the random variables is, their sum will follow a normal distribution. This also makes normal diffusion to be more common than anomalous diffusion.

Note that nothing was said about the units of D. If in Eq. 1.55, C represents the concentration with units $\left[\frac{mol}{m^3}\right]$ with t the time $[s]$ and x is the position $[m]$, then the diffusion coefficient D is given by $\left[\frac{m^2}{s}\right]$.

Incorrect dimensions are often encountered in fractional calculus, because, when we substitute (for example) the classical time derivative by its fractional counterpart, we alter the dimensions of the equation, and the meaning of D changes (see next subsection).

1.3.3 Anomalous Diffusion

Normal diffusion is the usual case when systems are at equilibrium, and anomalous diffusion occurs in more complex systems. A general relationship for all the different anomalous diffusion processes is still something under development, and, fractional calculus seems to be a good tool to fairly describe and understand some of these complex processes.

Although in nature we have several processes that follow a Gaussian distribution, there are cases where this normal distribution does not apply, and therefore, more general theories need to be derived.

Lets start with a simple example. Consider a free particle that travels with constant velocity v (undergoes no collisions and experiences no friction forces). The trajectory/location of the particle is given by $z(t)=vt$ and if we use Eq. 1.67 to compute the Mean Square Displacement (MSD), that from now on is represented by $<(z(t))^2>$, we have that $<(z(t))^2> \sim t^2$ (see Lemma 1.3.5). Therefore we say this process is superdiffusive (the exponent is bigger than 1 - figure 1.16). That are also experiments revealing that $<(z(t))^2> \sim t^{1/2}$, $<(z(t))^2> \sim t^{1/4}$ (subdiffusion - the exponent is smaller than 1 - figure 1.16) or that the MSD changes with time (see for example the work of Coupier et al. [71]).

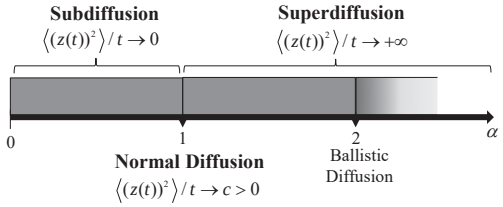


FIGURE 1.16: Subdiffusion, normal diffusion and superdiffusion.

This means that diffusion is a complex process, and a more generalized theory is needed. An example of anomalous diffusion is shown in figure 1.17. Note that the particle makes long jumps that are followed by a normal diffusion.

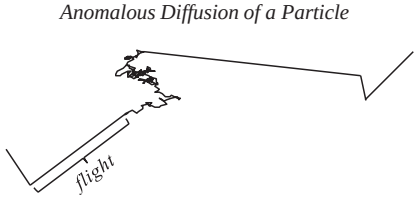


FIGURE 1.17: Anomalous diffusion of a particle.

Lemma 1.3.5 ***A Not so Random Movement of a Free Particle:*** *Let $z(t)$ be the position of one particle of ink ($z(0) = 0$). At each constant time step τ_i $(i = 1, 2, ...)$ the particle can only move/jump to the right by a distance of l:*

$$z(t) + l = z(t + \tau) = \ \ prob. = 1. \tag{1.62}$$

Therefore we can define the random variable

$$l_i = +l \ \ prob. = 1. \tag{1.63}$$

Since the particles have no memory (the previous step will not affect the next step), the random variables l_i are independent and identically distributed (iid).

Based on this, we have that the Mean Square Displacement is given by:

$$\mathbb{E}((z(t) - z(0))^2) =< (z(t) - z(0))^2 >= \tfrac{l^2}{\tau^2} t^2 \ , \tag{1.64}$$

meaning that this free particle shows a variance that is proportional to t^2.

Proof 1.3.5 *The position of the particle at $t = n\tau$ is given by $z(t) = z(0) + l_1 + ... + l_n = \sum_{k=1}^{n} l_k$. Therefore, we have that $\mathbb{E}(\sum_{k=1}^{n} l_k) = nl$.*

since

$$z(t) = z(0) + l_1 + ... + l_n = \sum_{k=1}^{n} l_k \tag{1.65}$$

we have that

$$\begin{aligned} \mathbb{E}((z(t) - z(0))^2) = & \ \mathbb{E}\left((\sum_{k=1}^{n} l_k)^2\right) \\ = & \ \mathbb{E}\left((l_1 + ... + l_n)(l_1 + ... + l_n)\right) \\ = & \ \mathbb{E}\left(l_1 l_1 + ... + l_n l_n + \sum_{i \neq j} l_i l_j\right) \\ = & \ \mathbb{E}\left(l_1^2\right) + ... + \mathbb{E}\left(l_n^2\right) + \sum_{i \neq j} \mathbb{E}(l_i l_j) \\ = & \ nl^2 + (n^2 - n)l^2 \\ = & \ \frac{l^2}{\tau^2} t^2 \end{aligned} \tag{1.66}$$

We will now tackle the case when anomalous diffusion is observed, that is,

$$< (z(t))^2 > \sim t^{\alpha} \tag{1.67}$$

with $\alpha > 0$ ($\alpha \neq 1$), but, it does not change with time (α is constant).

In order to justify the need of fractional calculus we will briefly describe a situation where the use of a fractional derivative in time (instead of the classical derivative) leads to anomalous diffusion, that is, $< (z(t))^2 > \sim t^{\alpha}$.

Lemma 1.3.6 *Consider the fractional subdiffusion equation given by*

$$\frac{\partial^{\alpha} C(x,t)}{\partial t^{\alpha}} = D_{\alpha} \frac{\partial^2 C(x,t)}{\partial x^2}, \ 0 < \alpha < 1, \ x \in \mathbb{R}, \, t > 0 \tag{1.68}$$

with D_{α} constant. Assume we have an infinite domain $-\infty \leq x \leq +\infty$ free of substance. At the initial instant $t = 0$ consider that $C(x,0) = \delta(x)$. Also, consider the boundary conditions:

$$\lim_{x \to \pm\infty} C(x,t) = 0. \tag{1.69}$$

The Mean Square Displacement is then given by:

$$< (z(t))^2 > = \frac{2D_{\alpha}}{\Gamma(1+\alpha)} t^{\alpha} \ . \tag{1.70}$$

Proof 1.3.6 *See for example the work by R. Metzler and J. Klafter [72].*

It is now clear that fractional calculus can be used to analyze anomalous diffusion. Although, one can not generalize this previous result, and say that fractional calculus will solve all anomalous diffusion problems. The time-fractional diffusion equation comes from a generalized Random Walk/Brownian Motion (the Continuous Time Random Walk (CTRW) model), where a particle can perform arbitrary jumps, and can wait before performing a jump (with varying waiting time). This variety of jumps and waiting times is complex, and to go from the CTRW to a fractional differential equation a certain distribution for the waiting time and jump length was assumed. A different choice of waiting time and jump length would not allow to write all the microscopic information in the compact form of

the fractional operator. Therefore, in the future, new and more general operators need to be derived, so that particular types of diffusion can be easily modeled by such general operators.

While these new operators are not derived, we must take advantage of the tools that we have at the present time, and therefore, we must study in detail fractional operators, such as the Caputo fractional derivative.

As seen before, the anomalous diffusion equation allows modelling both subdiffusive and superdiffusive processes. Examples of subdiffusive processes are, for example, the diffusion of proteins across cell membranes, diffusion of contaminants in groundwater, transient photocurrent in amorphous thin films that form the core of photocopier machines, etc, and, examples of supperdiffusive processes are, the flight of albatrosses, the movement of bacteria, etc. Due to the high number of such anomalous processes in our daily lives, we may quote Klafter and Sokolov [73] and say that "anomalous is normal!".

Due to the high number of publications on the subject, and the diversity of anomalous processes, in this work we had to choose/focus on only one type of diffusion. Therefore, we will only address the subdiffusive processes, where $\alpha < 1$ in Eq. 1.70.

Finally, it should be remarked that we may find experimentally subdiffusive Mean Square Displacements that do not scale with t^{α}, or show more that one scale, therefore, in this cases we also need to find a different time derivative operator (something that can give us a good macroscopic view of what is happening in the microscopic world).

These more complex phenomena will require the use of more advanced fractional tools, such as, for example, the distributed order operators, which are a continuous weighted sum of fractional derivatives. This topic will be addressed with detail in Chapter 3.

1.4 Motivation, Aim and Objectives

Due to the huge number of papers being published everyday on the subject of fractional calculus, the task of finding a subtopic to further develop and explore was not an easy task. The initial objective was to establish a bridge between Engineering and Fractional Calculus, by presenting an axiomatic definition of the physical processes under study and by developing new and more sophisticated numerical methods that allow the solution of the fractional differential equations involved. After a long and exhaustive literature review it was realized that most papers on anomalous diffusion either consider a constant diffusion coefficient D or the diffusion term $D(x)\frac{\partial^2 u}{\partial x^2}$ (which may lead to the wrong modeling of diffusion), instead of the correct diffusion term $\frac{\partial}{\partial x}(D(x)\frac{\partial u}{\partial x})$. This motivated us to develop a new numerical method for the solution of the Time-Fractional Diffusion Equation with varying diffusion coefficient and a diffusion term given by $\frac{\partial}{\partial x}(D(x)\frac{\partial u}{\partial x})$. Also, we considered Neumann boundary conditions and proved the solvability, stability and convergence of the method (most works only consider Dirichlet boundary conditions). We then used the new numerical method to study the diffusion of temperature in human tissue.

After getting familiarized with fractional differential equations and numerical methods for their solution, it was realized that although these equations have a huge potential in modeling physical phenomena, they present two major drawbacks that were poorly addressed in the literature. These are: (I) the potential singularities of the solution and (II) the fact the numerical solution of such equations is highly demanding in terms of computational time.

(I) few papers can be found in the literature addressing the singularity issues, and they can be categorized into four different approaches [74]: the use of refined meshes near the singularity, increasing in this way the order of convergence [75; 76; 77; 78; 79]; approximate the solution by nonpolynomials, capturing the potential solution behavior near the singularity [80; 81; 82; 83; 84; 85; 86; 87; 88]; Separate the solution into two parts: smooth and nonsmooth parts and force the time discretisation scheme to hold exactly for the nonsmooth part [89; 90; 91]; introduce a Correction to the starting steps of the time discretisation schemes in order to capture the singularity of the solution [92; 93; 94; 95; 96; 97]. It should be remarked that these works are related with the fractional differential equation of the form $D^{\alpha}(t)u(t) + Au(t) = f(t)$, $0 < t \leq T$ with $u(0) = u_0$. Due to the importance of this subject, it became the primary objective of this work, that is: *to obtain reliable numerical methods that can deal with the potential singularity of solutions of fractional differential equations, including the Time-Fractional Diffusion Equation*.
(II) The highly demanding computational effort needed to solve fractional differential equations (due to the non-local properties of these operators) has been poorly addressed in the literature, being finite differences the most common methods used for the numerical solution of fractional differential equations. In order to solve this issue we proposed a new numerical method based on the approximation of the solution by Chebyshev polynomials. The numerical method is tested on Distributed-Order differential equations, enhancing in this way the need for fast computations (since these distributed order operators are a continuous weighted sum of fractional derivatives). It should be remarked that Chebyshev polynomials were already presented in the literature for solving similar problems [98], but, a proof of convergence of the method could not be found, and therefore it was difficult to infer the fastness of the method and its robustness when in the presence of singular solutions. Therefore we derived the full convergence analysis of the numerical method, assuming the same regularity assumptions often encountered in finite differences methods. We concluded that this method is much faster when compared to traditional finite differences.

Since the regularity assumptions often used in finite differences and other methods poses limitations in the applicability of the method, we developed a new numerical method that does note pose any restriction in the solution. Based on a previous work by the group [83], we developed a numerical method for the solution of the Time-Fractional Diffusion Equation based on a nonpolynomial approximation of the solution. This method proved to be robust and independent of the order of the fractional derivative. The main issue of the method was that the computational effort was still high. Therefore, we developed a new hybrid numerical method that uses only a nonpolynomial approximation in the first discretized time interval (including the potential singular point, the origin in time), and, for the remaining intervals a polynomial approximation was used. The method was first tested in systems of fractional differential equations, and was later generalized to the Time-Fractional Diffusion Equation (using the method of lines to transform the equation into a system of fractional differential equations). We perform numerical tests and show that the method allows high convergence orders.

1.5 Structure of the Thesis

Chapter 1 In Chapter 1 we present the brief history of fractional calculus together with the mathematical preliminaries that are needed for this thesis to become self contained.

We then describe the basic functions of fractional calculus, and, we also discuss the different definitions of fractional derivatives. We present an axiomatic description of the physical phenomenon of anomalous diffusion and we discuss the application of fractional calculus in the modeling of such complex process.

Chapter 2 This chapter is dedicated to the Time-Fractional Diffusion Equation. We start by presenting the existence and uniqueness results of solutions to such equations; we derived a numerical method based on finite differences for the solution of this equation with space varying diffusion coefficient and Neumann boundary conditions, prove its convergence and stability, and show an application of this fractional model in describing the diffusion of temperature in human tissue. The typical substitution of a classical derivative by its fractional counterpart is discussed in light of the physics involved.

Chapter 3 We derive a numerical method (based on the approximation of the solutions with Chebyshev polynomials) for the solution of the distributed order fractional diffusion equation, with the aim of improving the speed of the computations. This type of equations allow the modeling of strong subdiffusive processes encountered in nature. We present a detailed analysis of the convergence of the method and compare the method with a classical finite difference approach in terms of speed-up.

Chapter 4 A numerical method for the solution of the systems of fractional ordinary differential equations and the Time-Fractional diffusion equation is presented, and, the convergence of the method is studied numerically. The numerical method is based on the method of lines (for the Time-Fractional diffusion equation) and the convergence order is independent of the order of the fractional derivative. The solution is viewed as a sum of non-polynomial functions. Based on the results obtained for the non-polynomial method, and with the aim of improving the speed-up of the numerical method, we also develop a new and more robust hybrid method that is much faster, can deal with the non regularity of the solutions, and, at the same time allows one to choose the degree of accuracy.

Chapter 5 In this Chapter we present the main conclusions and a discussion of the work developed.

Finite Difference Schemes: A Numerical Method for the Time-Fractional Diffusion Equation with Space Varying Diffusion Coefficient and Neumann boundary Conditions 2

2.1 Introduction

The Time-Fractional Diffusion Equation has been found in a broad variety of engineering, biological and physics processes where anomalous diffusion occurs (see previous chapter). This equation takes into account both subdiffusion and supperdiffusion, $0 < \alpha \leq 2$, and is given by (1D)

$$\frac{\partial^{\alpha}\phi\left(x,t\right)}{\partial t^{\alpha}} = D_{\alpha}\frac{\partial^{2}\phi\left(x,t\right)}{\partial x^{2}} \quad x \in \mathbb{R},\, t > 0 \tag{2.1}$$

where D_{α} stands for a general diffusion coefficient with dimensions $[length]^2$ / $[time]^{\alpha}$. It was studied by a number of authors since the 1980s: see, for example, Wyss (1986) [99], Nigmatullin (1986) [100], Schneider and Wyss (1989) [101], Mainardi (1995, 1996) [102; 103], Nigmatullin (2006) [104], Angulo et al. (2000) [105]. Other relevant works are: [106; 107; 72; 108; 109; 110; 111; 112; 113; 114; 115; 116; 117; 64; 118; 119; 120; 121].

Since the analytical solution of the fractional diffusion equation is known only for simple initial and boundary conditions [122; 123; 124], the ability to generate a numerical solution is crucial in real world applications. However, the computation of the numerical solution of fractional differential equations is not an easy task, mainly due to the nonlocal property of the fractional differential operator, since, by definition, the solution at a certain time depends on the solution at all earlier times. As a consequence, the full solution trajectory has to be stored in order to compute the solution at the current time level, resulting generally in very expensive computational methods. It is then very important to use reasonably high-order schemes for the time and space discretisation.

Finite difference methods seem to be the most popular for the numerical solution of time-fractional diffusion equations (see for example [125; 126; 127; 128; 129; 130; 131; 132;

78; 133]) although other numerical approaches have also appeared, such as, for example, finite element methods [134; 135], meshless collocation methods [136] and collocation spectral methods [137].

However, there is a lack of numerical methods for the solution of time fractional diffusion equations with Neumann boundary conditions and a space varying diffusion coefficient (following a standard 'Fickian' transport equation). For example, we have the work of Damor et al. [138] where they presented a method for the numerical solution of such equations (without a space varying diffusion coefficient). They do not provide any proof of convergence and stability of their method, and, they use a first order approximation for the discretisation of the Neumann boundary conditions. Another interesting work is the study proposed by Karatay et al. [139] where they present a new numerical scheme, based on the Crank-Nicholson method, for the solution of the time fractional heat equation.

Most of the works also usually consider the diffusion coefficient outside of the derivative operator $D_\alpha(x)\frac{\partial^2\phi(x,t)}{\partial x^2}$ while it should be $\frac{\partial}{\partial x}\left(D_\alpha(x)\frac{\partial\phi(x,t)}{\partial x}\right)$. A good discussion on this subject is provided in the work of B. Milligen et al. [140] entitled *On the applicability of Fick's law to diffusion in inhomogeneous systems*.

Figure 2.1: Courant, Friedrichs, Lewy

Finite difference approximations for derivatives were already known by Euler in 1768 (1D case) and were possibly extended to 2D by C. Runge in 1908. However, the true emphasis on the use of finite differences to solve PDE's was given in the fundamental paper by Courant, Friedrichs and Lewy (1928) on the solution of problems of by means of finite differences. Richard Courant (1888 – 1972) was a German American mathematician. Kurt Otto Friedrichs (1901 - 1982) was also a noted German American mathematician and the co-founder of the Courant Institute at New York University. Hans Lewy (1904 – 1988) was a Jewish German born American mathematician.

Therefore, the motivation of this chapter is the development of a numerical method based on finite differences for the solution of the fractional diffusion equation taking into account Neumann boundary conditions and the fact that diffusivity may vary in space, and also, to prove the convergence and stability of the method. The numerical method will then be used study the diffusion of temperature in tissues (using the bioheat equation), and also perform a critical analysis on the common procedure of substituting the classical time derivative by its fractional counterpart.

Next we present some results on the existence and uniqueness of solutions for the Time-Fractional Diffusion Equation, that are essential for developing the numerical solution.

2.2 Existence and Uniqueness of Solutions

Consider the generalized time-fractional diffusion equation given by (these results were obtained from Luchko [141; 142; 143]),

$$ {}_a^C D_x^\alpha u(t) = div(p(x)grad(u)) - q(x)u + F(x,t),\ 0 < \alpha < 1 \tag{2.2} $$

where div and $grad$ are usual divergent and gradient operators, $(x,t) \in \Omega = G \times (0,T)$, $G \subset \mathbb{R}^n$, $p \in C^1(\overline{G})$, $q \in C(\overline{G})$, $p(x) > 0$, $q(x) \geq 0$, $x \in \overline{G}$. Also, let S represent the boundary of G.

Consider the initial-boundary-value problem

$$\begin{aligned} u|_{t=0} = &\quad u_0(x), \;\; x \in \overline{G} \\ u|_S = &\quad v(x,t), \;\; (x,t) \in S \times [0,T]. \end{aligned} \tag{2.3}$$

Let us define the space $W_t^1((0,T]) = \{space\ of\ functions\ f \in C^1((0,T]) : \; f' \in L((0,T))\}$. A classical solution of this problem is a function $u = u(x,t)$ defined in the domain $\overline{G} \times [0,T]$ that belongs to the space $C(\overline{G} \times [0,T]) \bigcap W_t^1((0,T]) \bigcap C_x^2(G)$ and satisfies both Eq. 2.2 and initial and boundary conditions 2.3

Note that if this problem possesses a classical solution, then the functions F , u_0 and v given in the problem have to belong to the spaces $C(G \times (0,T))$, $C(\overline{G})$ and $C(S \times [0,T])$, respectively.

Theorem 2.2.1 ***Uniqueness of Solution:*** *The initial-boundary-value problem (Eqs. 2.2 and 2.3) possesses at most one classical solution. This solution continuously depends on the data given in the problem in the sense that if* $\|F - \tilde{F}\|_{C(\overline{\Omega})} \leq \varepsilon$, $\|u_0 - \overline{u}_0\|_{C(\overline{G})} \leq \varepsilon_0$, $\|v - \overline{v}\|_{C(S \times [0,T])} \leq \varepsilon_1$, *and* u *and* $\overline{u}$ *are the classical solutions of Eqs. 2.2 and 2.3 with the source functions* F *and* $\overline{F}$*, the initial conditions* u_0 *and* $\overline{u}_0$*, and the boundary conditions* v *and* $\overline{v}$*, respectively, then the norm estimate* $\|u - \overline{u}\|_{C(\overline{\Omega})} \leq \max\{\varepsilon_0, \varepsilon_1\} + \frac{T^\alpha}{G(1+\alpha)}\varepsilon$ *for the solutions* u *and* $\overline{u}$ *holds true.*

Let M_L be the space of the functions f that satisfy $X|_S = 0, \; X \in S$ and the inclusions $f \in C^1(\Omega) \bigcap C^2(G)$, $L(f) \in L^2(G)$.

Theorem 2.2.2 ***Existence of Solution:*** *Let an open domain* G *be a one-dimensional interval* $(0,l)$ *and* $u_0 \in M_L$ *. Then the classical solution of the initial boundary-value problem*

$$\begin{aligned} u|_{t=0} = &\quad u_0(x), \;\; 0 \leq x \leq l \\ u(0,t) = &\quad u(l,t) = 0, \;\; 0 \leq t \leq T \end{aligned} \tag{2.4}$$

for the generalized time-fractional diffusion equation

$${}_a^C D_x^\alpha u(t) = \frac{\partial}{\partial x}\left(p(x)\frac{\partial u}{\partial x}\right) - q(x)u < \alpha < 1 \tag{2.5}$$

exists and is given by the Fourier series in the form $u(x,t) = \sum_{i=1}^{\infty}(u_0, X_i)E_\alpha(-\lambda_i t^\alpha)X_i(x)$, *with* $X_i \in M_L$, $i = 1, 2, ...$ *being the eigenfunction corresponding to the eigenvalues* λ_i *of the eigenvalue problem*

$$\begin{aligned} L(X) = &\quad \lambda X \\ X|_S = &\quad 0, \;\; X \in S \end{aligned} \tag{2.6}$$

$(L(u) = -p(x)\dfrac{\partial^2 u}{\partial x^2} - \dfrac{\partial p(x)}{\partial x}\left(\dfrac{\partial u}{\partial x}\right) + q(x)u)$, *and,* E_α *being the Mittag-Leffler function (see Introduction Section - Eq. 1.13).*

A generalization of these results to more complex (Robin) boundary conditions was obtained by Jukka Kemppainen [144]. We now summarize his main results and remarks.

Consider the generalized time fractional diffusion equation given by,

$$ {}_a^C D_x^\alpha u(x,t) = \Delta u(x,t) + f(x,t),\ 0 < \alpha < 1 \tag{2.7} $$

with boundary and initial conditions,

$$ \begin{aligned} \tfrac{\partial u(x,t)}{\partial n(x)} + \beta(x,t)u(x,t) = &\quad g(x,t)\ on\ B = \Gamma \times (0,T] \\ u|_{t=0} = &\quad u_0(x),\ x \in \overline{G} \end{aligned} \tag{2.8} $$

where $(x,t) \in G \times (0,T]$, $G \subset \mathbb{R}^n$, $f,\ g,\ u_0(x)$ are any given functions, $G \subset \mathbb{R}^n$, $n \geq 2$, is a bounded domain with Lyapunov boundary $\Gamma \in C^{1+\lambda}$ $(0 < \lambda < 1)$.

Theorem 2.2.3 *Let $g \in C(\overline{B})$, $u_0(x) \in C^1(\overline{G})$ and $f \in C(\overline{B})$ such that $f(.,t)$ is Hölder continuous uniformly in $t \in [0,T]$ and $suppf(\cdot,t) \subset G$, $t \in [0,T]$. Then the time-fractional diffusion equation admits a unique classical solution and the solution depends continuously on the data in the following sense:*

$$ \|u(x,t)\|_{C(\overline{G})} \leq C \left(\|f\|_{C(\overline{G})} + \|g\|_{C(B)} + \|u_0\|_{C^1(\overline{G})} \right) \tag{2.9} $$

In the same paper Kemppainen [144] presents the following remark:

Remark 3.7. The same technique as above may be used for more general time-fractional diffusion equations, where Δ is replaced by a uniformly elliptic second-order differential operator in nondivergence form with bounded continuous real-valued coefficients depending on x.

2.3 A Numerical Method for the Fractional Diffusion Equation with Neumann Boundary Conditions and a Space Varying Diffusion Coefficient

2.3.1 Time-Fractional Diffusion Equation

Consider the fractional differential equation given by:

$$ \frac{\partial^\alpha T(x,t)}{\partial t^\alpha} = A \frac{\partial}{\partial x} \left(k\,(x)\, \frac{\partial T(x,t)}{\partial x} \right) - BT(x,t) + C \quad 0 < t < T^*,\ 0 < x < L, \tag{2.10} $$

where $\frac{\partial^\alpha}{\partial t^\alpha}$ is the fractional Caputo derivative of arbitrary real order α given by [48],

$$ \frac{\partial^\alpha T(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma\,(1-\alpha)} \int_0^t (t-s)^{-\alpha}\, \frac{\partial T(x,s)}{\partial s} ds \tag{2.11} $$

with $0 < \alpha < 1$, and A, B and C model parameters with suitable dimensions, so that the equation becomes dimensionally consistent. Note that $k\,(x)$ is a function of x, meaning that we can deal with possible anisotropy. The reason for using the variable T is because later this equation will be used to predict the diffusion of temperature.

Note that we are now using a more simple notation to represent the Caputo derivative. This is because from now on only the Caputo fractional derivative will be used.

2.3.2 Boundary Conditions

We assume Neumann boundary conditions (constant heat flux) given by:

$$-k(x)\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = q_0, \quad t>0 \tag{2.12}$$

$$-k(x)\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=L} = 0, \quad t>0, \tag{2.13}$$

and an initial condition,

$$T(x,0) = T_a, \quad x \in (0,L). \tag{2.14}$$

This way we are considering that at $x=0$ we have a constant heat flux, and that *far* from that region, the zero temperature gradient applies (we consider T to be the temperature). Besides the Neumann boundary condition, we also consider an oscillatory flux at the boundary, given by,

$$-k(x)\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = q_0 cos\left(\omega t\right), \quad t>0. \tag{2.15}$$

where ω is the heating frequency (one possible application of this type of boundary conditions is the tumor treatment by alternate cooling and heating [145]).

2.3.3 Numerical Solution

In order to obtain an approximate solution of Eq. (2.10), we need to approximate the time and spatial derivatives. For that, we consider a uniform space mesh on the interval $[0,L]$, defined by the gridpoints $x_i = i\Delta x$, $i=0,\ldots,N$, where $\Delta x = \frac{L}{N}$, and we approximate the space derivative by the second order finite difference (assuming $T \in C^4$ with respect to space):

$$\left.\frac{\partial}{\partial x}\left(k\left(x\right)\frac{\partial T(x,t)}{\partial x}\right)\right|_{x=x_i} = \frac{k_i^+ T(x_{i+1},t) - \left(k_i^+ + k_i^-\right)T(x_i,t) + k_i^- T(x_{i-1},t)}{\left(\Delta x\right)^2} + \mathcal{O}((\Delta x)^2) \tag{2.16}$$

where $k_i^+ = k\left(x_i + \frac{\Delta x}{2}\right)$ and $k_i^- = k\left(x_i - \frac{\Delta x}{2}\right)$. For the discretisation of the fractional time derivative we also assume a uniform mesh, with a time step $\Delta t = T^*/R$ and time gridpoints $t_l = l\Delta t$, $l=0,\,1,\ldots,R$, and, we use the backward finite difference formula provided by Diethelm [48] (assuming $T \in C^2$ with respect to time),

$$\frac{\partial^\alpha T(x,t)}{\partial t^\alpha} = \frac{(\triangle t)^{-\alpha}}{\Gamma(2-\alpha)}\sum_{m=0}^{l} a_{m,l}^{(\alpha)}\left(T\left(x,t_{l-m}\right) - T\left(x,0\right)\right) + \mathcal{O}((\Delta t)^{2-\alpha}) \tag{2.17}$$

where

$$a_{m,l}^{(\alpha)} = \begin{cases} 1, & m = 0, \\ (m+1)^{1-\alpha} - 2m^{1-\alpha} + (m-1)^{1-\alpha}, & 0 < m < l, \\ (1-\alpha)\, l^{-\alpha} - l^{1-\alpha} + (l-1)^{1-\alpha}, & m = l. \end{cases}$$

The coefficients $a_{m,l}^{(\alpha)}$ are such that

$$a_{m,l}^{(\alpha)} < 0, \quad m = 1,\, 2, ..., l-1 \tag{2.18}$$

$$\sum_{m=0}^{l-1} a_{m,l}^{(\alpha)} > 0, \;\; l = 1,\, 2, \ldots. \tag{2.19}$$

For a proof of these results see [146] and [147; 148]. These properties will be useful when deriving the stability and convergence of the proposed method. Since the fractional derivate is a nonlocal operator, an increase in the computational effort is expected. To solve this problem, parallel algorithms can be used. The interested reader on the topic of parallel computing of fractional derivatives may consult the work by Gong et al. [149] where a parallel algorithm for the Riesz fractional reaction-diffusion equation is presented and explained.

Denoting the approximate value of $T\left(x_i, t_l\right)$ by T_i^l, and $k\left(x_i \pm \frac{\Delta x}{2}\right)$ by $k_i^{\pm}$ and neglecting the $\mathcal{O}((\triangle x)^2)$ and $\mathcal{O}((\triangle t)^{2-\alpha})$ terms, the finite difference scheme is then given by,

$$\begin{aligned} \frac{(\triangle t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{m=0}^{l} a_{m,l}^{(\alpha)} \left(T_i^{l-m} - T_i^0\right) &= A \frac{k_i^+ T_{i+1}^l - \left(k_i^+ + k_i^-\right) T_i^l + k_i^- T_{i-1}^l}{(\Delta x)^2} \\ &+ f\left(x_i, t_l, T_i^l\right) \quad i = 1, ..., N-1,\; l = 1, ..., R, \end{aligned} \tag{2.20}$$

with $f\left(x_i, t_l, T(x_i, t_l)\right) \sim f\left(x_i, t_l, T_i^l\right) = -BT_i^l + C$.

For consistency with the order of the spatial discretisation at grid points $i = 2, ..., N-2$, we also assume a second order approximation for the Neumann boundary conditions. For that, a second order forward and backward finite difference formulae were used (assuming $T \in C^3$ with respect to space):,

$$\left.\frac{\partial T(x,t_l)}{\partial x}\right|_{x=0} = \frac{-T(x_2,t_l) + 4T(x_1,t_l) - 3T(x_0,t_l)}{2\Delta x} + \mathcal{O}((\Delta x)^2), \tag{2.21}$$

$$\left.\frac{\partial T(x,t_l)}{\partial x}\right|_{x=L} = \frac{3T(x_N,t_l) - 4T(x_{N-1},t_l) + T(x_{N-2},t_l)}{2\Delta x} + \mathcal{O}((\Delta x)^2) \tag{2.22}$$

This way we can obtain the following approximate expressions for the temperature at x_0 and x_N,

$$T_0^l \approx -\frac{1}{3} T_2^l + \frac{4}{3} T_1^l + \frac{2\Delta x f_0(t)}{3k(0)} \tag{2.23}$$

and

$$T_N^l \approx \frac{4}{3}T_{N-1}^l - \frac{1}{3}T_{N-2}^l - \frac{2\Delta x f_L(t)}{3k(L)} \tag{2.24}$$

where $f_0(t)$ stands for q_0 or $q_0 cos(\omega t)$ and $f_L(t)$ stands for 0. In order to keep the method as general as possible we will proceed using $f_0(t)$ and $f_L(t)$ (two functions of time) as the imposed fluxes.

The following lemma establishes the second order approximation at the boundaries.

Lemma 2.3.1 *Let $u(x)$ be a well behaved function, with continuous derivates up to a desired order ($u(x) \in C^4$). The discretization of the diffusion term at $x = x_1$ given by*

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial u(x)}{\partial x}\right)\Big|_{x=x_1} \simeq \frac{k_1^+ u(x_2) - \left(k_1^+ + k_1^-\right)u(x_1) + k_1^- u(x_0)}{(\Delta x)^2} \tag{2.25}$$

with

$$u(x_0) = \frac{4}{3}u(x_1) - \frac{1}{3}u(x_2) - \frac{2}{3}\Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) + \frac{2(\Delta x)^3}{9}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) \tag{2.26}$$

is a second order ($\mathcal{O}(\Delta x)^2$) approximation.

Proof 2.3.1 *Let us write $\frac{\partial}{\partial x}\left(k(x)\frac{\partial u(x)}{\partial x}\right) = f(x)$. From the Neumann boundary condition we know that*

$$k(x)\frac{\partial u(x)}{\partial x}\Big|_{x=x_0} = A \tag{2.27}$$

with A representing a general function. A Taylor series expansion of fucntion $u(x)$ centered in $x = x_0$ is given by:

$$\begin{aligned} u(x_1) = \quad & u(x_0) + \Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) + \frac{(\Delta x)^2}{2!}\left(\frac{\partial^2 u(x_0)}{\partial x^2}\right) \\ & + \frac{(\Delta x)^3}{3!}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) + \mathcal{O}((\Delta x)^4) \end{aligned} \tag{2.28}$$

$$\begin{aligned} u(x_2) = \quad & u(x_0) + 2\Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) + \frac{(2\Delta x)}{2!}\left(\frac{\partial u^2(x_0)}{\partial x^2}\right) \\ & + \frac{(2\Delta x)^3}{3!}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) + \mathcal{O}((\Delta x)^4) \end{aligned} \tag{2.29}$$

We want to prove that for the case when x_0 is not known (a Neumann boundary condition is provided at the boundary $x = x_0$), we can still obtain a second order approximation for the diffusive term at x_1.

By using Eqs. 2.28 and 2.29 we observe that

$$-\frac{3}{2}u(x_0) + 2u(x_1) - \frac{1}{2}u(x_2) = \Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) - \frac{2(\Delta x)^3}{3!}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) + O((\Delta x)^4) \tag{2.30}$$

and therefore we obtain the following approximation for the one-sided derivative

$$\left.\frac{\partial u(x)}{\partial x}\right|_{x=0} = \frac{-u(x_2)+4u(x_1)-3u(x_0)}{2h} + \mathcal{O}((\Delta x)^2) \tag{2.31}$$

and also an approximation for $u(x_0)$*,*

$$u(x_0) = \frac{4}{3}u(x_1) - \frac{1}{3}u(x_2) - \frac{2}{3}\Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) + \frac{2(\Delta x)^3}{9}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) + O((\Delta x)^4) \tag{2.32}$$

Making use of the initial condition, Eq. 2.27, the previous equation can be re-written in the following form:

$$u(x_0) = \frac{4}{3}u(x_1) - \frac{1}{3}u(x_2) - \frac{2\Delta x}{3}\frac{A}{k(x_0)} + \frac{2(\Delta x)^3}{9}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) + O((\Delta x)^4). \tag{2.33}$$

If $u(x_0)$ *is known, we have that*

$$f(x_1) = \frac{k_1^+ u(x_2) - \left(k_1^+ + k_1^-\right)u(x_1) + k_1^- u(x_0)}{(\Delta x)^2} + O((\Delta x)^2) \tag{2.34}$$

and, the substitution of Eq. 2.33 into Eq. 2.34 leads to the following expression,

$$\begin{aligned} f(x_1) = \; & \frac{k_1^+(u(x_2)-u(x_1)) - k_1^-(u(x_2)-u(x_1))}{(\Delta x)^2} \\ & + \frac{\frac{2}{3}k_1^-(u(x_2)-u(x_1))}{(\Delta x)^2} + \frac{-\frac{2k_1^-}{3}\frac{\Delta x A}{k(0)} + \frac{2k_1^- h^3}{9}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right)}{(\Delta x)^2} \\ & + O((\Delta x)^2) \end{aligned} \tag{2.35}$$

The following Taylor series expansion,

$$u(x_1) = u(x_0) + \Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) + \frac{(\Delta x)^2}{2!}\left(\frac{\partial^2 u(x_0)}{\partial x^2}\right) + \frac{(\Delta x)^3}{3!}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) + O((\Delta x)^4), \tag{2.36}$$

$$u(x_2) = u(x_0) + 2\Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) + \frac{(2\Delta x)^2}{2!}\left(\frac{\partial^2 u(x_0)}{\partial x^2}\right) + \frac{(2\Delta x)^3}{3!}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) + O((\Delta x)^4) \tag{2.37}$$

results in the difference:

$$u(x_2) - u(x_1) = \Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) + \frac{3(\Delta x)^2}{2}\left(\frac{\partial^2 u(x_0)}{\partial x^2}\right) + \frac{7(\Delta x)^3}{6}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right) + O((\Delta x)^4). \tag{2.38}$$

This leads to:

$$\begin{aligned} f(x_1) = \quad & \frac{k_1^+(u(x_2)-u(x_1)) - k_1^-(u(x_2)-u(x_1))}{(\Delta x)^2} \\ & + \frac{\frac{2}{3}k_1^-\left[\Delta x\left(\frac{\partial u(x_0)}{\partial x}\right) + \frac{3(\Delta x)^2}{2}\left(\frac{\partial^2 u(x_0)}{\partial x^2}\right) + \frac{7(\Delta x)^3}{6}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right)\right]}{(\Delta x)^2} \\ & + \frac{-\frac{2k_1^-}{3}\frac{\Delta x A}{k(0)} + \frac{2k_1^-(\Delta x)^3}{9}\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right)}{(\Delta x)^2} + O((\Delta x)^2) \end{aligned} \tag{2.39}$$

This equation can be further simplified:

$$\begin{aligned} f(x_1) = \quad & \frac{k_1^+(u(x_2)-u(x_1))}{(\Delta x)^2} - \frac{u(x_1)) - k_1^-(u(x_2)-u(x_1))}{(\Delta x)^2} \\ & + \frac{(\Delta x)^2 k_1^+\left(\frac{\partial^2 u(x_0)}{\partial x^2}\right)}{(\Delta x)^2} + \frac{(\Delta x)^3 k_1^-\left(\frac{\partial^3 u(x_0)}{\partial x^3}\right)}{(\Delta x)^2} + O((\Delta x)^2). \end{aligned} \tag{2.40}$$

We know that:

$$\begin{aligned} u(x_2) = \quad & u_1^+ + \frac{\Delta x}{2}\frac{\partial u_1^+}{\partial x} + \frac{(\Delta x/2)^2}{2!}\frac{\partial^2 u_1^+}{\partial x^2} \\ & + \frac{(\Delta x/2)^3}{3!}\frac{\partial^3 u_1^+}{\partial x^3} + O((\Delta x)^4) \end{aligned} \tag{2.41}$$

$$\begin{aligned} u(x_1) = \quad & u_1^+ - \frac{\Delta x}{2}\frac{\partial u_1^+}{\partial x} + \frac{(\Delta x/2)^2}{2!}\frac{\partial^2 u_1^+}{\partial x^2} \\ & - \frac{(\Delta x/2)^3}{3!}\frac{\partial^3 u_1^+}{\partial x^3} + O((\Delta x)^4) \end{aligned} \tag{2.42}$$

$$\begin{aligned} u(x_2) = \quad & u_1^- + \frac{3\Delta x}{2}\frac{\partial u_1^-}{\partial x} + \frac{(3\Delta x/2)^2}{2!}\frac{\partial^2 u_1^-}{\partial x^2} \\ & + \frac{(3\Delta x/2)^3}{3!}\frac{\partial^3 u_1^-}{\partial x^3} + O((\Delta x)^4) \end{aligned} \tag{2.43}$$

$$\begin{aligned} u(x_1) = \quad & u_1^- + \frac{\Delta x}{2}\frac{\partial u_1^-}{\partial x} + \frac{(\Delta x/2)^2}{2!}\frac{\partial^2 u_1^-}{\partial x^2} \\ & + \frac{(\Delta x/2)^3}{3!}\frac{\partial^3 u_1^-}{\partial x^3} + O((\Delta x)^4) \end{aligned} \tag{2.44}$$

with $u\left(x_{i\pm\frac{1}{2}}\right) = u_i^{\pm}$. *We can therefore obtain the following differences:*

$$u(x_2) - u(x_1) = \Delta x\frac{\partial u_1^+}{\partial x} + \frac{(\Delta x/2)^2}{3}\frac{\partial^2 u_1^+}{\partial x^2} + O((\Delta x)^4), \tag{2.45}$$

$$\begin{aligned} u(x_2) - u(x_1) = \quad & \Delta x\frac{\partial u_1^-}{\partial x} + (\Delta x)^2\frac{\partial^2 u_1^+}{\partial x^2} \\ & + \frac{13(\Delta x)^3}{24}\frac{\partial^3 u_1^-}{\partial x^3} + O((\Delta x)^4). \end{aligned} \tag{2.46}$$

If we insert Eq. 2.45 in the first term of Eq. 2.40 , Eq. 2.46 in the second term of Eq. 2.40 and taking into acount that

$$f(x_1) = \frac{k_1^+ \frac{\partial u_1^+}{\partial x} - k_1^- \frac{\partial u_1^-}{\partial x}}{\Delta x} + O((\Delta x)^2) \tag{2.47}$$

we obtain:

$$\begin{aligned} &\left| \frac{k_1^+(u(x_2)-u(x_1))}{(\Delta x)^2} - \frac{u(x_1)-k_1^-(u(x_2)-u(x_1))}{(\Delta x)^2} \right. \\ &\left. + \frac{(\Delta x)^2 k_1^+ \left(\frac{\partial^2 u(x_0)}{\partial x^2}\right)}{(\Delta x)^2} + \frac{(\Delta x)^3 k_1^- \left(\frac{\partial^3 u(x_0)}{\partial x^3}\right)}{(\Delta x)^2} - f(x_1) \right| = g(x) \end{aligned} \tag{2.48}$$

with

$$\begin{aligned} g(x) = \; & \frac{\frac{(\Delta x)^3}{24} k_1^+ \frac{\partial^3 u_1^+}{\partial x^3} - \frac{(\Delta x)^3}{24} k_1^- \frac{\partial^3 u_1^-}{\partial x^3}}{(\Delta x)^2} \\ & - k_1^- \left[\frac{(\Delta x)^2 \frac{\partial^2 u_1^-}{\partial x^2} - (\Delta x)^2 \frac{\partial^2 u(x_0)}{\partial x^2} + \frac{(\Delta x)^3}{2} \frac{\partial^3 u_1^-}{\partial x^3} - (\Delta x)^3 \frac{\partial^3 u(x_0)}{\partial x^3}}{(\Delta x)^2} \right] \\ & + O((\Delta x)^2). \end{aligned} \tag{2.49}$$

Since

$$\begin{aligned} &\frac{(\Delta x)^3}{24} k_1^+ \frac{\partial^3 u_1^+}{\partial x^3} - \frac{(\Delta x)^3}{24} k_1^- \frac{\partial^3 u_1^-}{\partial x^3} = O((\Delta x)^2) \\ &= \frac{(\Delta x)^2}{24} \left[\frac{\partial}{\partial x} \left(k(x_1) \frac{\partial^3 u(x_1)}{\partial x^3} \right) + O((\Delta x)^2) \right] \end{aligned} \tag{2.50}$$

and

$$(\Delta x)^2 \left(\frac{\partial^2 u(x_0)}{\partial x^2} \right) = (\Delta x)^2 \frac{\partial^2 u\left(x_{1-\frac{1}{2}}\right)}{\partial x^2} - \frac{(\Delta x)^3}{2} \frac{\partial^3 u\left(x_{1-\frac{1}{2}}\right)}{\partial x^3} + O((\Delta x)^4) \tag{2.51}$$

$$(\Delta x)^3 \left(\frac{\partial^3 u(x_0)}{\partial x^3} \right) = (\Delta x)^3 \frac{\partial^3 u\left(x_{1-\frac{1}{2}}\right)}{\partial x^3} + O((\Delta x)^4) \tag{2.52}$$

we have that,

$$\begin{aligned} &\left| \frac{k_1^+(u(x_2)-u(x_1))}{(\Delta x)^2} - \frac{u(x_1)-k_1^-(u(x_2)-u(x_1))}{(\Delta x)^2} \right. \\ &\left. + \frac{(\Delta x)^2 k_1^+ \left(\frac{\partial^2 u(x_0)}{\partial x^2}\right)}{(\Delta x)^2} + \frac{(\Delta x)^3 k_1^- \left(\frac{\partial^3 u(x_0)}{\partial x^3}\right)}{(\Delta x)^2} - f(x_1) \right| = O((\Delta x)^2), \end{aligned} \tag{2.53}$$

and therefore a second order ($\mathcal{O}((\Delta x)^2)$) approximation is obtained.

We now present the system of equations that we need to solve. Using (2.23) and (2.24) in equations (2.20), for $i = 1$ and $i = N - 1$ we obtain:

$$\frac{(\triangle t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{m=0}^{l} a_{m,l}^{(\alpha)} \left(T_1^{l-m} - T_1^0 \right) = \left(k_{\frac{3}{2}} - \frac{1}{3} k_{\frac{1}{2}} \right) D T_2^l - \left(\left(k_{\frac{3}{2}} - \frac{1}{3} k_{\frac{1}{2}} \right) D + B \right) T_1^l + 2 k_{\frac{1}{2}} D \frac{f_0(t)\,\Delta x}{3k_0} + C, \tag{2.54}$$

$$\frac{(\triangle t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{m=0}^{l} a_{m,l}^{(\alpha)} \left(T_{N-1}^{l-m} - T_{N-1}^0 \right) = - \left(\left(k_{\frac{2N-3}{2}} - \frac{1}{3} k_{\frac{2N-1}{2}} \right) D + B \right) T_{N-1}^l + \left(k_{\frac{2N-3}{2}} - \frac{1}{3} k_{\frac{2N-1}{2}} \right) D T_{N-2}^l - 2 k_{\frac{2N-1}{2}} D \frac{f_L(t_l)\,\Delta x}{3k_N} + C. \tag{2.55}$$

For $i = 2, ..., N-2$ we have:

$$\frac{(\triangle t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{m=0}^{l} a_{m,l}^{(\alpha)} \left(T_i^{l-m} - T_i^0 \right) = k_{i+\frac{1}{2}} D T_{i+1}^l - \left(\left(k_{i+\frac{1}{2}} + k_{i-\frac{1}{2}} \right) D + B \right) T_i^l + k_{i-\frac{1}{2}} D T_{i-1}^l + C, \tag{2.56}$$

where $D = \dfrac{A}{(\Delta x)^2}$.

Introducing the vectors

$$\begin{aligned} \vec{x} &= \left[\begin{array}{cccc} x_1 & x_2 & \dots & x_{N-1} \end{array} \right]^{\mathrm{T}}, \\ \mathbf{T}^l &= \left[\begin{array}{cccc} T_1^l & T_2^l & \cdots & T_{N-1}^l \end{array} \right]^{\mathrm{T}}, \\ \frac{\partial^2 \mathbf{T}}{\partial x^2}(\vec{x}, t_l) &\left[\begin{array}{cccc} \frac{\partial^2 T}{\partial x^2}(x_1, t_l) & \frac{\partial^2 T}{\partial x^2}(x_2, t_l) \cdots & \frac{\partial^2 T}{\partial x^2}(x_{N-1}, t_l) \end{array} \right]^{\mathrm{T}}, \end{aligned} \tag{2.57}$$

the right-hand-side (rhs) of system of equations (2.54)-(2.56) can now be written in a discretised matrix form (for a time level l), as:

$$A \frac{\partial^2 \mathbf{T}}{\partial x^2}(\vec{x}, t_l) - B\mathbf{T}^l + C \approx \mathbf{M}\mathbf{T}^l + \mathbf{S}^l, \tag{2.58}$$

where

$$\mathbf{S}^l = \left[\begin{array}{ccccc} C + 2k_{\frac{1}{2}} D \frac{\Delta x}{3k(0)} f_0(t_l) & C & \cdots & C & C - 2k_{\frac{2N-1}{2}} D \frac{\Delta x}{3k_0} f_L(t_l) \end{array} \right]^{\mathrm{T}} \tag{2.59}$$

and

$$\mathbf{M} = \left[\begin{array}{cccccc} \varphi_1(-1, -\frac{1}{3})D - B & \varphi_1(1, -\frac{1}{3})D & 0 & \dots & 0 & 0 \\ k_{\frac{5}{2}} D & -\varphi_2(1,1)D - B & k_{\frac{3}{2}} D & 0 & \dots & 0 \\ \dots & \ddots & \ddots & \ddots & \ddots & \dots \\ 0 & \ddots & k_{i+\frac{1}{2}} D & -\varphi_i(1,1)D - B & k_{i-\frac{1}{2}} D & \dots \\ 0 & \dots & \dots & 0 & \varphi_{N-1}(-\frac{1}{3}, 1)D & \varphi_{N-1}(\frac{1}{3}, -1)D - B \end{array} \right], \tag{2.60}$$

with $\varphi_i(w_1, w_2) = w_1 k_{i+\frac{1}{2}} + w_2 k_{i-\frac{1}{2}}$.

The approximation (2.17), at $(x,t) = (x_i, t_l)$, for the time fractional derivative can be written as,

$$\frac{\partial^\alpha T}{\partial t^\alpha}(x_i, t_l) \approx \frac{(\triangle t)^{-\alpha}}{\Gamma(2-\alpha)} \left(T_i^l + \sum_{m=1}^{l-1} a_{m,l}^{(\alpha)} \left(T_i^{l-m} \right) - \sum_{m=1}^{l-1} a_{m,l}^{(\alpha)} T_i^0 - T_i^0 \right), \tag{2.61}$$

or, in matrix form,

$$\frac{\partial^\alpha \mathbf{T}}{\partial t^\alpha}(\vec{x}, t_l) \approx \frac{(\triangle t)^{-\alpha}}{\Gamma(2-\alpha)} \left(\mathbf{T}^l + \sum_{m=1}^{l-1} a_{m,l}^{(\alpha)} \mathbf{T}^{l-m} - \sum_{m=1}^{l-1} a_{m,l}^{(\alpha)} \mathbf{T}^0 - \mathbf{T}^0 \right). \tag{2.62}$$

From the previous considerations we are now in position to describe the numerical scheme. Assume that we are at time level l and that we know the temperature field from the previous time levels, then from (2.58) and (2.62) the system of equations that needs to be solved can be written as

$$\mathbf{T}^l + \sum_{m=1}^{l-1} \left[a_{m,l}^{(\alpha)} \mathbf{T}^{l-m} \right] - \mathbf{T}^0 \sum_{m=1}^{l-1} a_{m,l}^{(\alpha)} - \mathbf{T}^0 = \Lambda \mathbf{M} \mathbf{T}^l + \Lambda \mathbf{S}^l \tag{2.63}$$

with $\Lambda = \dfrac{\Gamma(2-\alpha)}{(\triangle t)^{-\alpha}}$. Or, in an equivalent form,

$$(\mathbf{I} - \Lambda \mathbf{M}) \mathbf{T}^l = - \sum_{m=1}^{l-1} \left[a_{m,l}^{(\alpha)} \mathbf{T}^{l-m} \right] + \mathbf{T}^0 + \mathbf{T}^0 \sum_{m=1}^{l-1} a_{m,l}^{(\alpha)} + \Lambda \mathbf{S}^l \tag{2.64}$$

The matrix $\mathbf{I} - \Lambda \mathbf{M}$, where $\mathbf{I}$ is the $(N-1) \times (N-1)$ identity matrix, is a strictly diagonally dominant matrix. Therefore the matrix $\mathbf{I} - \Lambda \mathbf{M}$ is invertible and the system (2.64) admits a unique solution given by

$$\mathbf{T}^l = (\mathbf{I} - \Lambda \mathbf{M})^{-1} \left(- \sum_{m=1}^{l-1} \left[a_{m,l}^{(\alpha)} \mathbf{T}^{l-m} \right] + \mathbf{T}^0 + \mathbf{T}^0 \sum_{m=1}^{l-1} a_{m,l}^{(\alpha)} + \Lambda \mathbf{S}^l \right) \tag{2.65}$$

2.3.4 Stability and Convergence of the Difference Scheme

In this section we will prove the stability and convergence of the proposed method. Some of the ideas used in the demontrations were based on the excellent work by Huang et al. [150].

2.3.5 Stability of the Difference Scheme

For the proof of stability, the following lemmata will be used.

Lemma 2.3.1 *[150] Let* $\mathbf{L}$ *be an arbitrary square matrix. Then for any matrix norm, we have* $\rho(\mathbf{L}) \leq \|\mathbf{L}\|$ *where* $\rho(\mathbf{L})$ *represents the spectral radius of* $\mathbf{L}$*. Moreover for any* $\varepsilon > 0$ *there exists a norm, denoted by* $\|.\|_\varepsilon$*, such that* $\|\mathbf{L}\|_\varepsilon \leq \rho(\mathbf{L}) + \varepsilon$*.*

Let A be a complex $n \times n$ matrix, with entries a_{ij},. For $i \in \{1, \ldots, n\}$ let $R_i = \sum_{j \neq i} |a_{ij}|$ be the sum of the absolute values of the non-diagonal entries in the $i-th$ row. Let $D(a_{ii}, R_i)$ be the closed disc centered at a_{ii} with radius R_i. Such a disc is called a Gershgorin disc.

Lemma 2.3.2 *Every eigenvalue of A lies within at least one of the Gershgorin discs $D(a_{ii}, R_i)$.*

Theorem 2.3.1 *Let $0 < \varepsilon \leq \Delta t$, the scheme given by (2.65) is unconditionally stable with respect to the initial conditions.*

Proof 2.3.2 *For the proof of this result, we will assume the existence of two different vector solutions, $\mathbf{H}_1^l$ and $\mathbf{H}_2^l$ (that satisfy Eq. 2.65) with different initial conditions $\left(\mathbf{H}_1^0 \neq \mathbf{H}_2^0\right)$ but same boundary conditions. The difference $\mathbf{H}^l = \mathbf{H}_1^l - \mathbf{H}_2^l$ satisfies the following equation,*

$$(\mathbf{I} - \Lambda \mathbf{M})\, \mathbf{H}^l = -\sum_{m=1}^{l-1} \left[a_{m,l}^{(\alpha)} \mathbf{H}^{l-m} \right] + \mathbf{H}^0 + \mathbf{H}^0 \sum_{m=1}^{l-1} a_{m,l}^{(\alpha)} \tag{2.66}$$

From Lemma 2.3.1 we know that, given $\varepsilon > 0$, there exists a norm $\|.\|_\varepsilon$ such that

$$\left\| (\mathbf{I} - \Lambda \mathbf{M})^{-1} \right\|_\varepsilon \leq \rho \left((\mathbf{I} - \Lambda \mathbf{M})^{-1} \right) + \varepsilon. \tag{2.67}$$

Using (2.67), for $l = 1$ we obtain

$$\begin{aligned} \left\| \mathbf{H}^1 \right\|_\varepsilon = \left\| (\mathbf{I} - \Lambda \mathbf{M})^{-1} \mathbf{H}^0 \right\|_\varepsilon &\leq \left\| (\mathbf{I} - \Lambda \mathbf{M})^{-1} \right\|_\varepsilon \left\| \mathbf{H}^0 \right\|_\varepsilon \\ &\leq \left(\rho \left((\mathbf{I} - \Lambda \mathbf{M})^{-1} \right) + \varepsilon \right) \left\| \mathbf{H}^0 \right\|_\varepsilon \end{aligned} \tag{2.68}$$

Since Λ, D, B and k_i are all positive, using the Gerschgorin Theorem is straightforward to prove that $\rho\left(\mathbf{I} - \Lambda \mathbf{M}\right) > 1$ which implies

$$\rho \left((\mathbf{I} - \Lambda \mathbf{M})^{-1} \right) < 1. \tag{2.69}$$

Hence, from (2.68) it follows

$$\left\| \mathbf{H}^1 \right\|_\varepsilon \leq (1 + \varepsilon) \left\| \mathbf{H}^0 \right\|_\varepsilon. \tag{2.70}$$

Now, assume that the following relationship holds,

$$\left\| \mathbf{H}^k \right\|_\varepsilon \leq (1 + \varepsilon)^k \left\| \mathbf{H}^0 \right\|_\varepsilon \; k = 1, 2, ..., l \tag{2.71}$$

we will prove $\left\| \mathbf{H}^{l+1} \right\|_\varepsilon \leq (1 + \varepsilon)^{l+1} \left\| \mathbf{H}^0 \right\|_\varepsilon$.

From (2.18), (2.19), (2.69) and (2.71), it can be deduced that

$$\begin{aligned} \left\| \mathbf{H}^{l+1} \right\|_\varepsilon &\leq \left\| (\mathbf{I} - \Lambda \mathbf{M})^{-1} \right\|_\varepsilon \left\| \sum_{m=1}^{l} \left[\left(-a_{m,l+1}^{(\alpha)} \right) \mathbf{H}^{l+1-m} \right] + \mathbf{H}^0 + \mathbf{H}^0 \sum_{m=1}^{l} \left(a_{m,l+1}^{(\alpha)} \right) \right\|_\varepsilon \\ &\leq (1 + \varepsilon) \left(\left\| \sum_{m=1}^{l} \left[\left(-a_{m,l+1}^{(\alpha)} \right) \mathbf{H}^{l+1-m} \right] \right\|_\varepsilon + \left[1 + \sum_{m=1}^{l} \left(a_{m,l+1}^{(\alpha)} \right) \right] \left\| \mathbf{H}^0 \right\|_\varepsilon \right) \\ &\leq (1 + \varepsilon) \left(\left[\sum_{m=1}^{l} (-a_{m,l+1}^{(\alpha)}) \right] (1 + \varepsilon)^j \left\| \mathbf{H}^0 \right\|_\varepsilon + \left[1 + \sum_{m=1}^{l} (a_{m,l+1}^{(\alpha)}) \right] (1 + \varepsilon)^l \left\| \mathbf{H}^0 \right\|_\varepsilon \right) \\ &\leq (1 + \varepsilon)^{l+1} \left\| \mathbf{H}^0 \right\|_\varepsilon \leq e^{(l+1)\varepsilon} \left\| \mathbf{H}^0 \right\|_\varepsilon \end{aligned} \tag{2.72}$$

Assuming $0 < \varepsilon \leq \Delta t$*, from (2.72) it follows that*

$$\left\|\mathbf{H}^{l+1}\right\|_{\varepsilon} \leq e^{T^*} \left\|\mathbf{H}^{0}\right\|_{\varepsilon},$$

meaning that our numerical scheme is unconditionally stable with respect to the initial conditions.

2.3.6 Convergence Analysis

Let us define the vector of the errors at time step l:

$$\mathbf{e}^l = \left[e_1^l,\, e_2^l, ..., e_{N-1}^l\right], \quad l = 1, 2, ..., ,$$

where $e_i^l = T\left(x_i, t_l\right) - T_i^l \;\; l = 1, 2, ...,\; i = 1, ..., N-1$ is the error at each point of the mesh.

Let $\mathbf{T}_{an}^l = \left[\begin{array}{cccccc} T\left(x_1, t_l\right) & T\left(x_2, t_l\right) & \cdots & T\left(x_{N-2}, t_l\right) & T\left(x_{N-1}, t_l\right) \end{array}\right]^{\mathrm{T}}$ be the vector containing the exact solution for each node i (at time step l).

It can be easily seen that $\mathbf{T}_{an}^l$ satisfies the following equation,

$$\begin{array}{rl} \left(\mathbf{I} - \Lambda\mathbf{M}\right)\mathbf{T}_{an}^l = & -\sum_{m=1}^{l-1}\left[a_{m,l}^{(\alpha)}\mathbf{T}_{an}^{l-m}\right] + \mathbf{T}_{an}^0 + \mathbf{T}_{an}^0\sum_{m=1}^{l-1}a_{m,l}^{(\alpha)} \\ & +\Lambda\mathbf{S}^l + \Lambda\mathbf{R}^l \end{array} \tag{2.73}$$

where $\mathbf{R}^l = [R_1^l, \quad R_2^l, ..., R_{N-1}^l]$ is a $(N-1)\times 1$ vector containing the errors committed in the discretisation of the derivative operators. If $T(x,t)$ is sufficiently regular, from (2.16), (2.17), (2.21) and (2.22) it is straightforward prove that the truncation error at each point $(x_i, t_l),\; i = 1, \ldots, N-1$ satisfies

$$R_i^l = \mathcal{O}\left(\left(\Delta x\right)^2\right) + \mathcal{O}\left(\left(\triangle t\right)^{2-\alpha}\right). \tag{2.74}$$

On the other hand, the approximate solution $\mathbf{T}^l$ obtained from the proposed method satisfies

$$\left(\mathbf{I} - \Lambda\mathbf{M}\right)\mathbf{T}^l = -\sum_{m=1}^{l-1}\left[a_{m,l}^{(\alpha)}\mathbf{T}^{l-m}\right] + \mathbf{T}^0 + \mathbf{T}^0\sum_{m=1}^{l-1}a_{m,l}^{(\alpha)} + \Lambda\mathbf{S}^l. \tag{2.75}$$

Subtracting (2.75) from (2.73) we have (notice that $\mathbf{e}^0 = [0,\, 0, ..., 0]$),

$$\mathbf{e}^l = \left(\mathbf{I} - \Lambda\mathbf{M}\right)^{-1}\left(\sum_{m=1}^{l-1}\left[\left(-a_{m,l}^{(\alpha)}\right)\mathbf{e}^{l-m}\right] + \Lambda\mathbf{R}^l\right) \tag{2.76}$$

Therefore, for $l = 1, 2, \ldots, R$ we have

$$\begin{array}{rcl} \left\|\mathbf{e}^l\right\|_{\varepsilon} & \leq & \left(1+\varepsilon\right)\left\|\sum_{m=1}^{l-1}\left[\left(-a_{m,l}^{(\alpha)}\right)\mathbf{e}^{l-m}\right]\right\|_{\varepsilon} + \Lambda\left(1+\varepsilon\right)\left\|\mathbf{R}^l\right\|_{\varepsilon} \\ & \leq & \left(1+\varepsilon\right)\sum_{m=1}^{l-1}\left(-a_{m,l}^{(\alpha)}\right)\left\|\mathbf{e}^{l-m}\right\|_{\varepsilon} + \Lambda\left(1+\varepsilon\right)\left\|\mathbf{R}^l\right\|_{\varepsilon}, \end{array} \tag{2.77}$$

where ϵ is a positive constant such that $\varepsilon < \Delta t$.

Let us define a sequence $\{p_l\}_{l\in\mathbb{N}_0}$ such that $p_l - p_{l+1} = a^{(\alpha)}_{m,l+1}, \quad m = 0, 1, \ldots, l-1$. Then $p_l = (l+1)^{1-\alpha} - l^{1-\alpha}, \quad l = 0, 1, \ldots$, and from (2.18) we can conclude that p_l is a decreasing sequence. Taking this into account, in what follows we prove by induction on l, that

$$\left\|\mathbf{e}^l\right\|_\varepsilon \leq C\Lambda\,(1+\varepsilon)^l\, p_{l-1}^{-1}\left((\Delta t)^{2-\alpha} + (\Delta x)^2\right), \quad l = 0, 1, \ldots. \tag{2.78}$$

From (2.77) and (2.74) we obtain

$$\left\|\mathbf{e}^1\right\|_\varepsilon \leq \Lambda\,(1+\varepsilon)\left\|\mathbf{R}^1\right\|_\varepsilon \leq C\Lambda\,(1+\varepsilon)\, p_0^{-1}\left((\Delta t)^{2-\alpha} + (\Delta x)^2\right), \tag{2.79}$$

then (2.78) is valid for $l = 1$. Now, suppose we have

$$\left\|\mathbf{e}^j\right\|_\varepsilon \quad \leq C\,\Lambda\,(1+\varepsilon)\; p_{j-1}^{-1}\left((\Delta t)^{2-\alpha} + (\Delta x)^2\right), \quad j = 1, 2, \ldots, l \tag{2.80}$$

we want to prove that

$$\left\|\mathbf{e}^{l+1}\right\|_\varepsilon \quad \leq C\,\Lambda\,(1+\varepsilon)\; p_l^{-1}\left((\Delta t)^{2-\alpha} + (\Delta x)^2)\right)\,. \tag{2.81}$$

From (2.77), (2.74), (2.80), and using some properties of the sequences p_l and $a^{(\alpha)}_{m,j}$ (explained before), we obtain

$$\begin{aligned}
\left\|\mathbf{e}^{l+1}\right\|_\varepsilon &\leq (1+\varepsilon)\sum_{m=1}^{l}\left(-a^{(\alpha)}_{m,l+1}\right) C\Lambda\,(1+\varepsilon)^{l-m}\, p_{l-m-1}^{-1}\left((\Delta t)^{2-\alpha} + (\Delta x)^2\right) \\
&+ (1+\varepsilon)\, C\Lambda\left((\Delta t)^{2-\alpha} + (\Delta x)^2\right) \\
&\leq C\left((\Delta t)^{2-\alpha} + (\Delta x)^2\right)(1+\varepsilon)^{l+1}\, p_l^{-1}\left(\sum_{m=1}^{l}\left(-a^{(\alpha)}_{m,l+1}\right) + p_l\right)
\end{aligned} \tag{2.82}$$

Since

$$\sum_{m=1}^{l}\left(-a^{(\alpha)}_{m,l+1}\right) + p_l = (p_0 - p_1 + p_1 - p_2 + ... + p_{l-1} - p_l) + p_l = p_0 = 1,$$

from (2.82) it follows

$$\left\|\mathbf{e}^{l+1}\right\|_\varepsilon \leq C\,\left((\Delta t)^{2-\alpha} + (\Delta x)^2\right)(1+\varepsilon)^{l+1}\, p_l^{-1},$$

and by induction (2.78) is valid for $l \in \mathbb{N}$.

Theorem 2.3.2 *Let $0 < \varepsilon \leq \Delta t$, if the solution of (2.10) is of class C^2 with respect to t and of class C^4 with respect to x, then there exists a constant C_0 independent of Δx and Δt such that,*

$$\left\|\mathbf{e}^l\right\|_\varepsilon \leq C_0\left((\Delta t)^{2-\alpha} + (\Delta x)^2\right), \quad l = 0, 1, \ldots. \tag{2.83}$$

Proof 2.3.3 *From (2.78), the* $\left\|\mathbf{e}^l\right\|_\varepsilon$ *satisfies*

$$\begin{aligned}\left\|\mathbf{e}^l\right\|_\varepsilon &\leq \frac{l^{-\alpha}}{p_l} C\Gamma(2-\alpha) l^\alpha (\Delta t)^\alpha (1+\varepsilon)^l \left((\Delta t)^{2-\alpha} + (\Delta x)^2\right) \\ &\leq \frac{l^{-\alpha}}{p_l} C\Gamma(2-\alpha) T^{*\alpha} (1+\varepsilon)^l \left((\Delta t)^{2-\alpha} (\Delta x)^2\right), \quad l = 0, 1, \ldots.\end{aligned}$$

On the other hand,

$$\begin{aligned}\lim_{l\to\infty} \frac{l^{-\alpha}}{p_l} &= \lim_{l\to\infty} \frac{l^{-\alpha}}{(l+1)^{-\alpha} - l^{-\alpha}} \\ &= \frac{1}{1-\alpha} \lim_{l\to\infty} \left(1 - \frac{1}{l}\right)^\alpha = \frac{T^{*\alpha}}{1-\alpha}.\end{aligned} \tag{2.84}$$

Thus, for $0 < \varepsilon \leq \triangle t$, $(1+\varepsilon)^{n+1} \leq e^{T^*}$ *it follows (2.83), for some positive constant* C_0 *that does not depend on* Δt *and* Δx.

Note that the convergence order depends on the fractional order α. For a method presenting optimal order convergence without the need to impose inconvenient smoothness conditions on the solution, see the work by Ford et al. [83].

2.3.7 Methodology Assessment

In order to illustrate the effectiveness of the method, some examples for which the analytical solution is known are presented. The error is measured by determining the maximum error at the mesh points (x_i, t_l):

$$\varepsilon_{\Delta x, \Delta t} = \max_{i=1,\ldots,N,\, l=0,\ldots,R} \left|T(x_i, t_j) - T_i^l\right|, \tag{2.85}$$

where T_i^l is the numerical solution at (x_i, t_l).

Example 2.3.1

$$\begin{cases} \dfrac{\partial^\alpha T(x,t)}{\partial t^\alpha} = \dfrac{\partial}{\partial x}\left((x+1)\dfrac{\partial T(x,t)}{\partial x}\right) + t^{3/2}x^2\left(\dfrac{3}{2} - x\right) \\ \qquad\qquad -T(x,t) - 3t^{3/2}\left(1 - 3x^2\right) - \dfrac{3\sqrt{\pi}t^{3/2-\alpha}x^2(2x-3)}{8\Gamma\left(\frac{5}{2}-\alpha\right)} \\ T(x,0) = 0, \quad x \in (0,1) \\ \left.\dfrac{\partial T(x,t)}{\partial x}\right|_{x=0,1} = 0, \quad t \in (0,1) \end{cases} \tag{2.86}$$

whose analytical solution is $T(x,t) = t^{3/2}x^2\left(\frac{3}{2} - x\right)$, and,

Example 2.3.2

Table 2.1: Numerical results obtained for the problem given in Eq. 2.86, for two different values of α ($\frac{1}{2}$ and $\frac{3}{4}$): values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p, for the variable t ($\Delta x = 0.002$).

Step-sizes		$\alpha = 3/4$		$\alpha = 1/2$	
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	p	$\varepsilon_{\Delta x,\Delta t}$	p
1/16	0.002	0.00207	–	0.00185	–
1/32	0.002	0.00090	1.19	0.00075	1.33
1/64	0.002	0.00039	1.21	0.00030	1.35
1/128	0.002	0.00017	1.22	0.00012	1.35

$$
\begin{cases}
\dfrac{\partial^\alpha T(x,t)}{\partial t^\alpha} & = \dfrac{\partial}{\partial x}\left((x+1)\dfrac{\partial T(x,t)}{\partial x}\right) - \cos(t)\, t^2\left(x - \dfrac{x^4}{4}\right) \\
& -t^2\left(-1+3x^2+4x^3\right)\cos(t) \\
& -\dfrac{(-4+x^3)xt^{-\alpha}}{4}\left(\dfrac{2t^2\,{}_2F_3\left(\left\{1,\frac{3}{2}\right\},\left\{\frac{1}{2};\frac{3}{2}-\frac{\alpha}{2},2-\frac{\alpha}{2}\right\};-\dfrac{t^2}{4}\right)}{\Gamma(3-\alpha)}\right) \\
& +\dfrac{(-4+x^3)xt^{-\alpha}}{4}\left(\dfrac{6t^4\,{}_2F_3\left(\left\{2,\frac{5}{2}\right\},\left\{\frac{3}{2};\frac{5}{2}-\frac{\alpha}{2},3-\frac{\alpha}{2}\right\};-\dfrac{t^2}{4}\right)}{\Gamma(5-\alpha)}\right) \\
& -T(x,t)) \\
T(x,0) & = 0, \quad x \in (0,1) \\
\left.\dfrac{\partial T(x,t)}{\partial x}\right|_{x=0} & = t^2\cos(t), \quad \left.\dfrac{\partial T(x,t)}{\partial x}\right|_{x=1} = 0, \quad t \in (0,1)
\end{cases}
\tag{2.87}
$$

whose analytical solution is $T(x,t) = \cos(t)\, t^2\left(x - \frac{x^4}{4}\right)$, with ${}_2F_3\left(...;...;...\right)$ the generalised hypergeometric function.

In Tables 2.1 and 2.2, we show the time and space convergence orders obtained for Ex. 2.3.1 using two different values of α ($\frac{1}{2}$ and $\frac{3}{4}$). Note that the analytical solution is not smooth at $t = 0$, and therefore, we are expecting a reduction on the theoretical convergence order (the convergence order depends on α $\left(O\left((\triangle t)^{2-\alpha}\right)\right)$, and so, for a smooth function, we would obtain in the limit of a highly refined mesh, an experimental convergence order of 1.5 when $\alpha = 0.5$ and 1.25 when $\alpha = 0.75$).

For the space variable, we obtain an experimental convergence order of 2 (in the limit of a highly refined mesh), while for time, the convergence order slightly decreased, as expected, being 1.35 for $\alpha = 0.5$ and 1.22 for $\alpha = 0.75$. Nevertheless, the computations were easily performed, indicating that the method can deal with nonsmooth solutions.

Ex. 2.3.2 was also used to test the convergence order of the method. In this case, the imposed temperature flux is a sinusoidal function of time, that may be interpreted physically as a pulsating temperature applied at the surface of an object. In this case, the analytical solution is a smooth function in both time and space.

Table 2.2: Numerical results obtained for the problem given in Eq. 2.86, for two different values of α ($\frac{1}{2}$ and $\frac{3}{4}$): values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence q, for the variable x ($\Delta t = 0.001$).

Step sizes		$\alpha = 3/4$		$\alpha = 1/2$	
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	q	$\varepsilon_{\Delta x,\Delta t}$	q
0.001	1/8	0.02687	–	0.02929	–
0.001	1/16	0.00718	1.91	0.00780	1.91
0.001	1/32	0.00183	1.97	0.00201	1.96
0.001	1/64	0.00045	2.04	0.00051	1.99

Table 2.3: Numerical results obtained for the problem given in Eq. 2.87, for $\alpha = 0.9$: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p, for the variable t ($\Delta x = 0.002$).

Step-sizes		$\alpha = 0.9$	
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	p
1/10	0.002	0.00929	–
1/20	0.002	0.00449	1.05
1/40	0.002	0.00213	1.08
1/80	0.002	0.00100	1.09

Table 2.4: Numerical results obtained for the problem given in Eq. 2.87, for $\alpha = 0.9$: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p, for the variable x ($\Delta t = 0.001$).

Step sizes		$\alpha = 0.9$	
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	q
0.001	1/4	0.06052	–
0.001	1/8	0.01855	1.71
0.001	1/16	0.00513	1.85
0.001	1/32	0.00038	1.90

The results presented in Tables 2.3 and 2.4, show that the convergence orders obtained, match the theoretical predictions, reinforcing the robustness of the numerical method proposed.

Note that the numerical method was derived for the numerical solution of equations that are simpler than the ones presented in the two previous examples. Nevertheless, the numerical method proved to be robust, providing the theoretical results we were expecting. The reason for choosing these two examples, was based on the lack of analytical solutions for fractional differential equations with the structure of equation (2.10).

2.3.8 Case Study

In order to test the influence of the time-fractional derivative on the classical bioheat equation, we used as a case study, the heating of skin assuming we have a geometry as the one

shown in Fig. 2.2(a), where different layers of skin are shown.

From the practical method of measuring the body temperature with our own hands, to the use of highly sophisticated measuring devices, we can find diverse alternative possibilities and intense theoretical and experimental research work that resulted in major advances and increased knowledge of temperature distribution inside the human body. The pioneering work of Harry H. Pennes [151] in 1948 is the cornerstone of the mathematical modeling of temperature diffusion in tissues, but, as happens with most initial modeling approaches, it required some improvements.

Pennes' [151] bioheat transfer equation (see also [152], [153], [154], [155], [156], [157]), which describes the thermal distribution in human tissue, taking into account the influence of blood flow, (see Fig. 2.2(a)) is given by,

$$\rho_t c_t \frac{\partial T(x,t)}{\partial t} = k \frac{\partial^2 T(x,t)}{\partial x^2} + W_b c_b \left(T_a - T\right) + q_m, \quad t > 0, \;\; 0 < x < L, \tag{2.88}$$

where ρ_t, c_t are constants representing the density $\left[kg/m^3\right]$ and the specific heat $\left[J/\left(kg\,^\circ C\right)\right]$, respectively, and k is the tissue thermal conductivity$[J/(s.m\,^\circ C)]$; W_b is the mass flow rate of blood per unit volume of tissue $\left[kg/\left(s.m^3\right)\right]$; c_b is the blood specific heat; q_m is the metabolic heat generation per unit volume $\left[J/(s.m^3)\right]$; T_a represents the temperature of arterial blood $[^\circ C]$; T is the temperature and the term $W_b c_b \left(T_a - T\right)$ represents the blood perfusion. It is worth mentioning that the W_b constant was experimentally obtained by Pennes for a human forearm (he adjusted W_b until the temperature theoretical results matched the experimental ones).

The bioheat equation presented before (2.88) is now adapted, using the time-fractional derivative instead of the first-order time derivative, $\frac{\partial T(x,t)}{\partial t}$, generalizing in this way the original equation derived by Harry Pennes (Eq. 2.10 with with $0 < \alpha < 1$, and $A = \frac{1}{\rho_t c_t \tau^{\alpha-1}}$, $B = \frac{W_b c_b}{\rho_t c_t \tau^{\alpha-1}}$, and $C = \frac{W_b c_b T_a + q_m}{\rho_t c_t \tau^{\alpha-1}}$). It is worth-mentioning the fact that we have added a new parameter $\tau\,[s]$ to the equation, so that it becomes dimensionally consistent.

Case study I:

Three layers are considered, the epidermis, dermis, and, the subcutaneous tissue, with the space variable, x, ranging from 0 to $0.005\;[m]$; since the thermal conductivities of the epidermis, dermis and subcutaneous tissue, are given by 0.23, 0.45 and $0.19\;[W/(m\,^\circ C)]$, respectively, we will use a logistic function to obtain a smooth variation of the thermal conductivity on the transition regions (from one layer to another), allowing this way to test the robustness of the numerical method. The density and the specific heat are the ones from the subcutaneous region, that is, $\rho_t = 1000$, $c_t = 2675$. The thermal conductivity function is given by:

$$k\left(x\right) = 0.23 + \left(1 + e^{[m(-x+0.00008)]}\right)^{-1} 0.45 - \left(1 + e^{[m(-x+0.00208)]}\right)^{-1} 0.26 \tag{2.89}$$

and $L = 0.005\,[m]$ (with m a parameter that allows tuning the smoothness k between two layers. For this particular case we have considered $m = 100000$). We have also considered a blood perfusion rate of $W_b = 0.5$ [138], a specific heat of $c_b = 3770$, and an arterial blood

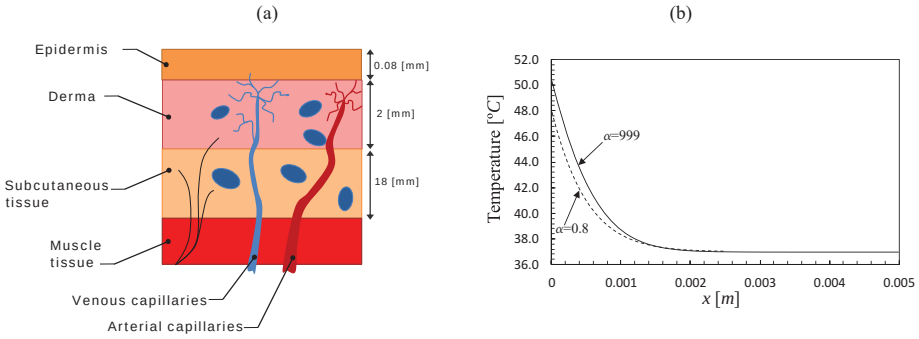


Figure 2.2: (a) Different skin layers. (b)Variation of temperature for constant $t = 2\,[s]$ and two different values of α, 0.999 and0.8 ($\tau = 1$).

temperature of $T_a = 37$ (note that the epidermis perfusion rate is zero [158]). Additionally, the metabolic heat generation q_m and the temperature flux q_0 on the skin surface are assumed to be, respectively, 368.1 and 5000 $\left[J/(s.m^3)\right]$.

Fig. 2.2 shows the variation of temperature along the different layers of skin, for $t = 2\,[s]$, and considering two different values of α (0.999 and 0.8).

Convergence was possible to obtain, and, we can now see that using a complex space varying thermal diffusion, with do not need an equation for each skin layer.

Case study II:

In this last case study, we used the experimental data provided by Barcroft and Edholme [159] for the temperature variation inside a human arm. One of their experiments consisted of measuring the temperature decrease of the subcutaneous tissue ($1\,cm$ below the skin surface) when the forearm is submersed in a $12°C$ water bath (see Fig. 2.3 (a)).

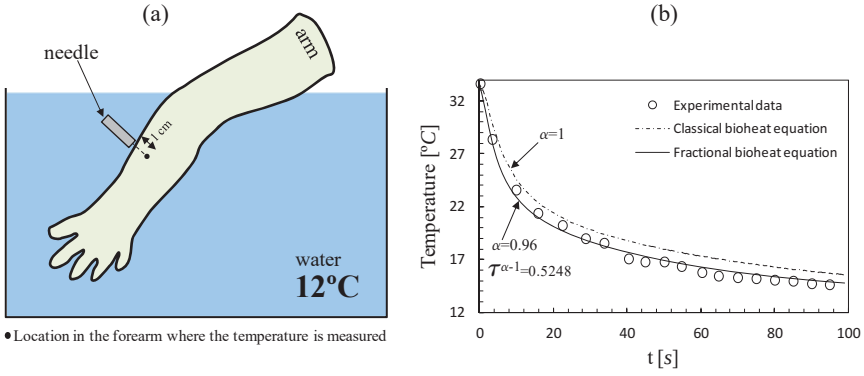


Figure 2.3: (a) Experimental setup. (b) Fitting experimental data (case study II).

For the numerical tests we have assumed a 1D problem, and, even then, good results were obtained by setting $\alpha = 0.96$ and and $\tau^{\alpha-1} = 0.5248$ (based on the data provided

in the papers [159] and [160] we have used the following parameters: initial temperature of $33.6C$, $\rho_t = c_t = 1\, g/cm^3$, $\rho_b = c_b = 1\, [cal.g^{-1}.C^{-1}]$, $q_m = 0.0001\, [cal.s^{-1}.cm^{-3}]$, $k = 0.0015\, cal.s^{-1}.cm^{-1}.C^{-1}$, $W_b c_b = 0.000016$). The boundary conditions are given by,

$$\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = 0, \tag{2.90}$$

$$\left. - k\, \frac{\partial T(x,t)}{\partial x}\right|_{x=4\,[cm]} = 0.0075\,(T-12)\,. \tag{2.91}$$

In Fig. 2.3 (b), we show that the proposed fractional bioheat equation can be used to improve the accuracy of the numerical predictions.

2.3.9 Conclusions and Discussion

A numerical method was devised to solve a general fractional diffusion equation equation, which was proved to be stable and convergent. The method can deal with the Neumann boundary conditions and the variation of the thermal diffusivity in space. We managed to obtain a better fit of experimental results by using the fractional bioheat equation, but, this conclusion should be explained with care. There is no doubt that the fractional derivative may improve the quality of the model, but we have added a new modeling parameter, and therefore, we can not say this is a better model when compared to the classical one.

The typical substitution of the classical derivative by a fractional derivative should be performed with care. First: there should be a physical reason for this substitution, and, second: the units of the parameters used in the equations are changed in the presence of the fractional derivative, therefore we can not used them as regular properties (see Fig. 2.4). A discussion on this subject is provided in [161].

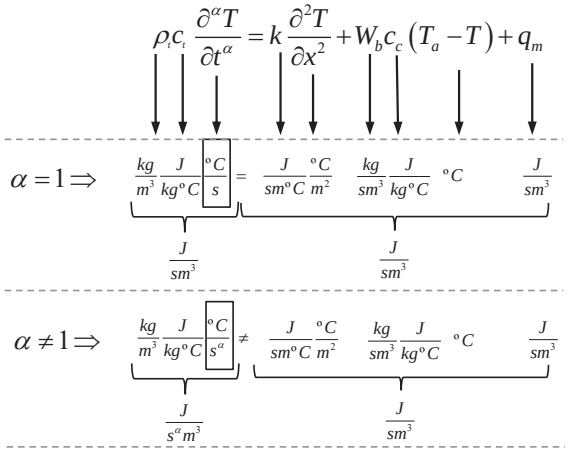


FIGURE 2.4: Dimensional analysis.

The main conclusion is that fractional derivatives can improve physical processes but a discussion on the results obtained and a comparison with the classical case should always be provided.

Regarding the numerical method, it should be highlighted the fact that when deriving the proofs of convergence and stability we have assumed certain regularity properties of the solution that may not be verified in reality. In this cases we are expecting the order of the method to decrease. This topic will be addressed later.

Chebyshev collocation methods: a faster numerical method 3

3.1 Introduction

The numerical method derived in the previous section taught us that the numerical solution of fractional differential equations is computational demanding. Therefore, different numerical techniques should be considered, besides finite differences. In order to enhance the fact that these computations are demanding we consider in this chapter an even more general operator, known as Distributed-Order fractional derivative.

FIGURE 3.1: Pafnuty Chebyshev

Pafnuty Lvovich Chebyshev was a Russian mathematician born in 1821. He suffered from gluteus medius lurch and therefore he limped and walked with a stick. His disability prevented him from playing with children therefore he devoted himself instead to mathematics. Chebyshev is known for his work in the fields of probability, statistics, mechanics, and number theory, mainly for the Chebyshev inequality and the Chebyshev polynomials. He was Professor of well-known students such as Aleksandr Lyapunov, and Andrei Markov, and, a lunar crater was named after him.

Next we present a brief justification on the need of this operator to model physical phenomena, followed by the existence and uniqueness results for the solution of Ditributed-Order Fractional Diffusion Equation. We then present the existing numerical methods for the solution of such equations, and, we propose a new numerical method that is faster than the typical finite-differences technique. We finish with the proof of convergence of the numerical method and perform some tests on the robustness of the method for singular solutions.

The Time-Fractional Diffusion Equation presented in the previous section models diffusion processes that follow $< (z(t))^2 > \sim t^{\alpha}$. In the real world, there are more complex systems that may present more than one characteristic scale, a mean square displacement that evolves with time (as is the case of complex systems where the morphology of the material changes along the process), etc. This means that fractional differential equations are a good tool for modeling some of the processes, but, in order to model correctly certain complex systems a more powerful mathematical tool should be used.

The answer to this problem of non-unique scalability was given by the creation of distributed order fractional differential equations [162; 163] that proved to be useful in modeling anomalous diffusion characterized by two or more scaling exponents in the mean squared displacement. A close look into the physics of some complex diffusive processes, suggests that an even more general theory for fractional derivatives should be devised, and, this will no doubt be developed in the near future [119; 108; 110; 64].

As Chechkin, Gorenflo and Sokolov [162] observed, *"the development of numerical schemes for solving distributed-order kinetic equations and for modelling sample paths of the random processes governed by these equations is also of importance."*, meaning that numerical schemes for the solution of this type of equation are demanded. This is the main motivation for this chapter, where we present a numerical method for the solution of the general distributed-order time fractional diffusion equation (the concept of distributed order was developed by Caputo [164] and further developed by Caputo, Bagley and Torvik [165; 166; 167; 168]),

$$\int_0^1 c(\alpha)\frac{\partial^{\alpha}u(x,t)}{\partial t^{\alpha}}\,d\alpha = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \quad 0 < t \leq a,\ 0 < x < b, \tag{3.1}$$

where the function $c(\alpha)$ acting as weight for the order of differentiation is such that ([169], [170]) $c(\alpha) \geq 0$ and $\int_0^1 c(\alpha)\,d\alpha = C > 0$. Obviously, if $c(\beta) = \dfrac{\delta(\alpha)}{D^{\alpha}}$, where $\delta()$ is the delta Dirac function, then (3.1) reduces to (2.1) (this means that the method derived in this chapter can also be used to solve the Time-Fractional Diffusion Equation, and, this particular case will be described later). Note that the dimensions of $c(\alpha)$ are $[time]^{\alpha}$ / $[length]^2$. For an alternative to these dimensions please consult the work of Chechkin et al. [163] where they use an extra constant that represents a characteristic time of the problem.

Here, we will be interested in the numerical approximation of this type of distributed-order equation with boundary conditions of Dirichlet type:

$$u(0,t) = \phi_0(t),\ u(b,t) = \phi_b(t), \quad 0 < t < a, \tag{3.2}$$

and initial condition

$$u(x,0) \quad = \quad g_0(x), \quad 0 < x < b. \tag{3.3}$$

3.2 Existence and Uniqueness of Solutions for the Distributed Order Diffusion Equation

We begin this section with some results on the well-posedness of the problem we intend to solve numerically. Such results are still very scarce and may be resumed in the following

theorems (adapted from [171]).
First, we define the spaces

$$W_t^1((0,a)) = \left\{ g \in C^1((0,a]) \text{ such that } g' \in L((0,a)) \right\}.$$
$$M_\Delta = \left\{ g \in C_t^1([0,a]) \cap C_x^2(0,b) \text{ such that } \frac{\partial^2 g}{\partial x^2} \in L^2((0,b)) \, and \, g(0,t) = g(b,t) = 0 \right\}.$$

Theorem 3.2.1 *Consider the distributed-order time fractional diffusion equation (3.1) with boundary conditions of Dirichlet type (3.2) and initial condition (3.3).*
If $f(x,t) \in C((0,b)\times(0,a))$, $\phi_0(t)$, $\phi_b(t) \in C([0,a])$ and $g_0(x) \in C([0,b])$, then the problem (3.1)-(3.3) possesses at most one solution $u(x,t) \in C_t([0,a]) \cap W_t^1((0,a)) \cap C_x^2((0,b))$. Moreover, that solution, if it exists, continuously depends on the data given in the problem as follows

$$\|u - \tilde{u}\|_\infty \leq \max\{\epsilon_0, \epsilon_1, \epsilon_2\} + \frac{a^\alpha}{C\,\Gamma(1+\alpha)}\epsilon, \tag{3.4}$$

for the solutions u and $\tilde{u}$ of the problem (3.1)-(3.3) with the data f, g_0, ϕ_0, ϕ_b and $\tilde{f}$, $\tilde{g_0}$, $\tilde{\phi}_0$, $\tilde{\phi}_b$, respectively, that satisfy the conditions $\|f - \tilde{f}\|_\infty \leq \epsilon$, $\|g_0 - \tilde{g_0}\|_\infty \leq \epsilon_0$, $\|\phi_0 - \tilde{\phi_0}\|_\infty \leq \epsilon_1$ and $\|\phi_b - \tilde{\phi_b}\|_\infty \leq \epsilon_2$.

In [171], Luchko also addressed the question of existence of solution. He considered the case where $\phi_0(x) = \phi_b(x) \equiv 0$ (mentioning that the more general case of non-vanishing functions ϕ could be reduced to this one) and he stated sufficient conditions for the existence of a formal solution, which could be regarded as a classical solution of the problem, that is, a function $u \in C_t([0,a]) \cap W_t^1((0,a)) \cap C_x^2((0,b))$ satisfying the differential equation together with the initial and bondary conditions.

Theorem 3.2.2 *If the conditions of Theorem 3.2.1 are satisfied and if the source function $f \in M_\Delta$ and $g_0 \in M_\Delta$, then there exists a solution $u(x,t)$ of the problem (3.1)-(3.3) that belongs to the space $C_t([0,a]) \cap W_t^1((0,a)) \cap C_x^2((0,b))$.*

3.3 Existing numerical methods for the solution of Distributed Order Fractional Differential Equations

With the growing interest on this type of equation, numerical methods started being developed, for example in the work by Diethelm and Ford [172] where they present a basic framework for the numerical solution of distributed order differential equations (see also [173; 174]). A more recent increase in interest in the use of distributed order differential equations (particularly in the case where the derivatives are given in the Caputo sense) led Ford and Morgado [175] to discuss the existence and uniqueness of solutions for this type of equation, and also to propose a numerical method for their approximation in the case where the initial conditions are not known (with boundary conditions being given away from the origin). Two years later, Katsikadelis [176] devised a numerical method for the solution of the distributed order FDE approximating them with a multi-term FDE (that is solved by adjusting appropriately the numerical method developed for multi-term FDEs). In the

same year, Liao et al. [177] investigated a class of modified Du Fort-Frankel-type schemes for fractional subdiffusion equations in the Jumarie modified Riemann-Liouville form with constant, variable or distributed fractional order.

In 2015, some papers were published on the numerical solution of distributed order FDEs. Morgado and Rebelo [147] presented an implicit scheme for the numerical approximation of the distributed order time-fractional reaction-diffusion equation with a nonlinear source term (see also [178]), Ye et al. presented two papers, one [179] considering the time distributed-order and Riesz space fractional diffusion on bounded domains with Dirichlet boundary conditions (deriving an implicit difference method for the multi-term time-space fractional diffusion equation) and the other [180] presenting a numerical method based on a compact difference scheme for a distributed order time-fractional diffusion-wave equation. Hu et al. [181] considered a new time distributed-order and two-sided space-fractional advection-dispersion equation that was solved numerically using an implicit method for the solution the multi-term fractional equation. Gao et al. published a series of papers [182; 183; 184] where: [182] two difference schemes were derived for both one-dimensional and two-dimensional distributed-order differential equations (he proved that the schemes are unconditionally stable and convergent); [183] the Grünwald formula was used to solve the one-dimensional distributed-order differential equations (two difference schemes were derived and the extrapolation method was applied to improve the approximate accuracy); [184] two alternating direction implicit difference schemes were derived for two-dimensional distributed-order fractional diffusion equations (he proved that the schemes are unconditionally stable and convergent). Wang et al. [185] derived and analysed a second-order accurate implicit numerical method for the Riesz space distributed-order advection-dispersion equation. Duong et al. [186] proposed a novel numerical scheme for analysing the behaviour of a distributed order linear single input single output control system under random forcing. The method is based on the operational matrix technique to handle stochastic distributed order systems. Jin et al. [187] presented a numerical solution of an initial boundary value problem for the distributed order time fractional diffusion equation. They developed a space semidiscrete scheme based on the standard Galerkin finite element method, and established error estimates for both smooth and nonsmooth initial data.

Finally, Chen et al. [188] developed a mixed finite difference/spectral method, and, Li et al. [189] proposed a numerical method for solving distributed order diffusion equations by using a classical numerical quadrature formula, and the resulting multi-term time-fractional diffusion equation were solved by the reproducing kernel method.

In almost all the methods described so far, only finite difference approximations have been considered for the fractional time derivative, and these methods may become computationally heavy due to the non-local property of fractional differential operators.

These authors assumed certain regularity assumptions on the solution in order to provide the convergence analysis of their numerical schemes, although it is widely known that the solution of fractional differential equations may be nonsmooth at $t = 0$ even if the data is infinitely smooth.

We consulted the few numerical methods existing in the literature for the numerical solution of this type of equations, and, with the exception of one paper, all assume a high regularity of the solution in order to prove the convergence and/or stability. For example, we have that: in [176] the convergence and the accuracy of the method for linear and nonlinear equations are demonstrated through well corroborated numerical results; in [177] the convergence of the method is obtained assuming the solution is $C_{x,t}^{4,2}$ (the same happens in

[147]). In [179] is assumed that the solution is $C^{6,3}_{x,t}$, in [183] $C^{4,3}_{x,t}$.

In the work of Jin et al. [187] a first order numerical method is presented based on convolution quadrature. Although in their method they do not require a restrictive regularity of the solution, they also report a drastic reduction in convergence when using nonsmooth data.

On the other hand, the idea of approximating the solution of fractional differential equations with truncated Chebyshev series has been widely exploited (see, for example, [190; 98] and the references cited therein), but to the best of our knowledge, a complete and detailed error analysis has not yet been provided.

It should be highlighted that the main aim of this chapter is to alleviate the computational costs of the previously described method, without imposing highly restrictive regularity assumptions on the solution.

Therefore, we present a new numerical method for the solution of the distributed order time-fractional diffusion equation, that is based on the approximation of the solution by a double Chebyshev truncated series, and the subsequent collocation of the resulting discretised system of equations at suitable collocation points. An error analysis is provided and a comparison with other methods used in the solution of this type of equation is also performed. A discussion on the regularity of the solution and the order of convergence are also performed.

3.4 Preliminaries

Here, we present some auxiliary results that will be used in the derivation of our proposed numerical scheme, which is based on the representation of the solution by a truncated Chebyshev series expansion. Hence, we begin this section with some results related to this approach.

Chebyshev polynomials of degree n, $T_n(z) = \cos(n \arccos(z))$, are defined on the interval $[-1, 1]$. In order to use them on the interval $[0, L]$, for any real $L > 0$, we introduce the change of variable $z = 2t/L - 1$ and obtain the so-called shifted Chebyshev polynomials $T_{L,n}(t) = T_n\left(\dfrac{2t}{L} - 1\right)$. These shifted Chebyshev polynomials can also be obtained from the following expression (see [98]):

$$T_{L,n}(t) = n \sum_{k=0}^{n} (-1)^{n-k} \frac{2^{2k}(n+k-1)!}{(2k)!(n-k)!L^k} t^k, \quad n = 1, 2, \ldots, \tag{3.5}$$

where

$$T_{L,i}(0) = (-1)^i \text{ and } T_{L,i}(L) = 1, \tag{3.6}$$

and satisfy the following orthogonality relation:

$$\int_0^L T_{L,j}(t) T_{L,k}(t) \omega_L(t) dt = \delta_{kj} h_k,$$

with $\omega_L(t) = \dfrac{1}{\sqrt{Lt - t^2}}$ and $h_0 = \pi$, $h_k = \frac{\pi}{2}$, $k = 1, 2, \ldots$.

The Chebyshev series expansion of a function $f(x, t)$, $(x, t) \in [-1, 1] \times [-1, 1]$, can be given by

$$f(x,t)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}a_{ij}T_i\left(t\right)T_j\left(x\right)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}a_{ij}T_{j\,i}\left(x,t\right), \tag{3.7}$$

where $T_{j\,i}\left(x,t\right)=T_i\left(t\right)T_j\left(x\right)$. In Mason [191] the proof of convergence of the series is provided, under the assumption that $f(x,t)$ is of bounded variation and that one of the partial derivatives is bounded (see also the works of Chen et al. [192; 193; 194]).
Generalising (3.7) for $(x,t)\in[0,b]\times[0,a]$ the series expansion is given by:

$$f(x,t)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}a_{ij}T_{a,i}(t)T_{b,j}(x)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}a_{ij}T_{j\,i}^{(b,a)}(x,t)(t), \tag{3.8}$$

where $T_{a,i}(t)=T_i\left(\dfrac{2t}{a}-1\right)$, $T_{b,j}(x)=T_j\left(\dfrac{2x}{b}-1\right)$ and $T_{j\,i}^{(b,a)}(x,t)=T_{a,i}(t)T_{b,j}(x)$.
The coefficients a_{ij} are given by

$$a_{ij}=\frac{e_i\,e_j\left\langle f(x,t),T_{j\,i}^{(b,a)}(x,t)\right\rangle}{\pi^2}=\frac{e_i\,e_j}{\pi^2}\int_0^a\int_0^b\frac{f(x,t)T_{a,i}(t)T_{b,j}(x)}{\sqrt{at-t^2}\sqrt{bx-x^2}}\,dx\,dt, \tag{3.9}$$

with $i,j=0,1,2,\ldots$ and,

$$e_i=\begin{cases}1, & i=0\\ 2, & i>0\end{cases}.$$

For computational purposes, only the first $(n+1)$ and $(m+1)$ terms of the series are considered, meaning that a function $f(x,t)$ of two independent variables, $(x,t)\in[-1,1]\times[-1,1]$, may be approximately expanded in terms of truncated double Chebyshev series

$$P_{n,m}\left(f\right)\left(x,t\right)\equiv f_{n,m}(x,t)=\sum_{i=0}^{n}\sum_{j=0}^{m}a_{ij}T_i(t)T_j(x), \tag{3.10}$$

or

$$P_{n,m}\left(f\right)\left(x,t\right)\equiv f_{n,m}(x,t)=\sum_{i=0}^{n}\sum_{j=0}^{m}a_{ij}T_{a,i}(t)T_{b,j}(x), \tag{3.11}$$

if $(x,t)\in[0,b]\times[0,a]$.

In the work of Sommariva et al. [195], it is stated that if f is continuous and of bounded variation, then for every $\varepsilon>0$, there exists an $n\left(\varepsilon\right)$, and a sequence $m_k=m\left(k;\varepsilon\right)$, such that $\left\|f-P_{n(\epsilon),m_k}\right\|_\infty\leq\varepsilon$, where $\left\|f\right\|_\infty=\max\limits_{(x,t)\in[-1,1]\times[-1,1]}\left|f(x,t)\right|$.
The adaptation of this result to rectangular domains $[0,b]\times[0,a]$ is straightforward. In that case we also define

$$\left\|f\right\|_\infty=\max_{(x,t)\in[0,b]\times[0,a]}\left|f(x,t)\right|.$$

Let $J=[0,b]\times[0,a]$ and define $E(J)$ as the space of all continuous real-valued functions endowed with the norm

$$\left\|f\right\|_*^2=\frac{1}{\pi^2}\int_0^a\int_0^b\left|f(x,t)\right|^2\frac{1}{\sqrt{at-t^2}}\frac{1}{\sqrt{bx-x^2}}\,dx\,dt. \tag{3.12}$$

In [192; 193; 194] Chen et al. provides upper bounds for the truncation error of the two-variable Chebyshev series expansion (3.11). This will give us an idea of the accuracy of this approximation of the solution, in the cases where it presents some regularity. The first result does not demand high regularity assumptions on the solution, which is the expected situation in the fractional setting.

Theorem 3.4.1 *Let g be in $E(J)$, with $J = [0,b] \times [0,a]$, and such that, $\frac{\partial^2 g}{\partial x \partial t} \in E(J)$. Let $P_{n,m}$ be defined by (3.11), then*

$$\|(I - P_{n,m})g\|_\infty \leq B_{nm} Q$$

where

$$B_{nm} = \gamma(m) + \gamma(n) + \gamma(0)\left(\gamma(n) + \gamma(m)\right), \tag{3.13}$$

$$Q = \max\left\{ \left\| \frac{dh}{dt} \right\|_*, \left\| \frac{dp}{dx} \right\|_*, \left\| \frac{\partial^2 g}{\partial x \partial t} \right\|_* \right\}, \tag{3.14}$$

and

$$\begin{aligned} \gamma^2(n) &= 2 \sum_{j \geq n+1} \frac{1}{j^2}, \\ h(t) &= \frac{1}{\pi} \int_0^b g(x,t) \frac{1}{\sqrt{at - t^2}} \frac{1}{\sqrt{bx - x^2}}\, dx, \\ p(x) &= \frac{1}{\pi} \int_0^a g(x,t) \frac{1}{\sqrt{at - t^2}} \frac{1}{\sqrt{bx - x^2}}\, dt. \end{aligned}$$

The next Theorem requires more smoothness conditions to be satisfied.

Theorem 3.4.2 *Let g be in $E(J)$, with $J = [0,b] \times [0,a]$, and such that, $\frac{\partial^{k+l} g}{\partial x^k \partial t^l}$, $\frac{\partial^s g}{\partial x^s}$, $\frac{\partial^s g}{\partial t^s} \in E(J)$, for $1 \leq k \leq p$, $1 \leq l \leq p$, $0 \leq s \leq 2p$, $p \geq 2$. Let $P_{n,m}$ be defined by (3.11), then*

$$\|(I - P_{n,m})g\|_\infty \leq \tilde{B}_{nm} \tilde{Q},$$

where

$$\tilde{B}_{nm} = 2\left(\frac{ba}{4}\right)^{2p} \left(\frac{1}{\sqrt{nm} \prod_{k=0}^{p-2}(n-k) \prod_{k=0}^{p-2}(m-k)} + \frac{\sqrt{n+1}}{\sqrt{m} \prod_{k=0}^{2p-2}(m-k)} + \frac{\sqrt{m+1}}{\sqrt{n} \prod_{k=0}^{2p-2}(n-k)} \right) \tag{3.15}$$

and

$$\tilde{Q} = \max\left\{\left\|\frac{\partial^{2p} g}{\partial x^p \partial t^p}\right\|_*, \left\|\frac{\partial^{2p} g}{\partial x^{2p}}\right\|_*, \left\|\frac{\partial^{2p} g}{\partial t^{2p}}\right\|_*\right\}. \tag{3.16}$$

Remark 3.4.1 *From Theorems 3.4.1 and 3.4.2, it is clear that, as in the univariate case, the smoother the function $g(x,t)$ is, the faster the method converges. It is clear from these two Theorems that, if a certain function is smooth then*

$$\|(I - P_{n,m})g\|_\infty \leq A_{nm} C,$$

where A_{nm} and C are given by (3.13) and (3.14) or (3.15) and (3.16) depending on the smoothness of the function being approximated.

If we consider $m = n$ we easily see that $B_{nm} \sim \frac{C_1}{\sqrt{n}}$ while $\tilde{B}_{nm} \sim \frac{C_2}{n^{2p-1}}$, with C_1 and C_2 constants.

3.5 The Numerical Scheme

In this section we describe the numerical method. As we will see, the method presented in this work is faster than the typical finite differences approaches, where we need to compute all the diffusion history at each time step (cf. section of numerical results).
If the source function f, and the functions ϕ_0, ϕ_b and g_0 related with the boundary and initial conditions, respectively, of the problem (3.1) satisfy the assumptions of Theorem 3.2.2 then the problem (3.1)-(3.3) has an unique solution $u(x,t) \in C_t([0,a]) \cap W_t^1((0,a)) \cap C_x^2((0,b))$. Furthermore if the solution u is a function of bounded variation, as we remarked previously, based on a result from [195], it can be approximated by the truncated series $u_{n,m}(x,t)$ defined in (3.11).

First, to deal with the integral term in (3.1), we use a Gauss-Legendre quadrature formula with s points, with associated weights and points denoted, respectively, by ω_q and β_q. Hence (3.1) is approximated with

$$\frac{1}{2}\sum_{q=1}^{s} \omega_q c\left(\frac{\beta_q + 1}{2}\right) \frac{\partial^{\frac{\beta_q+1}{2}} u_{n,m}(x,t)}{\partial t^{\frac{\beta_q+1}{2}}} = \frac{\partial^2 u_{n,m}(x,t)}{\partial x^2} + f(x,t). \tag{3.17}$$

Using (3.5) the following expressions can be derived:

$$\frac{\partial^\alpha u_{n,m}(x,t)}{\partial t^\alpha} = \sum_{i=\lceil\alpha\rceil}^{n}\sum_{j=0}^{m} a_{ij} T_{b,j}(x) \sum_{k=\lceil\alpha\rceil}^{i} w_{i,k}^{(\alpha)} t^{k-\alpha}, \tag{3.18}$$

$$\frac{\partial^2 u_{n,m}(x,t)}{\partial x^2} = \sum_{i=0}^{n}\sum_{j=2}^{m} a_{ij} T_{a,i}(t) \sum_{\gamma=2}^{j} \omega_{j,\gamma} x^{\gamma-2}, \tag{3.19}$$

where the weights $w_{i,k}^{(\alpha)}$ are defined by (see also [98])

$$w_{i,k}^{(\alpha)} = (-1)^{i-k} \frac{2^{2k} i (i+k-1)! \Gamma(k+1)}{(i-k)!(2k)!\Gamma(k+1-\alpha) a^k}, \tag{3.20}$$

and the weights $\omega_{j,\gamma}$ are given by

$$\omega_{j,\gamma} = (-1)^{j-\gamma}\frac{2^{2\gamma}j(j+\gamma-1)!\gamma(\gamma-1)}{(j-\gamma)!(2\gamma)!b^{\gamma}}. \tag{3.21}$$

Inserting (3.18) and (3.19) in (3.17), we obtain the following approximation of equation (3.1):

$$\frac{1}{2}\sum_{q=1}^{s}\omega_q c\left(\frac{\beta_q+1}{2}\right)\sum_{i=\lceil\frac{\beta_q+1}{2}\rceil}^{n}\sum_{j=0}^{m}a_{ij}T_{b,j}(x)\sum_{k=\lceil\frac{\beta_q+1}{2}\rceil}^{i}w_{i,k}^{(\frac{\beta_q+1}{2})}t^{k-\frac{\beta_q+1}{2}} =$$

$$\sum_{i=0}^{n}\sum_{j=2}^{m}a_{ij}T_{a,i}(t)\sum_{\gamma=2}^{j}\omega_{j,\gamma}x^{\gamma-2}+f(x,t). \tag{3.22}$$

In this case, since $\frac{\beta_q+1}{2}\in[0,1],\ q=1,\ldots,s$, then $\lceil\frac{\beta_q+1}{2}\rceil=1,\ q=1,\ldots,s$. Finally, in order to determine the coefficients a_{ij} of the truncated Chebyshev series expansion, we will use collocation.

For collocation points we consider, as usual, the Chebyschev points $t_p=\frac{a}{2}\left(\cos\left(\frac{\pi p}{n}\right)+1\right),\ p=0,\ldots,n$ and $x_\ell=\frac{b}{2}\left(\cos\left(\frac{\pi\ell}{m}\right)+1\right),\ \ell=0,\ldots,m$.

The coefficients $a_{ij},\ i=0,\ldots,n,\quad j=0,\ldots,m$, of the discrete solution are then computed by imposing that $u_{n,m}(x,t)$ satisfies the multi-term equation (3.22) at the collocation points (x_ℓ,t_p), $\ell=1,\ldots,m-1,\ p=0,\ldots,n-1$:

$$\frac{1}{2}\sum_{q=1}^{s}\omega_q c\left(\frac{\beta_q+1}{2}\right)\sum_{i=\lceil\frac{\beta_q+1}{2}\rceil}^{n}\sum_{j=0}^{m}a_{ij}T_{b,j}(x_\ell)\sum_{k=\lceil\frac{\beta_q+1}{2}\rceil}^{i}w_{i,k}^{(\frac{\beta_q+1}{2})}t_p^{k-\frac{\beta_q+1}{2}} =$$

$$\sum_{i=0}^{n}\sum_{j=2}^{m}a_{ij}T_{a,i}(t_p)\sum_{\gamma=2}^{j}\omega_{j,\gamma}x_\ell^{\gamma-2}+f(x_\ell,t_p). \tag{3.23}$$

On the other hand, we insist that the approximate solution, $u_{n,m}(x,t)$, satisfies the boundary and initial conditions at the collocation points placed at the boundary of the domain $[0,b]\times[0,a]$. Thus, using the fact that the shifted Chebyschev polynomials satisfy $T_{b,j}(0)=(-1)^j$ and $T_{b,j}(1)=1$, the coefficients a_{ij} that define the approximate solution $u_{n,m}(x,t)$ of u are such that it satisfies the system of equations (3.23) together with

$$\sum_{i=0}^{n}\sum_{j=0}^{m}a_{ij}T_{a,i}(t_p)(-1)^j=\phi_0(t_p), \tag{3.24}$$

$$\sum_{i=0}^{n}\sum_{j=0}^{m}a_{ij}T_{a,i}(t_p)=\phi_b(t_p), \tag{3.25}$$

$$\sum_{i=0}^{n}\sum_{j=0}^{m}a_{ij}(-1)^iT_{b,j}(x_\ell)=g_0(x_\ell), \tag{3.26}$$

$$p=0,\ldots,n-1,\ \ell=0,\ldots,m.$$

This way, we have $(n+1)\times(m+1)$ unknown coefficients a_{ij} and $(n+1)\times(m+1)$ equations.

Remark: For the particular case of the Time-Fractional Diffusion Equation, we have to solve

$$\frac{\partial^\alpha u_{n,m}(x,t)}{\partial t^\alpha} = \frac{\partial^2 u_{n,m}(x,t)}{\partial x^2} + f(x,t). \tag{3.27}$$

Substituting Eqs. (3.18)-(3.21) into Eq. (3.27) we obtain the following approximation of Eq. (3.27):

$$\sum_{i=\lceil\alpha\rceil}^{n}\sum_{j=0}^{m} a_{ij}T_{b,j}(x)\sum_{k=\lceil\alpha\rceil}^{i} w_{i,k}^{(\alpha)}t^{k-\alpha} = \sum_{i=0}^{n}\sum_{j=2}^{m} a_{ij}T_{a,i}(t)\sum_{\gamma=2}^{j}\omega_{j,\gamma}x^{\gamma-2} + f(x,t). \tag{3.28}$$

Using the previsous collocation method we arrive again at a system of $(n+1)\times(m+1)$ equations with $(n+1)\times(m+1)$ unknown coefficients a_{ij}.

3.6 Error Analysis

Let $u(x,t)$ be the exact solution of problem (3.1)-(3.3), $u_{n,m}(x,t)$ the truncated series representation of u, given by (3.11), and denote by $\hat{a}_{ij}$ the solution of the linear system of equations (3.23)-(3.26). Let us define the approximate solution obtained with the method described in the previous section as

$$\hat{u}_{n,m}(x,t) = \sum_{i=0}^{n}\sum_{j=0}^{m}\hat{a}_{ij}T_{a,i}(t)T_{b,j}(x), \quad (x,t)\in[0,b]\times[0,a]. \tag{3.29}$$

In Theorem 3.4.2 an error bound for the norm of the difference between the exact solution, $u(x,t)$, and the approximate solution $u_{n,m}(x,t)$ corresponding to the truncated Chebyshev series has been provided. In the numerical method described in the previous section, we have also replaced the time-fractional and the space derivatives of u by the time-fractional and the space derivatives of $u_{n,m}$. We begin this section with some auxiliary lemmas presenting error bound estimates for these approximations.
We can then use the results in the previous section, namely Theorem 3.4.1, Theorem 3.4.2 and Remark 3.4.1, to obtain some upper bounds on the approximations considered here. From Remark 3.4.1, the following two Lemmas are straightforward to obtain.

Lemma 3.6.1 *If $u(x,t)$ and at least the following partial derivative $\dfrac{\partial^4 u}{\partial t\,\partial x^3}$ are continuous on J, then:*

$$\left\|(I-P_{n,m})\,\frac{\partial^2 u}{\partial x^2}\right\|_\infty \le A_{nm}M_x,$$

where A_{nm} and M_x are defined according to Remark 3.4.1.

Lemma 3.6.2 *If $u(x,t)$ and at least the following partial derivative $\dfrac{\partial^3 u}{\partial t^2\,\partial x}$ are continuous on J, then:*

$$\left\|(I-P_{n,m})\,\frac{\partial u}{\partial t}\right\|_\infty \le A_{nm}M_t,$$

where A_{nm} and M_t are defined according to Remark 3.4.1.

Taking into account the definition of the Caputo derivative of order α of a function u, which for $0 < \alpha < 1$ reads

$$\frac{\partial^\alpha u(t,x)}{\partial x^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial u}{\partial s}(x,s)\, ds,$$

and Lemma 3.6.2 we obtain the following result:

Lemma 3.6.3 *If $u(x,t)$ and at least the following partial derivative $\dfrac{\partial^3 u}{\partial t^2\, \partial x}$ are continuous on J, then:*

$$\left\| (I - P_{n,m}) \frac{\partial^\alpha u}{\partial t^\alpha} \right\|_\infty \leq M_\alpha A_{nm},$$

with $M_\alpha = \dfrac{M_t\, a^{1-\alpha}}{\Gamma(1-\alpha)(1-\alpha)}$.

Proof 3.6.1

$$\begin{aligned}
\left\| (I - P_{n,m}) \frac{\partial^\alpha u}{\partial t^\alpha} \right\|_\infty &\leq \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \left\| (I - P_{n,m}) \frac{\partial u}{\partial s} \right\|_\infty ds \\
&\leq \frac{M_t\, A_{n,m}}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha}\, ds \\
&\leq \frac{M_t\, A_{nm}\, t^{1-\alpha}}{(1-\alpha)\Gamma(1-\alpha)} \leq \frac{M_t\, A_{nm}\, a^{1-\alpha}}{(1-\alpha)\Gamma(1-\alpha)}.
\end{aligned}$$

Before we present our main result in this section, we prove some auxiliary results.

Proposition 3.6.1 *The linear system of equations (3.23)-(3.26) can be equivalently written in the matrix form*

$$Az = B, \tag{3.30}$$

where A is invertible, B is the vector with the corresponding error for each one of the equations given in system of equations (3.23)-(3.26), z is the vector with components $(\hat{a}_{ij} - a_{ij})$, $i = 0, \ldots, n,\ j = 0, \ldots, m$, and the following estimate holds

$$\|[\hat{a}_{ij} - a_{ij}]\| \leq C_1 \left(\|R(s,x,t)\|_\infty + \|E(n,m,x,t)\|_\infty \right), \tag{3.31}$$

where $\|\cdot\|$ denotes the maximum vector or matrix norm, $R(s,x,t)$ is the error of the used s-point quadrature rule, and

$$\begin{aligned}
E(n,m,x,t) = \frac{1}{2} \sum_{q=1}^{s} \omega_q c \left(\frac{\beta_q + 1}{2} \right) (I - P_{n,m}) \left(\frac{\partial^{\frac{\beta_q+1}{2}}}{\partial t^{\frac{\beta_q+1}{2}}} u(x,t) \right) \\
+ (I - P_{n,m}) \left(\frac{\partial^2}{\partial x^2} u(x,t) \right).
\end{aligned} \tag{3.32}$$

Proof 3.6.2 *Let us define:*

$$\mathcal{L}_1(u(x,t)) = \int_0^1 c(\alpha)\,\frac{\partial^\alpha}{\partial t^\alpha}u(x,t)d\alpha - \frac{\partial^2}{\partial x^2}u(x,t),$$
$$\mathcal{L}_2(u(x,t)) = \frac{1}{2}\sum_{q=1}^{s}\omega_q c\left(\frac{\beta_q+1}{2}\right)\frac{\partial^{\frac{\beta_q+1}{2}}}{\partial t^{\frac{\beta_q+1}{2}}}u(x,t) - \frac{\partial^2}{\partial x^2}u(x,t). \quad (3.33)$$

Note that the collocation equations (3.23) can be written as

$$\begin{aligned}&\mathcal{L}_2(\hat{u}_{n,m}(x_\ell,t_p)) = f(x_\ell,t_p) = \mathcal{L}_1(u(x_\ell,t_p))\\ &\Leftrightarrow \mathcal{L}_2(\hat{u}_{n,m}(x_\ell,t_p)) = \mathcal{L}_1(u(x_\ell,t_p)) - \mathcal{L}_2(u(x_\ell,t_p)) + \mathcal{L}_2(u(x_\ell,t_p))\\ &\qquad\qquad - \mathcal{L}_2(u_{n,m}(x_\ell,t_p)) + \mathcal{L}_2(u_{n,m}(x_\ell,t_p))\\ &\ell = 1,\ldots,m-1, \quad p = 0,\ldots,n-1. \end{aligned} \quad (3.34)$$

and then

$$\begin{aligned}\mathcal{L}_2((\hat{u}_{n,m}-u_{n,m})(x_\ell,t_p)) &= [\mathcal{L}_1(u(x_\ell,t_p)) - \mathcal{L}_2(u(x_\ell,t_p))]\\ &\quad + [\mathcal{L}_2(u(x_\ell,t_p)) - \mathcal{L}_2(u_{n,m}(x_\ell,t_p))]\end{aligned} \quad (3.35)$$

It is obvious that $\mathcal{L}_1(u(x,t)) - \mathcal{L}_2(u(x,t))$ corresponds to the error of the used s-points quadrature rule, say $R(s,x,t)$, and then (see [196]):

$$\begin{aligned}[\mathcal{L}_1(u(x_\ell,t_p)) - \mathcal{L}_2(u(x_\ell,t_p))] &= R(s,x_\ell,t_p) = \frac{((s)!)^4}{(2s+1)((2s)!)^4}\frac{\partial^{2s}G}{\partial\alpha^{2s}}(\theta,x\ell,t_p)\\ &\approx \frac{\pi}{4^s}\frac{\partial^{2s}G}{\partial\alpha^{2s}}(\theta,x_\ell,t_p), \quad \theta\in[0,1],\end{aligned} \quad (3.36)$$

where the function G is defined by

$$G(\alpha,x,t) = c\left(\frac{\alpha+1}{2}\right)\frac{\partial^{\frac{\alpha+1}{2}}}{\partial t^{\frac{\alpha+1}{2}}}u(x,t). \quad (3.37)$$

On the other hand,

$$[\mathcal{L}_2(u(x_\ell,t_p)) - \mathcal{L}_2(u_{n,m}(x_\ell,t_p))] = E(n,m,x_\ell,t_p). \quad (3.38)$$

Substituting (3.36) and (3.38) in (3.35), we conclude that the collocation equations (3.23) can be written as:

$$\mathcal{L}_2((\hat{u}_{n,m}-u_{n,m})(x_\ell,t_p)) = R(s,x_\ell,t_p) + E(n,m,x_\ell,t_p). \quad (3.39)$$

Taking into account the boundary and initial conditions ((3.2) and (3.3)) and equations (3.24)-(3.26) we have that:

$$\begin{aligned}
\sum_{i=0}^{n}\sum_{j=0}^{m}(a_{ij}-\hat{a}_{ij})(-1)^j T_i(t_p) &= (\hat{u}_{n,m}-u_{n,m})(0,t_p) = (u-u_{n,m})(0,t_p) \\
&= (I-P_{n,m})\,(u(0,t_p)) = E(n,m,0,t_p) \quad (3.40)\\
\sum_{i=0}^{n}\sum_{j=0}^{m}(a_{ij}-\hat{a}_{ij})T_i(t_p) &= (\hat{u}_{n,m}-u_{n,m})(b,t_p) = (u-u_{n,m})(b,t_p) \\
&= (I-P_{n,m})\,(u(b,t_p)) = E(n,m,b,t_p), \quad (3.41)\\
\sum_{i=0}^{n}\sum_{j=0}^{m}(a_{ij}-\hat{a}_{ij})(-1)^i T_j(x_\ell) &= (\hat{u}_{n,m}-u_{n,m})(x_\ell,0) = (u-u_{n,m})(x_\ell,0) \\
&= (I-P_{n,m})\,(u(x_\ell,0)) \\
&= E_{(x_\ell,0)}(n,m,x_\ell,0), \quad (3.42)\\
&\quad p=0,\ldots,n-1,\ \ell=0,\ldots,m.
\end{aligned}$$

Then, from (3.35) and (3.40)-(3.42) it follows that equations (3.23)-(3.26) may be rewritten in the form (3.30), where the matrix A is given by (3.45) with

$$A_i^{t_p} = \sum_{q=1}^{s}\sum_{k=1}^{i}\omega_q c\left(\frac{\beta_q+1}{2}\right) w_{i,k}^{\binom{\beta_q+1}{2}} t_p^{k-\binom{\beta_q+1}{2}}, \quad (3.43)$$

and

$$B_m^{x_l} = \sum_{k=2}^{m}\omega_{m,k}x_l^{m-2} \quad (3.44)$$

,and, vector B is given by (3.46) (with $R_s^{x_\ell,t_p} = R(s,x_\ell,t_p)$ and $E_{n,m}^{x_\ell,t_p} = E(n,m,x_\ell,t_p)$).

It can be checked that A is an invertible matrix if the collocation points are all distinct. We have verified it computationally for several values of n and m.

$$\begin{bmatrix}
0 & 0 & -T_{a,0}^{t_0}B_2^{x_1} & \ldots & -T_{a,0}^{t_0}B_m^{x_1} & \ldots & T_{b,0}^{x_1}A_n^{t_0} & T_{b,1}^{x_1}A_n^{t_0} & T_{b,2}^{x_1}A_n^{t_0}-T_{a,n}^{t_0}B_2^{x_1} & \ldots & T_{b,m}^{x_1}A_n^{t_0}-T_{a,n}^{t_0}B_m^{x_1}\\
\vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \\
0 & 0 & -T_{a,0}^{t_0}B_2^{x_{m-1}} & \ldots & -T_{a,0}^{t_0}B_m^{x_{m-1}} & \ldots & T_{b,0}^{x_{m-1}}A_n^{t_0} & T_{b,1}^{x_{m-1}}A_n^{t_0} & T_{b,2}^{x_{m-1}}A_n^{t_0}-T_{a,n}^{t_0}B_2^{x_{m-1}} & \ldots & T_{b,m}^{x_{m-1}}A_n^{t_0}-T_{a,n}^{t_0}B_m^{x_{m-1}}\\
0 & 0 & -T_{a,0}^{t_1}B_2^{x_1} & \ldots & -T_{a,0}^{t_1}B_m^{x_1} & \ldots & T_{b,0}^{x_1}A_n^{t_1} & T_{b,1}^{x_1}A_n^{t_1} & T_{b,2}^{x_1}A_n^{t_1}-T_{a,n}^{t_1}B_2^{x_1} & \ldots & T_{b,m}^{x_1}A_n^{t_1}-T_{a,n}^{t_1}B_m^{x_1}\ldots\\
\vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\
0 & 0 & -T_{a,0}^{t_0}B_2^{x_{m-1}} & \ldots & -T_{a,0}^{t_1}B_m^{x_{m-1}} & \ldots & T_{b,0}^{x_{m-1}}A_n^{t_1} & T_{b,1}^{x_{m-1}}A_n^{t_1} & T_{b,2}^{x_{m-1}}A_n^{t_1}-T_{a,n}^{t_1}B_2^{x_{m-1}} & \ldots & T_{b,m}^{x_{m-1}}A_n^{t_1}-T_{a,n}^{t_1}B_m^{x_{m-1}}\\
\vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\
\vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\
0 & 0 & -T_{a,0}^{t_{n-1}}B_2^{x_1} & \ldots & -T_{a,0}^{t_{n-1}}B_m^{x_1} & \ldots & T_{b,0}^{x_1}A_n^{t_{n-1}} & T_{b,1}^{x_1}A_n^{t_{n-1}} & T_{b,2}^{x_1}A_n^{t_{n-1}}-T_{a,n}^{t_{n-1}}B_2^{x_1} & \ldots & T_{b,m}^{x_1}A_n^{t_{n-1}}-T_{a,n}^{t_{n-1}}B_m^{x_1}\\
\vdots & & \vdots & \vdots & & \ldots & \vdots & \vdots & \vdots & \vdots & \\
0 & 0 & -T_{a,0}^{t_{n-1}}B_2^{x_{m-1}} & \ldots & -T_{a,0}^{t_{n-1}}B_m^{x_{m-1}} & \ldots & T_{b,0}^{x_{m-1}}A_n^{t_{n-1}} & T_{b,1}^{x_{m-1}}A_n^{t_{n-1}} & T_{b,2}^{x_{m-1}}A_n^{t_{n-1}}-T_{a,n}^{t_{n-1}}B_2^{x_{m-1}} & \ldots & T_{b,m}^{x_{m-1}}A_n^{t_{n-1}}-T_{a,n}^{t_{n-1}}B_m^{x_{m-1}}\ldots\\
T_{a,0}^{t_0} & -T_{a,0}^{t_0} & T_{a,0}^{t_0} & \ldots & (-1)^m T_{a,0}^{t_0} & \ldots & T_{a,n}^{t_0} & -T_{a,n}^{t_0} & T_{a,n}^{t_0} & \ldots & (-1)^m T_{a,n}^{t_0}\\
\vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & \\
T_{a,0}^{t_{n-1}} & -T_{a,0}^{t_{n-1}} & T_{a,0}^{t_{n-1}} & \ldots & (-1)^m T_{a,0}^{t_{n-1}} & \ldots & T_{a,n}^{t_{n-1}} & -T_{a,n}^{t_{n-1}} & T_{a,n}^{t_{n-1}} & \ldots & (-1)^m T_{a,n}^{t_{n-1}}\\
T_{a,0}^{t_0} & T_{a,0}^{t_0} & T_{a,0}^{t_0} & \ldots & T_{a,0}^{t_0} & \ldots & T_{a,n}^{t_0} & T_{a,n}^{t_0} & T_{a,n}^{t_0} & \ldots & T_{a,n}^{t_0}\\
\vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & \\
T_{a,0}^{t_{n-1}} & T_{a,0}^{t_{n-1}} & T_{a,0}^{t_{n-1}} & \ldots & T_{a,0}^{t_{n-1}} & \ldots & T_{a,n}^{t_{n-1}} & T_{a,n}^{t_{n-1}} & T_{a,n}^{t_{n-1}} & \ldots & T_{a,n}^{t_{n-1}}\\
T_{b,0}^{x_1} & T_{b,1}^{x_1} & T_{b,2}^{x_1} & \ldots & T_{b,m}^{x_1} & \ldots & (-1)^n T_{b,0}^{x_1} & (-1)^n T_{b,1}^{x_1} & (-1)^n T_{b,2}^{x_1} & \ldots & (-1)^n T_{b,m}^{x_1}\\
\vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & \\
T_{b,0}^{x_{m-1}} & T_{b,1}^{x_{m-1}} & T_{b,2}^{x_{m-1}} & \ldots & T_{b,m}^{x_{m-1}} & \ldots & (-1)^n T_{b,0}^{x_{m-1}} & (-1)^n T_{b,1}^{x_{m-1}} & (-1)^n T_{b,2}^{x_{m-1}} & \ldots & (-1)^n T_{b,m}^{x_{m-1}}
\end{bmatrix} \quad (3.45)$$

$$\left[R_s^{x_1,t_0}+E_{n,m}^{x_1,t_0},\ldots,\ R_s^{x_{m-1},t_0}+E_{n,m}^{x_{m-1},t_{n-1}},\ E_{n,m}^{0,t_0},\ldots,E_{n,m}^{0,t_{n-1}},\right.$$
$$\left. E_{n,m}^{b,t_0},\ldots,E_{n,m}^{b,t_{n-1}},,\ E_{n,m}^{x_0,0},\ldots,E_{n,m}^{x_m,0}\right] \quad (3.46)$$

Being A an invertible matrix, then

$$\begin{aligned}\|z\| = \|[\hat{a}_{ij} - a_{ij}]\| &\leq \left\|A^{-1}\right\| \left(\|R(s, x_\ell, t_p)\| + \|E(n, m, x_\ell, t_p)\|\right) \\ &\leq C_1 \left(\|R(s, x, t)\|_\infty + \|E(n, m, x, t)\|_\infty\right).\end{aligned}$$

Proposition 3.6.2 *Let u be the solution of the problem (3.1)-(3.3). If*

- *$G(\alpha, x, t) \in C^{2s}([0, 1])$ (regarding the first variable α), for fixed $(x, t) \in [0, b] \times [0, a]$, with G defined by (3.37), and s coming from the s-point quadrature rule,*
- *$u(x, t)$, $\frac{\partial^3 u}{\partial t^2\, \partial x}$ and $\frac{\partial^4 u}{\partial t\, \partial x^3}$ are continuous on J,*

then,

$$\|u_{n,m} - \hat{u}_{n,m}\|_\infty \leq C_4 \left(4^{-s} + A_{nm}\right), \tag{3.47}$$

where A_{nm} is defined according to Remark 3.4.1.

Proof 3.6.3 *Note that since $\|T_{a,i}\| \leq 1$ and $\|T_{b,j}\| \leq 1$ we have*

$$\begin{aligned}\|\hat{u}_{n,m} - u_{n,m}\|_\infty &\leq \sum_{i=0}^{n}\sum_{j=0}^{m} |\hat{a}_{i,j} - a_{i,j}| \, \|T_{a,i}\|_\infty \, \|T_{b,j}\|_\infty \leq \|[\hat{a}_{i,j} - a_{i,j}]\|_1 \\ &\leq C^* \, \|[\hat{a}_{i,j} - a_{i,j}]\|_\infty \\ &\leq C^* C_1 \left(\|R(s, x, t)\|_\infty + \|E(n, m, x, t)\|_\infty\right).\end{aligned}$$

Under the conditions on the function G, from (3.36) it follows

$$\max_{(x,t)\in[0,b]\times[0,a]} |R(s, x, t)| = \|R(s, x, t)\|_\infty \leq \frac{C_2}{4^s}. \tag{3.48}$$

On the other hand, taking into account Lemmas 3.6.1 and 3.6.3 we easily come to the conclusion that

$$\|E(n, m, x, t)\|_\infty \leq C_3 A_{nm}. \tag{3.49}$$

Hence, the result is proved with $C_4 = \max\{C_2, C_3\}$.

Defining the error function,

$$e_{n,m}(x, t) = u(x, t) - \hat{u}_{n,m}(x, t),$$

we finally present our main result of this section.

Theorem 3.6.1 *Assume that all the conditions of Proposition 3.6.2 are satisfied. Then*

$$\|e_{n,m}\|_\infty \leq C \left(4^{-s} + A_{nm}\right). \tag{3.50}$$

Proof 3.6.4 *First note that:*

$$\|e_{n,m}\|_\infty \leq \|u - u_{n,m}\|_\infty + \|u_{n,m} - \hat{u}_{n,m}\|_\infty. \tag{3.51}$$

Under the conditions stated in Theorem 3.4.1 or Theorem 3.4.2 in the case of a smoother solution (see also Remark 3.4.1), the following upper bound for $\|u - u_{n,m}\|_\infty$ can be derived:

$$\|u - u_{n,m}\|_\infty \leq M \, A_{nm} \, C. \tag{3.52}$$

Taking this and the result in Proposition 3.6.2 into account, the theorem is proved.

3.7 Numerical Results

In order to analyse the accuracy of the proposed numerical method, we consider the L_∞ errors:

$$\|\mathbf{E}_{n,m}\|_\infty = \max_{i,j} |u(x_i,t_j) - u_{n,m}(x_i,t_j)|\,, \text{ for } (x_i,t_j) \in [0,b]\times[0,a].$$

In order to approximate the integral that defines the distributed order derivative we use a 3-point Gaussian quadrature formula.

To illustrate the theoretical results, we first consider examples in which the solution satisfies the required smoothness assumptions in the convergence analysis. Because we can expect the solution of fractional differential equations to be nonsmooth we also consider some examples with nonsmooth solutions to check the performance of the present numerical method in such cases.

3.7.1 The Time-Fractional Diffusion Equation

In this subsection we consider some examples in order to illustrate the performance and feasibility of the proposed method for the Time-Fractional Diffusion Equation. We also compare the results obtained with the Chebyschev method with the results obtained with the implicite finite difference scheme by Ford et al. [178]. For that we consider the following two examples (with a regular and a singular solution):

Example 3.7.1

$$f(x,t) = t^2\left(-\frac{2x\left(x^2-1\right)t^{-\alpha}\cos(x)}{\Gamma(3-\alpha)} - x\left(\left(x^2-7\right)\cos(x)+6x\sin(x)\right)+2\sin(x)\right),$$

with analytical solution given by $u(x,t) = t^2 x\left(1-x^2\right)\cos(x), \quad (x,t)\in[0,1]\times[0,1].$

Example 3.7.2

$$f(x,t) = t^\alpha\left(2\sin(x) - x\left(\left(x^2-7\right)\cos(x)+6x\sin(x)\right)\right) + \frac{\pi x\left(x^2-1\right)\csc(\pi\alpha)\cos(x)}{\Gamma(-\alpha)},$$

with analytical solution given by $u(x,t) = x\left(1-x^2\right)t^\alpha\cos(x), \quad (x,t)\in[0,1]\times[0,1].$

The first example (regular solution) clearly benefits the approximation with Chebyschev polynomials sinde the analytical solution is made of polynomial and the $Cos(x)$ function. In order to compare the performance of both methods (finite differences and Chebyschev collocation methods) in solving the Time-Fractional Diffusion Equation, we show in Table 3.1 the L_∞ error, the simulation time and speed-up obtained for Example 3.7.1. We tried to obtain errors of the same order for the two methods, so that a fair comparison could be performed.

As we can see, the Chebyschev collocation method is much faster, and, the finite difference approach becomes impossible to use if high accuracy is needed. Note the speed-up of ≈ 60000 (with a higher error obtained for the finite difference method).

The second example (singular solution), presents a typical singular solution of a fractional differential equation. Again, we compared the performance of both methods, and the results obtained are shown in Table 3.2.

Table 3.1: Numerical solution of Example 3.7.1 using the implicit finite difference and Chebyschev collocation methods. The results are presented in terms of L_∞ error, the simulation time and speed-up (SU). We have considered $\alpha = 0.5$.

Finite Difference Method			Chebyschev Collocation Method			
$\tau = h$	L_∞ error	time (s)	$m = n$	L_∞ error	time (s)	SU
0.0033	$5.42 \cdot 10^{-6}$	732.4	6	$8.38 \cdot 10^{-6}$	0.2	446.2
0.0017	$1.65 \cdot 10^{-6}$	22425.3	7	$4.61 \cdot 10^{-7}$	0.375	59800

Table 3.2: Numerical solution of Example 3.7.2 using the implicit finite difference and Chebyschev collocation methods. The results are presented in terms of L_∞ error, the simulation time and speed-up (SU). We have considered $\alpha = 0.5$.

Finite Difference Method			Chebyschev Collocation Method			
$\tau = h$	L_∞ error	time (s)	$m = n$	L_∞ error	time (s)	SU
0.0125	$4.00 \cdot 10^{-3}$	5.4	10	$4.61 \cdot 10^{-3}$	2.8	1.9
0.0063	$3.31 \cdot 10^{-3}$	40.9	15	$1.16 \cdot 10^{-3}$	21.7	1.9
0.0031	$2.66 \cdot 10^{-3}$	1398.9	20	$9.60 \cdot 10^{-4}$	95.7	14.6

We have obtained speed-up up to ≈ 15, and, we obtained a lower error, which translates in an even higher speed-up value.

From these results it is obvious that finite differences are a fair method to solve the Time-Fractional Diffusion Equation (at least the method proposed in this work), but, the high computation times make it impossible to use when high accuracy is needed. This scenario is expected to get worse in the case of distributed-order subdiffusion equations, as explained next.

3.7.2 The Distributed-Order Time-Fractional Diffusion Equation

First we present the L_∞ error obtained for the examples shown below, and then we study in more detail the examples whose solutions do not satisfy the regularity assumptions required for the theoretical convergence analysis. Even for these cases the numerical method showed reasonable results.

Example 3.7.3

$$c(\alpha) = \Gamma(4-\alpha); \quad f(x,t) = t^2\left(\frac{x(6t + t\log(t) - 6)\sin(x)}{\log(t)} - 2t\cos(x)\right),$$

with analytical solution given by $u(x,t) = t^3 x sin(x), \quad (x,t) \in [0,1] \times [0,1]$.

Example 3.7.4

$$c(\alpha) = \Gamma\left(\frac{7}{2} - \alpha\right); \quad f(x,t) = \frac{t^{3/2}\left(15\sqrt{\pi}(t-1)(x-1)^2 x + 16t(2-3x)\log(t)\right)}{8\log(t)},$$

with analytical solution given by $u(x,t) = t^{5/2}x(1-x)^2, \quad (x,t) \in [0,1] \times [0,1]$.

Example 3.7.5

$$c(\alpha) = \Gamma\left(\frac{5}{2} - \alpha\right);$$

$$f(x,t) = \frac{\sqrt{t}(x-1)2\,(3\sqrt{\pi}(t-1)(x-1)2x2 - 8t(5x(3x-2)+1)\log(t))}{4\log(t)},$$

with analytical solution given by $u(x,t) = t^{3/2}x^2(1-x)^4, \quad (x,t) \in [0,1]\times[0,1]$. *Note that in this case the solution does not satisfy the smoothness conditions required in the convergence analysis of the method described in the previous sections. Even so, we tested the method in this example and in the next section we compare the obtained numerical results with the ones obtained with the finite difference scheme in [178] (Note that this example does not satisfy also the regularity assumptions demanded in the convergence analysis in [178]).*

	$\|\mathbf{E}_{n,m}\|_\infty$		
$n=m$	Example 3.7.3	Example 3.7.4	Example 3.7.5
1	$3.142\cdot10^{-1}$	$1.481\cdot10^{-2}$	$2.193\cdot10^{-2}$
3	$3.469\cdot10^{-3}$	$3.313\cdot10^{-4}$	$1.297\cdot10^{-2}$
5	$8.382\cdot10^{-6}$	$2.397\cdot10^{-5}$	$1.207\cdot10^{-3}$
7	$1.275\cdot10^{-8}$	$4.761\cdot10^{-6}$	$1.059\cdot10^{-5}$
9	$1.020\cdot10^{-11}$	$1.429\cdot10^{-6}$	$4.473\cdot10^{-6}$
11	$3.709\cdot10^{-14}$	$4.402\cdot10^{-7}$	$1.685\cdot10^{-6}$

Table 3.3: The errors $\|\mathbf{E}_{n,m}\|_\infty$, for several values of n and m, from Examples 3.7.3, 3.7.4 and 3.7.5.

In Table 3.3 we list the L_∞ errors obtained with the proposed method, for examples 3.7.3, 3.7.4 and 3.7.5, with several values of n and m. It can be observed that the error is smaller for the biggest values of m and n, that we consider. Thus, the overall errors can be made smaller by adding new terms from the series (3.11) that approximate $u(x,t)$. This leads us to the conclusion that the convergence of the method can be observed even if the solution does not satisfy the regularity assumptions required for the convergence analysis.

However we observe more accuracy and faster convergence for the examples whose solutions are more regular. For example 3.7.3 the solution is $C^\infty([0,1])$, and therefore, the rules dictated by the convergence analysis presented before can be applied and we observe that is possible to reduce the absolute error to very small values ($\sim 10^{-14}$) with a reasonable number of terms in the double Chebyshev series.
In Figure 3.2 we present the absolute error for the Chebyschev series $|u_{10,10}(x,t)|$ obtained for the examples 3.7.3, 3.7.4 and 3.7.5. As we expected the absolute error is smaller for the solution that presents more regularity.

Let us consider a final set of examples whose first derivative with respect to time is not defined at $t=0$. Since estimates for the error, when the solution is non-smooth at $t=0$, are not available in the literature, we have performed a large set of computations considering solutions with an increasing degree of singularity (d).

Example 3.7.6

$$c(\alpha) = \Gamma\left(\frac{d+1}{d} - \alpha\right);$$

$$f(x,t) = \frac{(x-1)^2\left(\frac{(t-1)(x-1)^2x^2\Gamma\left(\frac{d+1}{d}\right)}{\log(t)} - 2t(5x(3x-2)+1)\right)}{t^{d/d+1}},$$

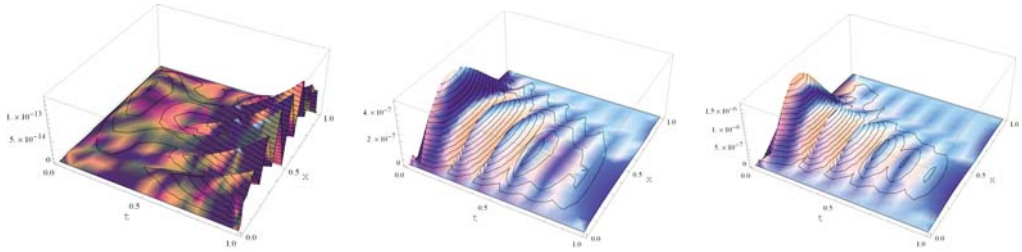


Figure 3.2: Plot of error function $|u(x,t) - u_{10,10}(x,t)|$. Left: Example 3.7.3. Center: Example 3.7.4. Right: Example 3.7.5.

with analytical solution given by $u(x,t) = t^{1/d}(1-x)^4x^2;, \quad (x,t) \in [0,1] \times [0,1]$. *The following set of values for* d *were considered* $d = \{1, 2, 3, ..., 9, 10, 12, 14, 16, ..., 28, 30\}$.

The error $\|\boldsymbol{E}_{n,m}\|_\infty$ obtained is shown in Figure 3.3. It can be seen that the error decreases asymptotically with the increase of $1/d$, and that a slow convergence is obtained with the increase of $m = n$. Although slow, convergence can be observed, even for the most critical case.

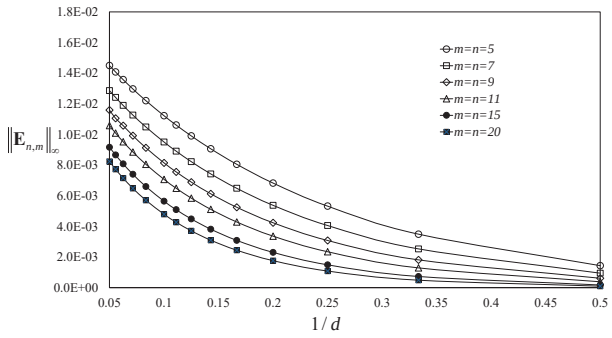


Figure 3.3: Variation of the error $\|\boldsymbol{E}_{n,m}\|_\infty$ with an increasing degree of the singularity.

3.7.2.1 Comparison with an Implicit Finite Difference Scheme

The method presented in this work was compared with the implicit numerical method proposed for these problems in [178]. For the numerical method proposed in [178] we consider a finite difference scheme of order $2-\alpha$ to approximate each fractional derivative, the midpoint rule (with stepsize h) to approximate the integral and a finite difference scheme of order 2 to approximate the second derivative in space. All the numerical experiments have been coded in MATHEMATICA and run on a personal computer with processor Intel(R) Core(TM) i5, 2.60 GHz under operating system MICROSOFT WINDOWS 8.1.

In Tables 3.4 and 3.5 we list the maximum of the absolute errors in the points of the considered time and space mesh, that is, points (x_i, t_j), where $x_i = i\Delta x$, $t_j = j\Delta t$, being Δx and Δt the space and time stepsizes respectively.

Δt	$h = \Delta x$	Implicite finite diff. scheme		Chebyshev Expansion		
				$m = n = 5$	$m = n = 7$	$m = n = 9$
		$\|E\|$	CPU	$\|E\|$	$\|E\|$	$\|E\|$
0.25	0.5	$5.06 \cdot 10^{-3}$	0.010	$8.402 \cdot 10^{-6}$	$1.275 \cdot 10^{-8}$	$9.431 \cdot 10^{-12}$
0.0625	0.25	$1.60 \cdot 10^{-3}$	0.875	$7.440 \cdot 10^{-6}$	$1.275 \cdot 10^{-8}$	$9.431 \cdot 10^{-12}$
0.015625	0.125	$2.80 \cdot 10^{-4}$	74.766	$7.440 \cdot 10^{-6}$	$1.275 \cdot 10^{-8}$	$9.431 \cdot 10^{-12}$
0.00390625	0.0625	$4.97 \cdot 10^{-5}$	4938.58	$8.225 \cdot 10^{-6}$	$1.275 \cdot 10^{-8}$	$9.7358 \cdot 10^{-12}$
				CPU: 6.828	CPU: 37.281	CPU: 125.031

Table 3.4: Maximum of errors ($\|E\|$) and running-time (CPU) in seconds, obtained for Example 3.7.3.

Δt	$h = \Delta x$	Implicite finite diff. scheme		Chebyshev Expansion		
				$m = n = 5$	$m = n = 7$	$m = n = 9$
		$\|E\|$	CPU	$\|E\|$	$\|E\|$	$\|E\|$
0.25	0.5	$8.40 \cdot 10^{-3}$	0.016	$1.007 \cdot 10^{-3}$	$2.054 \cdot 10^{-6}$	$6.001 \cdot 10^{-7}$
0.0625	0.25	$2.45 \cdot 10^{-3}$	0.734	$1.074 \cdot 10^{-3}$	$5.705 \cdot 10^{-6}$	$2.199 \cdot 10^{-6}$
0.015625	0.125	$6.36 \cdot 10^{-4}$	70.75	$1.074 \cdot 10^{-3}$	$1.048 \cdot 10^{-5}$	$5.071 \cdot 10^{-6}$
0.00390625	0.0625	$1.62 \cdot 10^{-4}$	5347	$1.185 \cdot 10^{-3}$	$1.05 \cdot 10^{-5}$	$5.338 \cdot 10^{-6}$
				CPU: 4.391	CPU: 21.531	CPU: 72.766

Table 3.5: Maximum of errors ($\|E\|$) and running-time (CPU) in seconds, obtained for Example 3.7.5.

We also compare these results with the ones obtained with the proposed method (considering several values of n and m), by computing the maximum of the absolute errors in the same mesh points where the absolute errors for the finite difference scheme were computed. The computational cost of each method is also presented.

From the results listed in Tables 3.4 and 3.5, we observe that with the method proposed in this work we can obtain an approximate solution with more accuracy and, by looking at the relative CPU times, with a lower computational cost.

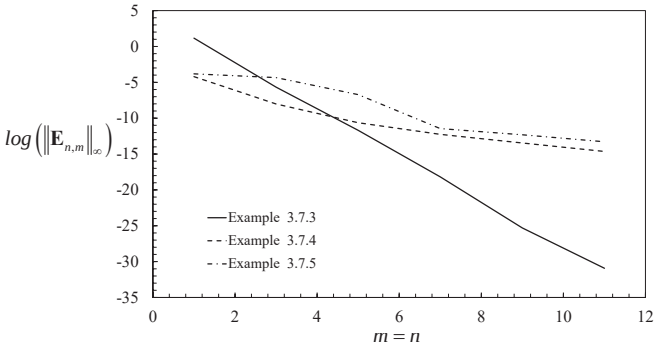


FIGURE 3.4: Variation of the logarithm of the error $\|\boldsymbol{E}_{n,m}\|_\infty$ with $m = n$, for Examples 3.7.3, 3.7.4 and 3.7.5

The experimental convergence order of the method can be seen in figure 3.4. As ex-

pected, the convergence slows for the less regular solutions.

3.8 Conclusions

In this chapter we have presented a new numerical method for the solution of distributed order time-fractional diffusion equations, based on the approximation of the solution by a Chebyshev truncated double series, and the subsequent collocation of the resulting discretised system of equations at suitable collocation points. We review the existing papers on the subject of numerical solution for this type of equations, and, we also present a detailed error analysis for the proposed numerical method.

The error analysis assumes a certain regularity of the solution, that is not always verified. This fact is explored and numerical tests are performed in order to evaluate how the method behaves with highly singular solutions. It was always observed convergence.

Up to now we have improved the issue of demanding computations, but, the regularity of the solution was not properly addressed. In the next Chapter we present a new numerical method that can deal with both the computational effort and the potential singularities of the solution.

Nonpolynomial Approximation Methods: a fast numerical approach for singular and smooth solutions 4

4.1 Introduction

In the previous Chapters we were concerned with the applications of fractional calculus to real world phenomena, and we have not presented a proper method to deal with the potential singularities of the solution.

In order to solve this issue the group developed the work *L.L. Ferrás, N.J. Ford, M.L. Morgado, M. Rebelo, A Numerical Method for the Solution of the Time-Fractional Diffusion Equation. B. Murgante et al. (Eds.): ICCSA 2014, Part I, Lecture Notes in Computer Science 8579 (2014) 117–131*, where it was provided a generalization of the nonpolynomial method (derived by Ford et al. [83] for fractional ordinary differential equations - *N.J. Ford, M.L. Morgado, M. Rebelo, Nonpolynomial collocation approximation of solutions to fractional differential equations, Fract. Calc. Appl. Anal. 16 (2013) 874-891*) to deal with the Time-Fractional diffusion equation. The numerical method takes into account the nonsmoothness of solutions, but, the computations are heavy.

Therefore, here we are concerned with the numerical solution of both (systems of) fractional ordinary differential equations and fractional partial differential equations, by addressing both the nonsmoothness of the solutions and the high computational effort needed to solve them numerically. Therefore, we extended the work by Ford et al. [83] to solve systems of fractional ODE's, and, at the same time we propose a method to decrease the computational effort. The methodology developed for systems of fractional ODE's is then used to solve the Time-Fractional Diffusion Equation (that is transformed into a system of equations by using the method of lines). This way we develop a robust method to solve some of the most used fractional differential equations, to solve physical problems.

The Chapter is organized as follows: we first present a brief description of the method used in [83] and then develop a new hybrid and faster numerical method for solving systems of ordinary differential equations. Finally, a new nonpolynomial numerical method for the solution of the the Time-Fractional diffusion equation is presented and improved. The method makes use of both polynomials and nonpolynomials, decreasing in this way the

computational effort of the original nonpolynomial method.

4.2 Preliminaries

Consider the fractional ordinary differential equation given by:

$$D^{\alpha}y(t) = f(t, y(t)), \quad t \in (0, T], \tag{4.1}$$
$$y(0) = y_0, \tag{4.2}$$

with smooth initial data and $\alpha > 0$.

Lemma 4.2.1 *[48] Assume that the solution y of (4.1-4.2) exists and is unique on $[0, T]$, for a certain $T > 0$. If $\alpha = \frac{p}{q}$, where $p \geq 1$ and $q \geq 2$ are two relatively prime integers and if each right-hand side function f can be written in the form $f(t, y(t)) = \overline{f}(t^{1/q}, y(t))$, where $\overline{f}$ is analytic in a neighborhood of $(0, y(0))$, then the unique solution of the problem (4.1-4.2), can be represented in terms of powers of $t^{1/q}$:*

$$y(t) = \sum_{k=0}^{\infty} a_k t^{k/q}, t \in [0, r), \tag{4.3}$$

where $r < T$ and a_k, $k \geq 0$ are constants.

Based on Lemma 4.2.1 we have the following important remark:

1. First, it should be noted that if the order of the fractional derivative α is not of the form $\alpha = \frac{p}{q}$, with $p \geq 1$ and $q \geq 2$ two relatively prime integers, we can always replace α with the nearest rational number of this form, since as it has been proved in [45], the solution of (4.1)-(4.2) depends continuously on the order of the derivative.

2. Second, from the above Lemma it follows that for $m \in \mathbb{N}$ fixed, the solution of (4.1)-(4.2) can be written in the form $y(t) = y^{(1)}(t) + y^{(2)}(t)$, where $y^{(1)} \in C^m([0, T])$, for a certain $m \geq 1$, and $y^{(2)}$ is the nonsmooth part of y.
   Obviously, this result also holds if instead of a single differential equation, we have a system of multiple equations.

Also, remember that assuming that the right hand-side function $f(t, y)$ is continuous on $[0, T] \times \mathbb{R}$, then the differential equation (4.1)-(4.2) is equivalent to the singular Volterra integral equation:

$$y(t) = y_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t - s)^{\alpha - 1} f(s, y(s))\, ds, \quad t \in (0, T]. \tag{4.4}$$

Given $m \in \mathbb{N}$, we seek a numerical solution of (4.4) on the $\ell-$dimensional space

$$V_m^{\alpha} = span\left\{t^{v_k}, k = 1, .., \ell\right\},$$

where $v_k \in \{i + j\alpha : i, j \in \mathbb{N}_0, i + j\alpha < m\}$. Taking into account the potential non-regularity of the solution y it makes sense to approximate the unique continuous solution of (4.4) by

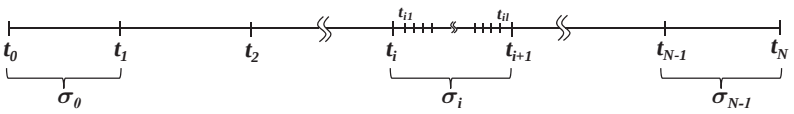


FIGURE 4.1: Schematic of the time partition.

an element of V_m^α, for a certain $m \in \mathbb{N}$.

In what follows we will use this information to derive numerical methods for systems of fractional differential equations and also for the Time-Fractional Diffusion Equation.

4.3 Fractional Ordinary Differential Equations

4.3.1 A Nonpolynomial Collocation Method

In this subsection we will briefly describe the numerical method proposed in [83] for ordinary differential equations.

Consider the time interval, $[0, T]$, is partitioned into N subintervals represented by $\sigma_i = (t_i, t_{i+1}]$, $i = 1, \ldots, N-1$, of equal size τ (with $\sigma_0 = [0, t_1]$).

On each subinterval σ_i we define ℓ collocation points (Fig. 4.1) $t_{ik} = t_i + c_k$, $k = 1, .., \ell$, where the collocation parameters $c_k \in [0,\ 1]$.

Let $V_{\tau,m}^\alpha = \left\{v :\ v|_{\sigma_i} \in V_m^\alpha, i = 1, .., N-1\right\}$, we seek a function $u \in V_{\tau,m}^\alpha$ such that

$$\begin{aligned} &u(t_{ik}) = y(0) + \frac{1}{\Gamma(\alpha)} \int_0^{t_{ik}} (t_{ik} - s)^{\alpha-1} f(s, u(s))\, ds, \\ &i = 0, 1,\ ...,\ N-1,\ k = 1, 2,\ ..., \ell. \end{aligned} \tag{4.5}$$

It will be convenient to introduce the following projection operator $P_\tau : C([0, T]) \to \mathcal{V}_{\tau,m}^\alpha$, defined by:

$$(P_\tau g)(s) = \sum_{k=1}^{\ell} \mathcal{L}_{ik}(s) g(t_{ik}), \quad s \in \sigma_i,$$

where the Lagrange functions $\mathcal{L}_{ik} \in V_m^\alpha$ are defined by

$$\mathcal{L}_{ik}(t) = \sum_{p=1}^{\ell} \beta_{pk}^i t^{\nu_p}, \tag{4.6}$$

where, for each $i = 1, ..., N-1$ $k = 1, \ldots, \ell$, the coefficients β_{pk}^i may be obtained by solving the linear system $\mathcal{L}_{ik}(t_{ij}) = \delta_{jk}$, $k, j = 1, ..., \ell$. By definition we have that the operator $P_\tau g(t_{ik}) = g(t_{ik})$. As an approximation of $f(s, u(s))$, on each subinterval σ_i $i = 0, ..., N-1$, we consider

$$f(s,u(s)) \approx P_\tau f(s) = \sum_{k=1}^{\ell} \mathcal{L}_{ik}(s) f(t_{ik}, u(t_{ik})). \tag{4.7}$$

For $s \in [t_i, t_{ik}]$, $i = 0, 1, ..., N-1$, $k = 1, ..., \ell$ we use

$$f(s,u(s)) \approx P_\tau f(s) = \sum_{\gamma=1}^{\ell} \mathcal{L}_{i\gamma}^{k}(s) f(t_i + \tau c_\gamma c_k, u(t_i + \tau c_\gamma c_k)). \tag{4.8}$$

where $\mathcal{L}_{i\gamma}^{k} i = 0, 1, ..., N-1$, $k = 1, ..., \ell$, $\gamma = 1, ..., \ell$ are the Lagrange function associated with points $t_i + \tau c_\gamma c_k$ defined similarly to (4.6). By considering the two previous approximations of the function $f(s, u(s))$, we have that an approximation to Equation 4.5 is given by

$$\begin{aligned} v\left(t_{ik}\right) &= y(0) + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{i-1} \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} \int_{t_j}^{t_{j+1}} (t_{ik} - s)^{\alpha-1} s^{v_p} ds \beta_{\gamma p}^{i} f(t_{j\gamma}, v(t_{j\gamma})), \\ &+ \frac{1}{\Gamma(\alpha)} \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} \int_{t_i}^{t_{ik}} (t_{ik} - s)^{\alpha-1} s^{v_p} ds \beta_{\gamma p}^{ik} f(t_i + \tau c_\gamma c_k, v(t_i + \tau c_\gamma c_k)). \end{aligned} \tag{4.9}$$

By defining the weights

$$\begin{aligned} w_{ik}^{j,p} &= \frac{1}{\Gamma(\alpha)} \int_{t_j}^{t_{j+1}} (t_{ik} - s)^{\alpha-1} s^{\nu_p} ds, \quad j < i, \\ w_{ik}^{i,p} &= \frac{1}{\Gamma(\alpha)} \int_{t_i}^{t_{ik}} (t_{ik} - s)^{\alpha-1} s^{\nu_p} ds, \ i = 0, 1, ..., N-1, \ k = 1, ..., \ell, \end{aligned}$$

the previous equation can be re-written as

$$\begin{aligned} v\left(t_{ik}\right) &= y(0) + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{i-1} \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} w_{ik}^{j,p} \beta_{\gamma p}^{i} f(t_{j\gamma}, v(t_{j\gamma})), \\ &+ \frac{1}{\Gamma(\alpha)} \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} w_{ik}^{i,p} \beta_{\gamma p}^{ik} f(t_i + \tau c_\gamma c_k, v(t_i + \tau c_\gamma c_k)). \end{aligned} \tag{4.10}$$

After solving (4.10), an approximation to the solution of (4.5) will be given by

$$y(s) \approx \sum_{k=1}^{\ell} y_{jk} \mathcal{L}_{jk}(s), \ s \in \sigma_j, \ j = 0, ..., N-1.$$

This numerical method gives a convergence order that is independent of the order α of the fractional differential equation, as shown in the following theorem by Ford et al. [83]:

Theorem 4.3.1 *Let y be the solution of (4.1-4.2), with $f(t, y(t)) = \beta y(t) + g(t)$, and $v \in V_m^\alpha$ the approximate solution obtained with the nonpolynomial method described before, with a stepsize τ. Then, for sufficiently small τ, there exists a positive constant C independent of τ such that,*

$$\|y - v\|_\infty \leq C\tau^m. \tag{4.11}$$

The numerical method is robust, and solves the problem of potential singularities. Also, we have extended the work of Ford et al. [83] to solve systems of ODE's. The major drawback of this numerical method is that it is computational demanding. Therefore, in the next subsection we provide a faster numerical method that works for both Fractional ODE's and systems of Fractional ODE's.

4.3.2 A Hybrid Collocation Method for the Solution of Systems of Fractional Ordinary Differential Equations

We now present a numerical method for systems of fractional ordinary differential equations which is able to attain the same accuracy with both smooth and nonsmooth solutions. The method consists of a nonpolynomial approximation near the origin, reflecting the singular behavior of the solution near that point, and in the remaining domain, we use a polynomial approximation. As it is natural and shown later, this reduces the computational effort while keeping the ability to deal with potential singularities of the solution.

Based on the previous method and taking into account a generalization of Lemma 4.2.1 we present a hybrid numerical method for linear systems of ordinary differential equations:

$$D^\alpha \mathbf{y}(t) = A\mathbf{y}(t) + \mathbf{F}(t), \quad t \in (0, T] \tag{4.12}$$

$$\mathbf{y}(0) = \mathbf{y_0}, \tag{4.13}$$

where A is a constant matrix $A = [a_{ij}]_{i,j=1,\ldots,n}$, and $\mathbf{y} = [y_1\ y_2 \ldots y_n]^T$. The function $\mathbf{F}$ can be written as $\mathbf{F}(t) = [f_1(t)\ f_2(t) ... f_n(t)]^T$ and $\mathbf{y_0} = [y_{01}\ y_{02} \ldots y_{0n}]^T$, where $y_{0i} = y_i(0),\ i = 1, ..., n$.

In this case, in order to approximate the solution of (4.12)-(4.13) we consider a nonuniform mesh on $[0, T]$, as in [80]. Let i_0 be an integer such that $\left(\frac{N}{i_0}\right)^{\frac{m}{\alpha}} \leq N$ and $\left(\frac{N}{i_0-1}\right)^{\frac{m}{\alpha}} > N$ and let $N' = N - i_0 + 1$. The partition on $[0, T]$ is defined through the meshpoints:

$$t_0 = 0,\ t_i = \left(\frac{i_0 + i - 1}{N}\right)^{\frac{m}{\alpha}} T, \quad i = 1, 2, \ldots, N' - 1, \tag{4.14}$$

and the N' subintervals:

$$\sigma_0 = [0, t_1], \quad \sigma_i = (t_i, t_{i+1}],\ i = 1, 2, \ldots, N' - 1, \tag{4.15}$$

with lengths $\tau_i = t_{i+1} - t_i$, $i = 0, 1, \ldots, N' - 1$. Let us define the maximum value of τ_i as $\tau = \max\{\tau_i,\ i = 0, 1, \ldots, N' - 1\}$.
Note that the integer i_0 satisfies the condition

$$N^{1-\alpha/m} \leq i_0 \leq N(N-1)^{-\alpha/m},$$

and from this inequality we can prove that there exists a positive constant c such that

$$\tau_i \leq c(i + i_0 - 2)^{\frac{m-\alpha}{\alpha}} N^{-\frac{m}{\alpha}} \leq cN^{-1}. \tag{4.16}$$

Taking Lemma 4.2.1 into account, if near the origin we approximate the solution of (4.12)-(4.13) with a function spanned by elements of space V_m^α, then it will reflect the potential nonsmooth properties of the solution near the singularity. Therefore, we define the space

$$S_\tau^m\left([0,T]\right)=\left\{u\in C([0,T]):\ u\big|_{\sigma_0}\in V_m^\alpha\big|_{\sigma_0},\ \ u\big|_{\sigma_l}\in\mathcal{P}_{m-1}\big|_{\sigma_l},\ l=1,2,\ldots,N'-1\right\},$$

where $\mathcal{P}_{m-1}$ is the space of polynomials of degree less than or equal to $m-1$ and σ_i, $i=0,1,....,N'-1$, are defined by (4.15).
The idea of the method is to approximate the solution of (4.12)-(4.13) by a function v such that $v\in S_\tau^m$. In order to define v we proceed as follows.
On the first interval of the partition, σ_0, we define ℓ collocation points $t_{0j}=c_j\tau_0,\ \ j=1,\ldots,\ell,\ c_j\in[0,1]$, and on the remaining intervals σ_l, $l=1,\ldots,N'-1$, we consider m collocation points $t_{lj}=t_l+c_j\tau_l,\ \ j=1,\ldots,m,\ c_j\in[0,1]$.

Noting that each equation of system (4.12) can be written as

$$y_i(t)=y_{0i}+\frac{1}{\Gamma(\alpha)}\int_0^t(t-s)^{\alpha-1}\left(\sum_{k=1}^n a_{ik}y_k(s)+f_i(s)\right)\,ds,\tag{4.17}$$

we will then seek for a function $v=[v_1\ v_2\ldots v_n]^T$ such that $v_i\in S_\tau^m\left([0,T]\right)$, $i=1,2,\ldots,n$, that satisfies

$$\begin{aligned}v_i(t_{0j}) &= y_{0i}+\frac{1}{\Gamma(\alpha)}\int_0^{t_{0j}}(t_{0j}-s)^{\alpha-1}\left(\sum_{k=1}^n a_{ik}v_k(s)+f_i(s)\right)\,ds, &(4.18)\\ &\quad j=1,\ldots,\ell,\\ v_i(t_{pj}) &= y_0+\frac{1}{\Gamma(\alpha)}\int_0^{t_{pj}}(t_{pj}-s)^{\alpha-1}\left(\sum_{k=1}^n a_{ik}v_k(s)+f_i(s)\right)\,ds, &(4.19)\\ &\quad p=1,\ldots,N'-1,\ j=1,\ldots,m.\end{aligned}$$

In order to obtain approximations for each $v_i(t_{0j})$, $i=1,\ldots,n$, $j=1,\ldots,\ell$, we define the Lagrange functions, $\mathcal{L}_{0j}\big|_{\sigma_0}\in\mathcal{V}_m^\alpha\big|_{\sigma_0},\ j=1,\ldots,\ell$, such that

$$\mathcal{L}_{0j}(t_{0k})=\delta_{jk},\ k=1,\ldots,\ell.\tag{4.20}$$

Then, we can write

$$\mathcal{L}_{0j}(t)=\sum_{i=1}^{\ell}\beta_{ji}t^{\nu_i},$$

where, for each $j=1,\ldots,\ell$, the coefficients β_{ji} may be obtained by solving the linear system (4.20).
It will be convenient to introduce the following projection operator
$P_\tau:C([0,T])\to\mathcal{V}_m^\alpha\big|_{\sigma_0}$, defined by (see [80]):

$$\left(P_\tau g\right)(s)=\sum_{k=1}^{\ell}\mathcal{L}_{0k}(s)g(t_{0k}),\quad s\in\sigma_0=[0,\tau_0].$$

Hence, for $t \in \sigma_0$, we use the following representation for $v_i \in \mathcal{V}_m^\alpha\big|_{\sigma_0}$, $i = 1, \ldots, n$:

$$v_i(t) = \sum_{k=1}^{\ell} v_i(t_{0k}) \mathcal{L}_{0k}(t). \tag{4.21}$$

On the remaining subintervals of the partition, σ_j, $j = 1, \ldots, N' - 1$, each y_i will be approximated by $v_i \in \mathcal{P}_{m-1}$:

$$v_i(t) = \sum_{\gamma=1}^{m} L_{j\gamma}(t) v_i(t_{j\gamma}), \quad t \in \sigma_j, \tag{4.22}$$

where $L_{j\gamma}$, $j = 1, \ldots, N'-1$, $\gamma = 1, \ldots, m$, are the Lagrange polynomials associated with the collocations points $t_{j\gamma} = t_j + \tau_j c_\gamma$, defined by

$$L_{j\gamma}(t) = \prod_{\substack{p=1 \\ p \neq \gamma}}^{m} \frac{t - t_{jp}}{t_{j\gamma} - t_{jp}}. \tag{4.23}$$

We also define the operators $P_j : C([0,T]) \to \mathcal{P}_{m-1}$ by

$$\left(P_j g\right)(s) = \sum_{\gamma=1}^{m} L_{j\gamma} g\left(t_{j\gamma}\right), \quad s \in \tau_j,\ j = 1, ..., N' - 1. \tag{4.24}$$

The values $v_i(t_{0k})$, $k = 1, ...\ell$ and $v_i(t_{lk})$, $l = 1, ...N'-1$, $k = 1, ..., m$, with $i = 1, \ldots, n$, are obtained by imposing that the functions $v_i(t)$ at the collocation points satisfy the integral equations:

$$\begin{aligned}
v_i(t_{0j}) &= y_{0i} + \frac{1}{\Gamma(\alpha)} \int_0^{t_{0j}} (t_{0j} - s)^{\alpha-1} \left(\sum_{p=1}^{n} a_{ip} \sum_{\gamma=1}^{\ell} v_p(t_{0\gamma}) \mathcal{L}_{0\gamma}(s) + f_i(s) \right) ds, \\
& j = 1, \ldots \ell,
\end{aligned}$$

$$\begin{aligned}
v_i(t_{lk}) &= y_{0i} + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_{lk} - s)^{\alpha-1} \left(\sum_{p=1}^{n} a_{ip} \sum_{\gamma=1}^{\ell} v_p(t_{0\gamma}) \mathcal{L}_{0\gamma}(s) \right) ds \\
&+ \frac{1}{\Gamma(\alpha)} \sum_{j=1}^{l-1} \int_{t_j}^{t_{j+1}} (t_{lk} - s)^{\alpha-1} \left(\sum_{p=1}^{n} a_{ip} \sum_{\gamma=1}^{m} L_{j\gamma}(s) v_p(t_{j\gamma}) \right) ds \\
&+ \frac{1}{\Gamma(\alpha)} \int_{t_l}^{t_{lk}} (t_{lk} - s)^{\alpha-1} \left(\sum_{p=1}^{n} a_{ip} \sum_{\gamma=1}^{m} L_{l\gamma}^{(k)}(s) v_p(t_l + \tau c_k c_\gamma) \right) ds, \\
&+ \frac{1}{\Gamma(\alpha)} \int_0^{t_{lk}} (t_{lk} - s)^{\alpha-1} f_i(s) ds, \\
& \quad l = 1, \ldots, N' - 1,\ k = 1, \ldots, m,
\end{aligned} \tag{4.25}$$

where $L_{l\gamma}^{(k)}$, $l = 1, \ldots, N' - 1$, $\gamma = 1, \ldots, m$, are the Lagrange polynomials associated with the points $t_l + \tau_l c_\gamma c_k$ defined similarly to (4.23).

After solving (4.25) and (4.25), the approximate solution of system (4.12)-(4.13), $v = [v_i]_{i=1}^n$ is given by:

$$v_i(t) = \begin{cases} \sum_{k=1}^{\ell} v_i(t_{0k})\mathcal{L}_{0k}(t), & t \in \sigma_0, \\ \sum_{k=1}^{m} v_i(t_{jk})L_{jk}(t), & t \in \sigma_j,\ j = 1, \ldots, N' - 1. \end{cases} \tag{4.26}$$

4.3.2.1 Convergence Analysis

In what follows, we present the convergence analysis of the hybrid method presented for ordinary fractional order systems. In order to do that, we first introduce some notation and some useful lemmas.
For each vector x, and matrix A, we denote

$$\|x\| = \|x\|_\infty = \max_i \{|x_i|\}, \quad \|A\| = \|A\|_\infty = \max_i \left\{ \sum_j |a_{ij}| \right\}$$

and for $f \in C([a,b])$ we define the maximum norm of a continuous function defined by $\|f\|_{[a,b]} = \max_{t\in[a,b]} |f(t)|$.

In the convergence analysis we shall need an auxiliary lemma from [80].

Theorem 4.3.2 *Let $\mathcal{L}_{0k}$, $k = 1, ..., \ell$, be the Lagrange functions defined by (4.20) and $\sigma_0 = [0, t_1]$. There exists a positive constant Δ_0 such that*

$$\|\mathcal{L}_{0k}\|_{\sigma_0} \leq \Delta_0, \quad k = 1, \ldots, \ell. \tag{4.27}$$

Furthermore, given $m \in \mathbb{N}$ and $f(t) = f_1(t) + f_2(t)$, where $f_1 \in C^m([0,T])$ and $f_2 \in V_m^\alpha$, we have

$$\|f - P_\tau f\|_{\sigma_0} \leq \bar{c}\tau_0^m \left\| f_1^{(m)} \right\|_{\sigma_0}, \tag{4.28}$$

for some positive constant $\bar{c}$.

We now provide an estimate for the error at the first subinterval of the mesh. For each $j = 1, \ldots, \ell$, we analyse the error at the collocation points t_{0j}:

$$e_{0j} = \left[e_{0j}^1\, e_{0j}^2\, \ldots\, e_{0j}^n\right]^T,$$

where $e_{0j}^i = y_i(t_{0j}) - v_i(t_{0j}),\ i = 1, 2, \ldots, n.$

Lemma 4.3.1 *Let $y = [y_k]_{k=1}^n$ be the solution of (4.12)-(4.13), and $v = [v_k]_{k=1}^n$ the approximate solution obtained by the hybrid collocation method and defined by (4.26). On the subinterval σ_0, we have*

$$\max_{1\leq k\leq n} \|y_k - v_k\|_{\sigma_0} \leq CN^{-m}, \tag{4.29}$$

where C is a positive constant that does not depend on N.

Proof 4.3.1 *Taking (4.17) and (4.18) into account, we have, for $i = 1, \ldots, n$ and $j = 1, \ldots, l$,*

$$\begin{aligned}\left|e_{0j}^{i}\right| = |y_i(t_{0j}) - v_i(t_{0,j})| &\leq \frac{1}{\Gamma(\alpha)} \int_0^{t_{0j}} (t_{0j} - s)^{\alpha-1} \sum_{k=1}^{n} |a_{ik}| \, |y_k(s) - v_k(s)| \; ds \\ &\leq \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{n} |a_{ik}| \, \|y_k - v_k\|_{\sigma_0} \int_0^{t_{0j}} (t_{0j} - s)^{\alpha-1} \; ds \\ &\leq \frac{t_{0j}^{\alpha}}{\Gamma(\alpha+1)} \sum_{k=1}^{n} |a_{ik}| \, \|y_k - v_k\|_{\sigma_0} \end{aligned} \tag{4.30}$$

Let us now analyse $\|y_k - v_k\|_{\sigma_0}$, $k = 1, \ldots, n$. First, note that

$$\|y_k - v_k\|_{\sigma_0} \leq \|y_k - P_\tau y_k\|_{\sigma_0} + \|P_\tau y_k - v_k\|_{\sigma_0} \, . \tag{4.31}$$

Because we are assuming that y_k, $k = 1, \ldots, n$, is of the form $y_k(t) = y_k^{(1)}(t) + y_k^{(2)}(t)$, where $y_k^{(1)}(t) \in C^{(m)}([0, T])$ and $y_k^{(2)}(t) \in \mathcal{V}_m^{\alpha}$, from Theorem 4.3.2 we obtain

$$\|y_k - P_\tau y_k\|_{\sigma_0} \leq c_1 \tau_0^m \left\| \frac{d^m}{dt^m} y_k^{(1)} \right\|_{\sigma_0} . \tag{4.32}$$

On the other hand, since $v_k \in \mathcal{V}_m^{\alpha}$, then $v_k = P_\tau v_k$, and therefore, from Theorem 4.3.2, we have

$$\begin{aligned}\|P_\tau y_k - v_k\|_{\sigma_0} &\leq \max_{j=1,\ldots,\ell} \|\mathcal{L}_{0j}\|_{\sigma_0} \sum_{j=1}^{\ell} |y_k(t_{0j}) - v_k(t_{0j})| \\ &\leq \Delta_0 \sum_{j=1}^{\ell} |y_k(t_{0j}) - v_k(t_{0j})| \, , \end{aligned} \tag{4.33}$$

with Δ_0 given by (4.27). Using (4.33) and (4.32) in (4.31), we obtain

$$\|y_k - v_k\|_{\sigma_0} \leq c_1 \tau_0^m C_d + \Delta_0 \sum_{j=1}^{\ell} |y_k(t_{0j}) - v_k(t_{0j})| \, , \quad k = 1, ..., n, \tag{4.34}$$

where C_d is a positive constant defined by $C_d = \max\limits_{1 \leq k \leq n} \left\| \frac{d^m}{dt^m} y_k^{(1)} \right\|_{\sigma_0}$.
Substituting in (4.30), we have, for $i = 1, \ldots, n$ and $j = 1, \ldots, \ell$,

$$\left|e_{0j}^{i}\right| \leq \frac{t_{0j}^{\alpha}}{\Gamma(\alpha+1)} \left(c_1 C_d \tau_0^m \sum_{k=1}^{n} |a_{ik}| + \Delta_0 \sum_{k=1}^{n} |a_{ik}| \sum_{j=1}^{\ell} \left|e_{0j}^{k}\right| \right) .$$

Then, from the last inequality and from the fact that $\tau_0 \leq cN^{-1}$, where c is a positive constant that does not depend on N (see [80]), we have

$$\max_{1 \leq i \leq n} \left|e_{0j}^{i}\right| \leq C_1 N^{-m} + C_2 \sum_{j=1}^{\ell} \max_{1 \leq k \leq n} \left|e_{0j}^{k}\right| ,$$

where C_1 and C_2 are positive constants does not depend on N. Hence it follows

$$\max_{1\le j\le \ell}\max_{1\le i\le n}\left|e^i_{0j}\right| \le C_1 N^{-m} + C_3 \max_{1\le j\le \ell}\max_{1\le k\le n}\left|e^k_{0j}\right|,$$

where $C_3 = \ell C_2$.

Hence, for sufficiently large N, there exists a positive constant C_4 such that

$$\max_{1\le j\le \ell}\max_{1\le i\le n}\left|e^i_{0j}\right| \le C_4 N^{-m},$$

and therefore, from (4.34) we thus obtain

$$\max_{1\le k\le n}\|y_k - v_k\|_{\sigma_0} \le C_5\, N^{-m},$$

where C_5 is a positive constant does not depend on N, and the result is proved .

Let us now analyse the error at the remaining subintervals of the mesh.

For each $j = 1, \ldots, m$ and $k = 1, \ldots, N' - 1$, we analyse the error at the collocation points t_{kj}:

$$e_{kj} = \left[e^1_{kj}\, e^2_{kj}\, \ldots\, e^n_{kj}\right]^T,$$

where $e^i_{kj} = y_i(t_{kj}) - v_i(t_{kj}),\ i = 1, 2, \ldots, n.$

Lemma 4.3.2 *Let $y = [y_k]_{k=1}^n$ be the solution of (4.12)-(4.13), and $v = [v_k]_{k=1}^n$ the approximate solution obtained by the hybrid collocation method and defined by (4.26). On the subinterval σ_k, $k = 1, \ldots, N' - 1$, we have*

$$\max_{1\le i\le n}\|y_i - v_i\|_{\sigma_k} \le CN^{-m}, \tag{4.35}$$

where C is a positive constant that does not depend on N.

Proof 4.3.2 *From (4.17) and (4.19) we have, for $j = 1, \ldots, m$ and $k = 1, \ldots, N' - 1$:*

$$\begin{aligned} e^i_{kj} &= y_i(t_{kj}) - v_i(t_{kj}) = \frac{1}{\Gamma(\alpha)}\int_0^{t_1}(t_{kj}-s)^{\alpha-1}\sum_{l=1}^n a_{il}\left(y_l(s) - v_l(s)\right)\, ds \\ &+ \frac{1}{\Gamma(\alpha)}\sum_{\gamma=1}^{k-1}\int_{t_\gamma}^{t_{\gamma+1}}(t_{kj}-s)^{\alpha-1}\sum_{l=1}^n a_{il}\left(y_l(s) - P_\gamma(y_l)(s) + P_\gamma(y_l)(s) - v_l(s)\right)\, ds + \\ &+ \frac{1}{\Gamma(\alpha)}\int_{t_k}^{t_{kj}}(t_{kj}-s)^{\alpha-1}\sum_{l=1}^n a_{il}\left(y_l(s) - P_k(y_l)(s) + P_k(y_l)(s) - v_l(s)\right)\, ds, \end{aligned}$$

where P_γ, $\gamma = 1, \ldots N' - 1$, is the interpolation operator defined by (4.24).
Since $\tau_i \le c\, N^{-1}$ (see (4.16)) we have, for $k = 1, \ldots, N' - 1$,

$$\int_{t_\gamma}^{t_{\gamma+1}}(t_{kj}-s)^{\alpha-1}ds \le \bar{c}\,\tau^\alpha(k-\gamma)^{\alpha-1} \le \bar{c}_1\, N^{-\alpha}(k-\gamma)^{\alpha-1}, \quad \gamma = 1, \ldots, k-1,$$

$$\int_{t_k}^{t_{kj}}(t_{kj}-s)^{\alpha-1}ds \le \bar{c}\,\tau^\alpha \le \bar{c}_1\, N^{-\alpha}, \quad j = 1, \ldots, m,$$

where $\bar{c}_1$ is a positive constant does not depend on N. On the other hand, since $v_l \in \mathcal{P}_{m-1}$ then

$P_\gamma(v_l)(s) = v_l(s),\ s \in \tau_\sigma, \quad \sigma = 1, ..., N' - 1$, *and hence for* $s \in \sigma_\gamma,\ \gamma = 1, 2, ..., N' - 1$ *we have*

$$P_\sigma(y_l)(s) - v_l(s) = \sum_{j=1}^{m} L_{\gamma j}(s) \left(y_l(t_{\gamma j}) - y_l(t_{\gamma j}) \right),\ \sigma = 1, ..., N' - 1.$$

Then, taking modulus and using the above bounds we obtain

$$\begin{aligned}
\left| e_{kj}^i \right| &\leq \frac{1}{\Gamma(\alpha)} \sum_{l=1}^{n} |a_{il}| \left\| y_l - v_l \right\|_{\sigma_0} \int_0^{t_1} (t_{kj} - s)^{\alpha-1} ds \\
&+ \frac{1}{\Gamma(\alpha)} \sum_{l=1}^{n} |a_{il}| \sum_{\gamma=1}^{k-1} \left\| y_l - P_\gamma(y_l) \right\|_{\sigma_\gamma} \int_{t_\gamma}^{t_{\gamma+1}} (t_{kj} - s)^{\alpha-1} ds \\
&+ \frac{1}{\Gamma(\alpha)} \sum_{l=1}^{n} |a_{il}| \left\| y_l - P_k(y_l) \right\|_{\sigma_k} \int_{t_k}^{t_{kj}} (t_{kj} - s)^{\alpha-1} ds \\
&+ \frac{m \Delta_m \bar{c}_1}{\Gamma(\alpha)} N^{-\alpha} \sum_{l=1}^{n} |a_{il}| \sum_{\gamma=1}^{k-1} (k - \gamma)^{\alpha-1} \max_{p=1,...,m} \left| e_{\gamma p}^l \right| \\
&+ \frac{m \Delta_m \tau^\alpha}{\Gamma(\alpha + 1)} \sum_{l=1}^{n} |a_{il}| \max_{p=1,...,m} \left| e_{kp}^l \right|, \qquad (4.36)
\end{aligned}$$

where Δ_m *is the Lebesgue constant associated with the collocation parameters* $c_1, ..., c_m$.

From Theorem 4.3.2 follows $\left\| y_l - v_l \right\|_{\sigma_0} \leq C\, N^{-m}$, $l = 1, \ldots, n$. *Let us now investigate what happens with* $\left\| y_l - P_\gamma(y_l) \right\|_{\sigma_\gamma}$, $l = 1, \ldots, n$, $\gamma = 1, \ldots, N' - 1$.

From the classical interpolation theory and because, as mentioned earlier, $\tau_i \leq c\, N^{-1}$, $i = 1, \ldots, N' - 1$, *we have*

$$\begin{aligned}
\left\| y_l - P_\gamma(y_l) \right\|_{\sigma_\gamma} \leq d_1 \tau_\gamma^m \max_{t \in \sigma_\gamma} \left| \frac{d^m y}{dt^m}(t) \right| \leq d_2 \tau_\gamma^m \max_{t \in \sigma_\gamma} \left| t^{\alpha-m} \right| \leq d_2 \tau_\gamma^m t_\gamma^{\alpha-m} \\
= d_2 \tau_\gamma^m \left(\frac{i_0 + \gamma - 1}{N} \right)^{\frac{m}{\alpha}(\alpha-m)}, \qquad (4.37)
\end{aligned}$$

where we have also used the argument in [199] that says that if a certain function f *for which* $f(t) = f_1(t) + f_2(t)$, *where* $f_1 \in C^m([0, T])$ *and* $f_2 \in V_m^\alpha$, *then* $\left| f^{(m)}(t) \right| \leq c\, t^{\alpha-m}$ *for* $t \geq t_1$.

Using estimate (4.16) stating that $\tau_i \leq c\, (i + i_0 - 2)^{\frac{m}{\alpha}-1} N^{-\frac{m}{\alpha}}$, *we easily achieve the estimate*

$$\left\| y_l - P_\gamma(y_l) \right\|_{\sigma_\gamma} \leq \bar{c}_2\, N^{-m},\ \gamma = 1, ..., N' - 1, \qquad (4.38)$$

for some positive constant $\bar{c}_2$ *that does not depend on* N.

Using the results (4.3.1) and (4.38) in (4.36), for N *sufficiently large,follows*

$$\max_{i=1,...,n} \max_{p=1,...,m} \left| e_{kp}^i \right| \leq \bar{C}_2 N^{-m} + \bar{C}_3 N^{-\alpha} \sum_{\gamma=1}^{k-1} (k - \gamma)^{\alpha-1} \max_{i=1,...,n} \max_{p=1,...,m} \left| e_{\gamma p}^l \right|, \qquad (4.39)$$

where $\bar{C}_2$ *and* $\bar{C}_3$ *are positive constants. Applying a standard weakly singular discrete Gronwall inequality, leads to the following result*

$$\max_{i=1,...,n} \max_{p=1,...,m} \left| e_{kp}^i \right| \leq \bar{C}_4\, N^{-m}. \qquad (4.40)$$

On the other hand, using the interpolation error (4.38) and definition of the interpolation operator P_γ we obtain, for $\gamma = 1, \ldots, N' - 1$,

$$\max_{k=1,\ldots,n} \|y_k - v_k\|_{\sigma_\gamma} \leq \bar{c}_2 N^{-m} + m\Delta_m \max_{k=1,\ldots,n} \max_{j=1,\ldots,m} \left| e^k_{\gamma j} \right|, \tag{4.41}$$

and therefore, from (4.40) we thus obtain for $k = 1, \ldots, n$

$$\|y_k - v_k\|_{\sigma_\gamma} \leq \bar{C}_5 N^{-m},\ \gamma = 1, ..., N', \tag{4.42}$$

where $\bar{C}_5$ is a positive constant does not depend on N, and the result is proved.

4.3.2.2 Numerical Results

In order to illustrate the feasibility of the method, some examples for which the analytical solution is known are presented together with a comparison with the hereafter designated by nonpolynomial method.
The numerical error is measured by determining the maximum error at the mesh points t_j:

$$\varepsilon_\tau = \max_{i=1,\ldots,n} \max_{p=1,\ldots,N'} |y_i(t_p) - v_i(t_p)| \tag{4.43}$$

where v_i is the approximate solution, for the i-th spatial function, obtained by the hybrid method.

Example 4.3.1

$$\begin{cases} D^{\frac{1}{2}} y(t) = \frac{1}{2} y(t), \quad t > 0 \\ y(0) = 1. \end{cases}$$

whose analytical solution is $y(t) = E_{1/2}(0.5\sqrt{t})$, and

Example 4.3.2

$$\begin{cases} D^\alpha y_1(t) = y_2(t) \\ D^\alpha y_2(t) = -y_1(t) - y_2(t) + t^{\alpha+1} + \frac{\pi \csc(\pi\alpha) t^{1-\alpha}}{\Gamma(-\alpha-1)\Gamma(2-\alpha)} + \frac{\pi t \csc(\pi\alpha)}{\Gamma(-\alpha-1)}, \end{cases} \tag{4.44}$$

$y_1(0) = 0$, $y_2(0) = 0$. *The analytical solution is given by $y_1(t) = t^{1+\alpha}$ and $y_2(t) = \pi\alpha(\alpha + 1)t \csc(\pi\alpha)/\Gamma(1-\alpha)$.*

For the numerical solution of example 1 we consider the spaces $\mathcal{V}_2^\alpha$, $\mathcal{V}_3^\alpha$, $\mathcal{V}_4^\alpha$, $\mathcal{V}_5^\alpha$, $\mathcal{V}_6^\alpha$. From Table 4.10 we observe that the nonpolynomial method provides a better convergence rate for smaller stepsizes, but, the speed-up (SU - ratio between the nonpolynomial and hybrid computational times) obtained with the hybrid method is really high (upt to 450x). Note also that the maximum and minimum condition number of the matrices involved ($\kappa(A) = \|A\|_\infty \left\|A^{-1}\right\|_\infty$) obtained for each simulation show that the hybrid method provides better conditioned matrices. Although the $\kappa(A)_{max}$ looks similar for both methods, it should be remarked that right after the first time-step we obtain the value of $\kappa(A)_{min}$ for the hybrid method, while for the nonpolynomial method the $\kappa(A)$ is slowly decreasing along time-steps. For $m = 4$ it was impossible to obtain convergence for certain values of N in the nonpolynomial method. The number of significant digits lost along the iterative procedure lead to badly conditioned matrices. For the hybrid method that problem could be solved by increasing the number of significant digits.

Table 4.1: Hybrid and nonpolynomial collocation methods for example 4.3.1 with three different values of m: values of the maximum of the absolute errors at the mesh points, the experimental orders of convergence p and speed-up (SU).

Stepsizes		hybrid($m=2$)					nonpolynomial($m=2$)			
N	N'	ε_τ	p	SU	$\kappa(A)_{min}$	$\kappa(A)_{max}$	ε_τ	p	$\kappa(A)_{min}$	$\kappa(A)_{max}$
10	5	$1.47 \cdot 10^{-3}$	–	10.2	1.19	16.9	$5.70 \cdot 10^{-5}$	-	4.92	26.87
20	11	$4.45 \cdot 10^{-4}$	1.72	52.5	1.09	9.58	$1.42 \cdot 10^{-5}$	2.00	3.56	16.84
40	25	$1.21 \cdot 10^{-4}$	1.88	114.9	1.04	5.33	$3.56 \cdot 10^{-6}$	2.00	2.70	10.71
80	54	$3.15 \cdot 10^{-5}$	1.94	175.7	1.02	3.69	$8.90 \cdot 10^{-7}$	2.00	2.14	7.01
160	116	$8.05 \cdot 10^{-6}$	1.97	156.5	1.01	2.67	$2.23 \cdot 10^{-7}$	2.00	1.78	4.78
Stepsizes		hybrid($m=3$)					nonpolynomial($m=3$)			
N	N'	ε_τ	p	SU	$\kappa(A)_{min}$	$\kappa(A)_{max}$	ε_τ	p	$\kappa(A)_{min}$	$\kappa(A)_{max}$
10	4	$5.01 \cdot 10^{-4}$	–	39.9	1.47	135.5	$1.50 \cdot 10^{-9}$	-	3.36	115.52
20	8	$7.65 \cdot 10^{-5}$	2.71	270.3	1.23	88.04	$1.50 \cdot 10^{-10}$	3.33	2.44	59.97
40	19	$1.05 \cdot 10^{-5}$	2.86	363.0	1.10	35.42	$1.60 \cdot 10^{-11}$	3.23	1.93	32.45
80	42	$1.39 \cdot 10^{-6}$	2.92	450.7	1.05	19.43	$1.80 \cdot 10^{-12}$	3.16	1.62	18.37
160	92	$1.78 \cdot 10^{-7}$	2.96	406.4	1.02	11.15	$2.07 \cdot 10^{-13}$	3.12	1.42	10.93
Stepsizes		hybrid($m=4$)					nonpolynomial($m=4$)			
N	N'	ε_τ	p	SU	$\kappa(A)_{min}$	$\kappa(A)_{max}$	ε_τ	p	$\kappa(A)_{min}$	$\kappa(A)_{max}$
10	3	$2.23 \cdot 10^{-4}$	–	67.0	2.14	426.1	$3.83 \cdot 10^{-13}$	-	1.48	253.57
20	7	$1.77 \cdot 10^{-5}$	3.65	122.2	1.38	148.5	$1.64 \cdot 10^{-14}$	4.54	1.31	129.68
40	15	$1.23 \cdot 10^{-6}$	3.84	-	1.18	85.18	–	-	–	–
80	34	$8.14 \cdot 10^{-8}$	3.92	-	1.08	41.44	–	-	–	–
160	76	$5.23 \cdot 10^{-9}$	3.96	-	1.04	21.26	–	-	–	–

Table 4.2: Hybrid collocation method for example 4.3.1 with two different values of m: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p.

Stepsizes		hybrid($m=5$)			
N	N'	ε_τ	p	$\kappa(A)_{min}$	$\kappa(A)_{max}$
10	3	$2.13 \cdot 10^{-5}$	–	3.35	$1.05 \cdot 10^{6}$
20	6	$8.51 \cdot 10^{-7}$	4.65	1.85	$5.36 \cdot 10^{5}$
40	13	$2.96 \cdot 10^{-8}$	4.85	1.37	$2.63 \cdot 10^{5}$
80	29	$9.78 \cdot 10^{-10}$	4.92	1.17	$1.23 \cdot 10^{5}$
160	64	$3.16 \cdot 10^{-11}$	4.95	1.08	$6.10 \cdot 10^{4}$

Stepsizes		hybrid($m=6$)			
N	N'	ε_τ	p	$\kappa(A)_{min}$	$\kappa(A)_{max}$
10	2	$1.38 \cdot 10^{-5}$	–	128.46	$4.81 \cdot 10^{8}$
20	5	$3.72 \cdot 10^{-7}$	5.21	14.95	$1.07 \cdot 10^{8}$
40	11	$6.66 \cdot 10^{-9}$	5.80	2.48	$4.79 \cdot 10^{7}$
80	25	$1.16 \cdot 10^{-10}$	5.84	1.63	$2.05 \cdot 10^{7}$

We were able to perform computations up to $m = 6$ by using the hybrid method. The simulations were fast and the new method proved to be robust.

Next we consider the second example where a systems of equations is considered.

The numerical method was used to solve Example 2 with $m = 4$ by considering $\alpha = 1/4, 1/2, 2/3$. The error and the experimental convergence order are listed in table 4.3. As expected we have obtained an optimal convergence order that is independent of α.

We obtained speed-ups that go up to 173x. Note that SU is not provided for the case $\alpha = 1/4$ because the simulation time for the nonpolynomial method became really high.

Now that we have shown the feasibility of using the hybrid method for the solution of systems of ordinary fractional differential equations, we will analise its application to time-fractional diffusion equations.

Table 4.3: Error, speed-up (SU) and convergence order (p) obtained for the numerical solution of Example 4.3.2 [197] using the Hybrid and nonpolynomial collocation methods, for $\alpha = 1/4, 1/2, 2/3$.

Stepsizes	hybrid($\alpha = 1/4$)			hybrid($\alpha = 1/2$)				hybrid($\alpha = 2/3$)			
N	N'	ε_τ	p	N'	ε_τ	p	SU	N'	ε_τ	p	SU
64	15	$2.11 \cdot 10^{-6}$	3.70	26	$1.94 \cdot 10^{-7}$	3.86	56.6	32	$5.53 \cdot 10^{-8}$	3.90	142.2
128	34	$1.45 \cdot 10^{-7}$	3.86	59	$1.27 \cdot 10^{-8}$	3.93	51.0	71	$3.58 \cdot 10^{-9}$	3.95	162.4
256	75	$9.43 \cdot 10^{-9}$	3.94	128	$8.13 \cdot 10^{-10}$	3.97	52.2	155	$2.28 \cdot 10^{-10}$	3.97	170.2
512	166	$6.00 \cdot 10^{-10}$	3.97	278	$5.14 \cdot 10^{-11}$	3.98	60.0	331	$1.44 \cdot 10^{-11}$	3.99	173.4

4.4 Fractional Partial Differential Equations: the Time-Fractional Diffusion Equation

In this Section we propose a numerical method for the solution of the Time-Fractional diffusion equation given by:

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = D_\alpha \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \quad t > 0, \;\; 0 \leq x \leq L, \tag{4.45}$$

with initial condition:

$$u(x,0) = g(x), \tag{4.46}$$

and boundary conditions:

$$u(0,t) = u_0, \;\; u(L,t) = u_L, \tag{4.47}$$

where we assume that D_α, u_0 and u_L are constants, the order of the fractional derivative satisfies $0 < \alpha < 1$, and the fractional derivative is again given in the Caputo sense, that is:

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial u(x,s)}{\partial s} \, ds.$$

The recently published book [200], contains a survey of numerical methods for partial differential equations, where the time fractional diffusion equation is included. Even so, there is still a lack of highly accurate numerical methods for the time fractional diffusion equation when compared to other kinds of equation, motivating us to contribute to this field. In this work we derive a method that was developed in the work *L.L. Ferrás, N.J. Ford, M.L. Morgado, M. Rebelo, A Numerical Method for the Solution of the Time-Fractional Diffusion Equation. B. Murgante et al. (Eds.): ICCSA 2014, Part I, Lecture Notes in Computer Science 8579 (2014) 117–131* and that can deal with potential singularities of the solution and also allows fast computations.

The method is similar to the nonpolynomial method shown before, with the main difference being the use of the method of lines for the numerical approximation of (4.45). The method of lines (MOL) is a widely known and standard computational approach for solving time-dependent partial differential equations (PDEs), that proceeds in two separate steps: first, spatial derivatives are approximated using, for instance, finite difference (FD) or finite element (FE) techniques. Second, the resulting system of semi-discrete ordinary differential equations (ODEs) in the initial value variable is integrated in time, t. For the integration in time t, we will use here the recent nonpolynomial collocation method proposed in [83].

The method is later extended to deal with graded meshes and we also consider an hybrid version where near the singularity the non-polynomial method is used and *far* from the singularity we assume the solution can be written as a combination of polynomials.

4.4.1 A Nonpolynomial Collocation Method for the Solution of the Time-Fractional Diffusion Equation

In this section we describe the numerical method for the approximation of the solution of (4.45), (4.46), (4.47). Although throughout the text we will always assume the existence and uniqueness of the solution, these matters will not be addressed here. For the interested reader we refer to the papers [142; 143], and the references therein.
As is usual in the method of lines, we first approximate the space derivative. In order to do that we consider a uniform space mesh on the interval $[0, L]$, defined by the gridpoints $x_i = i\Delta x$, $i = 0, \ldots, n$, where $\Delta x = \dfrac{L}{n}$, and we approximate the space derivative by the second order finite difference:

$$\frac{\partial^2 u(x_i,t)}{\partial x^2} \approx \frac{u(x_{i+1},t) - 2u(x_i,t) + u(x_{i-1},t)}{(\Delta x)^2}, \quad i = 1, \ldots, n-1. \tag{4.48}$$

Substituting in (4.45), and denoting by $y_i(t) \approx u(x_i, t)$, we obtain the following system of $n-1$ ODEs:

$$\frac{\partial^\alpha y_i(t)}{\partial t^\alpha} = D\frac{y_{i+1}(t) - 2y_i(t) + y_{i-1}(t)}{(\Delta x)^2} + f(x_i,t), \quad i = 1, \ldots, n-1. \tag{4.49}$$

Note that from the boundary conditions (4.47), we have $y_0(t) = u_0$, $y_n(t) = u_L$ and from the initial condition (4.46), we obtain:

$$y_i(0) = g(x_i), \;\; i = 1, \ldots, n-1, \tag{4.50}$$

and therefore, the solution of the $n-1$ initial value problems (4.49)-(4.50) may be determined by using any initial value problem solver. Here we will use the nonpolynomial collocation method recently proposed in [83], that may be outlined, in this case, as follows. For each $n \in \mathbf{N}$ and $t \geq 0$ we define

$$\mathbf{y}(t) = [y_0(t)\; y_1(t)\; y_2(t)\; \ldots\; y_{n-1}(t)\; y_n(t)] = [u_0\; y_1(t)\; y_2(t)\; \ldots\; y_{n-1}(t)\; u_L]\,.$$

Thus, the system (4.49), (4.50) can be rewritten as follows

$$\begin{cases} \dfrac{\partial^\alpha y_i(t)}{\partial t^\alpha} = F_i(t, \mathbf{y}(t)), \quad i = 1, \ldots, n-1, \\ y_i(0) = g(x_i), \;\; i = 1, \ldots, n-1, \end{cases} \tag{4.51}$$

where each function F_i is defined by

$$F_i(t, \mathbf{y}(t)) = D\frac{y_{i+1}(t) - 2y_i(t) + y_{i-1}(t)}{(\Delta x)^2} + f(x_i,t),\; i = 1, \ldots, n-1. \tag{4.52}$$

Hence, we end up with a system of $(n-1)$ fractional ordinary differential equations to solve. In what follows we suppose that there exists a $T > 0$ such that the system (4.51) has a unique continuous solution $\mathbf{y}$ on the interval $[0, T]$.

Again, assuming that the functions $F_i(s, \mathbf{y}(s))$ are continuous on $[0, T]$, the system of equations (4.51) is equivalent to a system of Volterra integral equations of the second kind [60]:

$$y_i\,(t) = y_i(0) + \frac{1}{\Gamma(\alpha)}\int_0^t (t-s)^{\alpha-1} F_i(s, \mathbf{y}(s))ds, \quad i = 1, \ldots, n-1, \tag{4.53}$$

where $y_i(0) = g(x_i),\ i = 1, \ldots, n-1$.
We will use the non-polynomial collocation method, recently proposed in [83], to approximate the solution of (4.53) and, consequently, the solution of the system of ODEs (4.51).

Although the method was described in the first Section of this Chapter, we will now adapt the method to this type of system of equations, and therefore, some concepts will be repeated.

Again, the time interval, $[0, T]$, is then partitioned into N subintervals, $\sigma_0 = [0, t_0]$, $\sigma_i = (t_i, t_{i+1}],\ i = 1, \ldots, N-1$, of equal size h. On each subinterval σ_i we define ℓ collocation points $t_{ik} = t_i + c_k \Delta t$, $k = 1, .., \ell$, where the collocation parameters $c_k \in [0,\ 1]$. We seek a vector solution,

$$\mathbf{u}(t) = \left(u_1\left(x_1, t\right),\ u_2\left(x_2, t\right),\ ...,\ u_{n-1}\left(x_{n-1}, t\right)\right) \tag{4.54}$$

such that $u_j\left(x_j, t\right) \in V_{\tau,m}^{\alpha}\ (j = 1, .., n-1)$, which means

$$u_j\left(x_j, t\right) = \sum_{k=1}^{\ell} a_{ik}^{j} t^{\upsilon_k},\ t \in \sigma_i,\ i = 1, \ldots, n-1.$$

In order to compute the coefficients $\mathbf{a}_{ik} = [a_{ik}^1, \ldots, a_{ik}^n]$ we impose the condition that the function $\mathbf{u}(t)$ must satisfy the system (4.53) at the collocation points t_{ik}:

$$\begin{aligned} & u_j\left(x_j, t_{ik}\right) = y_j(0) + \frac{1}{\Gamma(\alpha)} \int_0^{t_{ik}} (t_{ik} - s)^{\alpha-1} F_j\left(s, \mathbf{u}\left(s\right)\right) ds, \\ & i = 0, 1,\ ...,\ N-1,\ k = 1, 2,\ ..., \ell,\ j = 1, 2,\ ...n-1. \end{aligned} \tag{4.55}$$

For each i we obtain an $\ell\left(n-1\right)$ system of equations. We consider an approximation of each function $F_j\left(s, u\left(s\right)\right)$ on the space $V_{\Delta t,m}^{\alpha}$ (a detailed explanation of this subject can be found in [83]). The approximation $\widehat{u} \in V_{\Delta t,m}^{\alpha}$ is such that

$$\begin{aligned} \hat{u}_j\left(t_{ik}\right) &= y_j\left(0\right) + \sum_{\varsigma=1}^{i-1} \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} w_{ik}^{\varsigma,p} \beta_{\gamma p}^{\varsigma} F_j\left(t_\varsigma + \Delta t c_\gamma, \hat{u}\left(t_\varsigma + \Delta t c_\gamma\right)\right) \\ &+ \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} w_{ik}^{i,p} \beta_{\gamma p}^{ik} F_j\left(t_i + \Delta t c_k c_\gamma, \hat{u}\left(t_i + \Delta t c_k c_\gamma\right)\right), \\ & j = 1, \ldots, n-1,\ i = 0, \ldots, N-1,\ k = 1, \ldots, \ell. \end{aligned} \tag{4.56}$$

where

$$\begin{aligned} w_{ik}^{\sigma,p} &= \frac{1}{\Gamma(\alpha)} \int_{t_j}^{t_{\sigma+1}} (t_{ik} - s)^{\alpha-1} s^{\nu_p} ds, \quad j < i, \\ w_{ik}^{i,p} &= \frac{1}{\Gamma(\alpha)} \int_{t_i}^{t_{ik}} (t_{ik} - s)^{\alpha-1} s^{\nu_p} ds,\ i = 0, 1, ..., N-1,\ k = 1, ..., \ell, \end{aligned}$$

and $\beta_{\gamma p}^{\varsigma},\ \beta_{\gamma p}^{ik}$ are defined as in [83]. A schematic of the resulting system of equations (when F_j is linear) is shown in Fig. 4.2.

After solving (4.56), that is, after having determined for each $j = 1, \ldots, n-1$, the coefficients $\hat{u}_j\left(t_{ik}\right)$, $i = 0, \ldots, N-1,\ k = 1, \ldots \ell$, each component of the solution $\mathbf{y}$ is approximated by

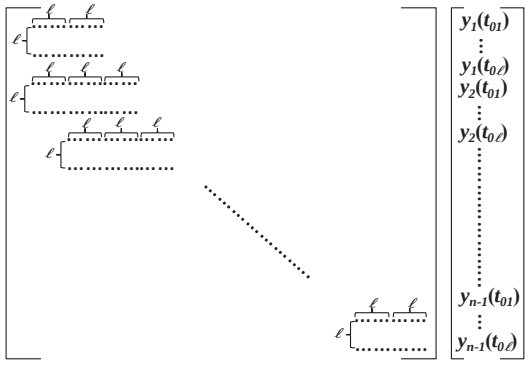


FIGURE 4.2: Schematic of the system of equations obtained for each subinterval σ_i (only non-zero entries are shown).

$$y_j(t) \approx \widehat{u}_j(t) = \sum_{k=1}^{\ell} y_{ik}^j \left(t_{ik}\right) L_{ik}\left(t\right), \quad t \in \sigma_i,\ i = 0, 1,\ ..., N-1,\ j = 1, \ldots, n-1, \tag{4.57}$$

where $y_{ik}^j = \widehat{u}_j\left(t_{ik}\right)$ and $L_{ik} \in V_m^\alpha$ are the Lagrange functions defined as in [83].

Before presenting some numerical results we remark the following: in [83] it was proved that the convergence order of the non-polynomial collocation method was m when a solution of a linear ordinary fractional differential equation of the type $D^\alpha y(t) = \beta y(t) + f(t)$ can be written as $y(t) = y_1(t) + y_2(t)$, $y_1 \in C^m([0,T])$ and $y_2 \in V_m^\alpha$.
In this work we need to solve a system of $(n-1)$ linear equations (see (4.51)), and we expect to obtain the same order m in time when working on V_m^α. Indeed, from Lemma 4.2.1, each component of the solution $\mathbf{y}$ may be written in the form $y_i(t) = y_i^1(t) + y_i^2(t)$, for a fixed integer m, $y_i^1 \in C^m([0,T])$ and $y_i^2 \in V_m^\alpha$.

4.4.1.1 Numerical Results

In order to illustrate the feasibility of the method, some examples for which the analytical solution is known are presented. The numerical error is measured by determining the maximum error at the mesh points (x_i, t_j):

$$\varepsilon_{\Delta x, \Delta t} = \max_{i=1,..,n,\, j=1,...,N} \left|u(x_i, t_j) - y_i\left(t_j\right)\right|,\ N = \frac{1}{\Delta t},\ n = \frac{L}{\Delta x} \tag{4.58}$$

where y_i is the numerical solution obtained for the i-th spatial function defined by (4.57). We consider two examples:

Example 4.4.1

$$\begin{cases} \dfrac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \dfrac{\partial^2 u(x,t)}{\partial x^2} + \dfrac{\Gamma(4+\alpha)}{6} x^4(2-x)t^3 - 4x^2(6-5x)t^{3+\alpha}, \quad t > 0,\ 0 \le x \le 2, \\ u(x,0) = 0, \\ u(0,t) = u(2,t) = 0. \end{cases}$$

whose analytical solution is $u(x,t) = x^4(2-x)t^{3+\alpha}$, *and*

Example 4.4.2

$$\begin{cases} \dfrac{\partial^{1/2}u(x,t)}{\partial t^{1/2}} = \dfrac{\partial^2 u(x,t)}{\partial x^2} + \dfrac{3\Gamma(1/2)}{4}tx^4(x-1) - 4x^2(5x-3)t^{3/2}, \quad t>0,\ 0\le x\le 1, \\ u(x,0)=0, \\ u(0,t)=u(1,t)=0, \end{cases}$$

whose analytical solution is nonsmooth at $t=0$ *and given by* $u(x,t)=x^4(x-1)t^{3/2}$.

We will use the method presented in the previous section with $m=1,2,3$ and we will compare the numerical results with the ones obtained with the method presented in [132].

4.4.1.2 Non-polynomial Collocation Method

In this subsection we present the numerical results obtained for these two examples on the spaces $V^{\alpha}_{1,\Delta t}$, $V^{\alpha}_{2,\Delta t}$ and $V^{\alpha}_{3,\Delta t}$.

The collocation parameters that we have used are listed below.

- For $\alpha=1/3$ we consider $c_1=0.15$, $c_2=0.3$, $c_3=0.4$, $c_4=0.5$, $c_5=0.7$, $c_6=0.85$ for $m=2$;
- For $\alpha=1/2$ we consider $c_1=0.25$, $c_2=0.5$ for $m=1$, $c_1=0.15$, $c_2=0.25$, $c_3=0.5$, $c_4=0.75$ for $m=2$ and $c_1=0.15$, $c_2=0.3$, $c_3=0.4$, $c_4=0.5$, $c_5=0.7$, $c_6=0.85$ for $m=3$;
- For $\alpha=2/3$ we consider $c_1=0.15$, $c_2=0.3$, $c_3=0.5$, $c_4=0.7$, $c_5=0.85$ for $m=2$;

For each case, the estimates for the time and space convergence orders were computed and denoted by p and q, respectively.

In table 4.9 we present the numerical results obtained, by the described method on the space V^{α}_{2}, for example 4.4.1 for three different values of the order of the time derivative, α. As expected we can determine $p\sim 2$ experimentally (not dependent on the order of the fractional derivative) and $q\sim 2$.

Table 4.4: Non-polynomial collocation method on the space V^{α}_{2} for example 4.4.1 with three different values of α: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p and q related with the stepsizes Δt and Δx, respectively.

Stepsizes		$\alpha=2/3$		$\alpha=1/2$		$\alpha=1/3$	
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	$p=q$	$\varepsilon_{\Delta x,\Delta t}$	$p=q$	$\varepsilon_{\Delta x,\Delta t}$	$p=q$
0.5	0.5	$3.92\cdot 10^{-1}$	–	$4.53\cdot 10^{-1}$	–	$4.74\cdot 10^{-1}$	–
0.25	0.25	$1.03\cdot 10^{-1}$	1.94	$1.16\cdot 10^{-1}$	1.96	$1.27\cdot 10^{-1}$	1.90
0.125	0.125	$2.61\cdot 10^{-2}$	1.97	$2.92\cdot 10^{-2}$	1.99	$3.18\cdot 10^{-2}$	1.99
0.0625	0.0625	$6.54\cdot 10^{-3}$	2.00	$7.31\cdot 10^{-3}$	2.00	$8.00\cdot 10^{-3}$	1.99

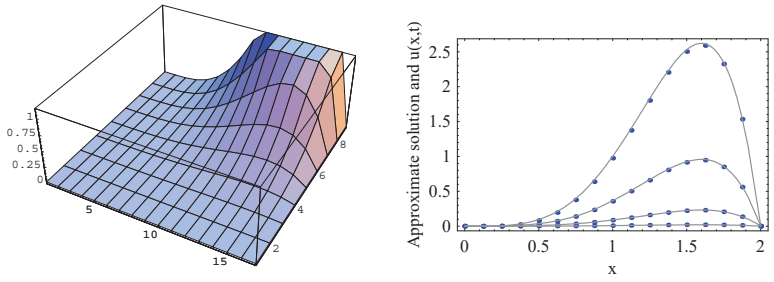


FIGURE 4.3: Approximate solution of example 4.4.1, with $\alpha = 1/2$, obtained with the non-polynomial collocation method on the space $V^{1/2}_{2,0.125}$ with $\Delta x = 0.125$. **Left:** Plot of the approximate solution. **Right:** Exact solution (*gray line*) and approximate solution (*blue points*).

In Fig. 4.4.1.2 (a) the approximate solution of example 4.4.1, with $\alpha = 1/2$, obtained with the non-polynomial collocation method on the space $V^{\alpha}_{2,0.125}$ with $\Delta x = 0.125$ is displayed. Fig. 4.4.1.2 (b) shows the exact and numerical solutions at the points $(x, 0.25i),\ i = 1, 2 \ldots, 4$. From Fig. 4.4.1.2 (b), it can be seen that the numerical solution is in good agreement with the exact one.

In Fig. 4.4 we show the absolute errors related with the approximate solution, of example 4.4.1, that belong to the space $V^{\alpha}_{2,0.125}$ and obtained by the proposed method. From Fig. 4.4 it can be seen that the absolute errors obtained for the several values of α are very similar.

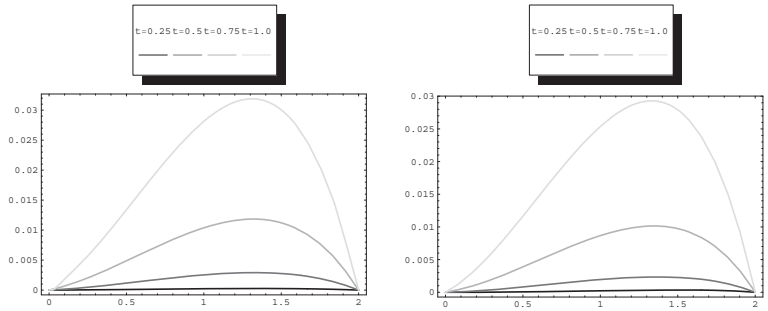
In table 4.5, we present the maximum of the absolute errors at the mesh points and the experimental orders of convergence, for example 4.4.2, whose analytical solution is nonsmooth at $t = 0$. Even so, the expected time convergence order is observed.

Table 4.5: Non-polynomial collocation method on the spaces V^{α}_1 and V^{α}_2 for example 4.4.2: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p and q related with the stepsizes Δt and Δx, respectively.

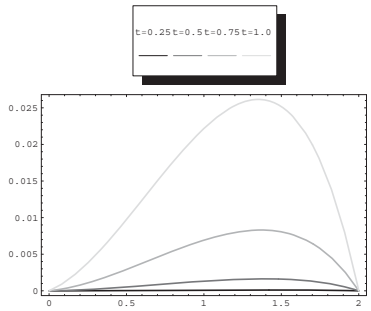
Collocation on the space V^{α}_1					Collocation on the space V^{α}_2			
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	p	q	Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	$p = q$
0.25	0.25	$2.04 \cdot 10^{-2}$	–	-	0.25	0.25	$2.04 \cdot 10^{-2}$	–
0.0625	0.125	$5.48 \cdot 10^{-3}$	0.95	1.90	0.125	0.125	$5.55 \cdot 10^{-3}$	1.88
0.0156225	0.0625	$1.39 \cdot 10^{-3}$	0.99	1.98	0.0625	0.0625	$1.39 \cdot 10^{-3}$	2.00
0.00390625	0.03125	$3.11 \cdot 10^{-4}$	1.08	2.16	0.03125	0.03125	$3.48 \cdot 10^{-4}$	2.00

In Fig. 4.5 (a) the approximate solution of example 4.4.2, obtained with the non-polynomial collocation method on the space $V^{\alpha}_{2,0.0625}$ with $\Delta x = \Delta t = 0.0625$ is displayed. Fig. 4.5 (b) shows the exact and numerical solutions at the points $(x, 0.25 \cdot i),\ i = 1, 2 \ldots, 4$, and we can observe that the numerical solution obtained by the proposed method is in good agreement with the exact solution.

In Fig. 4.6 we compare the absolute errors at the points $(x, i \cdot 0.25),\ i = 1, 2, \ldots, 4$ (bottom to top), obtained by the application of the non-polynomial collocation method on



$\alpha = 1/3$ $\alpha = 1/2$



$\alpha = 2/3$

Figure 4.4: Absolute errors for the approximate solution of example 4.4.1, for several values of α, obtained with the non-polynomial collocation method on the space $V^{\alpha}_{2,0.125}$ with $\Delta x = 0.125$.

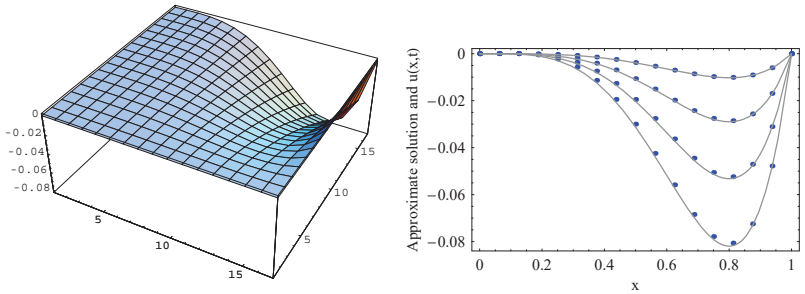


Figure 4.5: Approximate solution of example 4.4.2 obtained with the non-polynomial collocation method on the space $V^{1/2}_{2,0.0625}$ with $\Delta x = \Delta t = 0.0625$. **Left:** Plot of approximate solution. **Right:** Exact solution (*gray line*) and approximate solution (*blue points*).

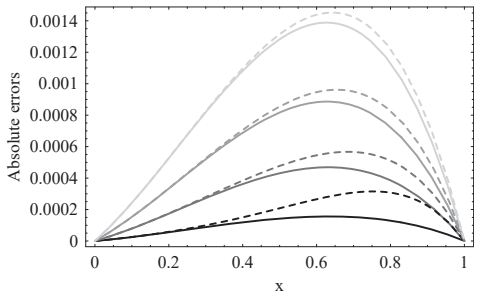


FIGURE 4.6: Absolute errors for the approximate solution of example 4.4.2 obtained with the non-polynomial collocation method on the spaces $V^{1/2}_{1,0.0625}$ (dashed line) and $V^{1/2}_{2,0.0625}$ (solid line), with $\Delta x = \Delta t = 0.0625$.

the spaces $V^{1/2}_{1,0.0625}$ and $V^{1/2}_{2,0.0625}$, and we observe that the error decreases on the second approximation, as expected.

We present some results for both examples ($m = 3$ and $\alpha = 1/2$), which are listed in table 4.6. As expected, the experimental order of convergence, with respect to the time variable, is 3.

Table 4.6: Non-polynomial collocation method on the space $V^{\frac{1}{2}}_{3,\Delta t}$ for examples 4.4.1 and 4.4.2: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p and q related with the stepsizes $\Delta t = (\Delta x)^{\frac{2}{3}}$ and Δx, respectively.

Example 4.4.1					Example 4.4.2				
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	p	q	Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	p	q
0.5	0.5	$4.34 \cdot 10^{-1}$	–	–	0.3333	0.25	$2.04 \cdot 10^{-2}$	–	–
0.3333	0.25	$1.15 \cdot 10^{-1}$	2.87	1.91	0.25	0.125	$5.55 \cdot 10^{-3}$	2.82	1.88
0.25	0.125	$2.91 \cdot 10^{-2}$	2.98	1.98	0.1429	0.0625	$1.39 \cdot 10^{-3}$	3.0	2.0
0.01429	0.0625	$7.21 \cdot 10^{-3}$	3.02	2.01	0.09091	0.03125	$3.57 \cdot 10^{-4}$	2.94	1.96

4.4.1.3 Comparison with Other Methods

The method proposed in this work was also compared with other methods available in the literature. As mentioned in the Introduction, finite difference methods are the most popular for the numerical approximation of this kind of equation. Here, we compare the numerical results obtained using the method described before with the ones obtained in the paper [132], where the author claims first order accuracy in time and second order in space. This convergence order can be observed in tables 4.7 and 4.8, where we present some results of numerical experiments with the method described in [132], obtained for examples 4.4.1 and 4.4.2, respectively, for different values of the stepsizes Δt and Δx.

4.4.1.4 Conclusions

A new numerical method has been developed for the solution of the time-fractional diffusion equation. This consists of the method of lines combined with a non-polynomial

Table 4.7: Method in [132] for example 4.4.1 with several values of α: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence q and p related with the stepsizes Δx and $\Delta t = (\Delta x)^2$, respectively.

Stepsizes		$\alpha = 2/3$			$\alpha = 1/2$			$\alpha = 1/3$		
Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	p	q	$\varepsilon_{\Delta x,\Delta t}$	p	q	$\varepsilon_{\Delta x,\Delta t}$	p	q
$1/4$	$1/2$	$2.75 \cdot 10^{-1}$	–	–	$3.76 \cdot 10^{-1}$	–	–	$4.47 \cdot 10^{-1}$	–	–
$1/16$	$1/4$	$7.71 \cdot 10^{-2}$	0.92	1.83	$1.05 \cdot 10^{-1}$	0.92	1.85	$1.23 \cdot 10^{-1}$	0.93	1.87
$1/64$	$1/8$	$2.16 \cdot 10^{-2}$	0.92	1.83	$2.76 \cdot 10^{-2}$	0.96	1.92	$3.13 \cdot 10^{-2}$	0.98	1.97
$1/256$	$1/16$	$5.81 \cdot 10^{-3}$	0.95	1.90	$7.10 \cdot 10^{-3}$	0.98	1.96	$7.95 \cdot 10^{-3}$	0.99	1.98

Table 4.8: Method in [132] for example 4.4.2: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence q and p related with the stepsizes Δx and $\Delta t = (\Delta x)^2$, respectively.

Δt	Δx	$\varepsilon_{\Delta x,\Delta t}$	p	q
$1/16$	$1/4$	$2.04 \cdot 10^{-2}$	-	-
$1/64$	$1/8$	$5.55 \cdot 10^{-3}$	0.94	1.88
$1/256$	$1/16$	$1.39 \cdot 10^{-3}$	1.00	2.00
$1/1024$	$1/32$	$3.47 \cdot 10^{-4}$	1.00	2.00

collocation method. The method presented here may be extended easily to other types of fractional PDEs, to problems with different boundary conditions and to equations with higher space dimension. From the numerical results we can see that the order of convergence of the time approximation is m if the solution can be written as a sum of a regular function and a function that belongs to the space V_m^α with respect to the time variable. Also, as expected, the spacial convergence order is 2.

4.4.2 A Hybrid Numerical Scheme for the Time-Fractional Diffusion Equation

In order to approximate the solution of (4.45)-(4.47), using a hybrid method, we just need to combine the previous Section with the method proposed for systems of Fractional ODE's. Therefore, consider on the interval $[0, T]$ the mesh defined by (4.14). We will then seek for a function $v = [v_1\ v_2 \dots v_n]^T$ such that $v_i \in S_\tau^m([0, T])$, $i = 1, 2, \dots, n$, that satisfies

$$\begin{aligned} v_i(t_{pj}) &= y_0 + \frac{D}{\Gamma(\alpha)} \int_0^{t_{pj}} (t_{pj} - s)^{\alpha-1} \left(\frac{v_{i+1}(s) - 2v_i(s) + v_{i-1}(s)}{h^2} + f(x_i, s) \right) ds, \\ & \quad p = 0, \dots, N' - 1,\ j = 1, \dots, m_p \end{aligned}$$

where $m_0 = \ell$ and $m_p = m\, p = 1, ..., N' - 1$.

4.4.2.1 Numerical Results

In order to illustrate the feasibility and performance of the method we will now compare the results obtained with the hybrid and classical nonpolynomial methods. The numerical error is measured by determining the maximum error at the mesh points (x_i, t_j):

$$\varepsilon_{h,\tau} = \max_{i=1,\dots,n,\, j=1,\dots,N} |u(x_i, t_j) - y_i(t_j)|,\ N = \frac{1}{\tau},\ n = \frac{L}{h} \tag{4.59}$$

where y_i is the numerical solution obtained for the i-th spatial function and $u(x_i, t_j)$ is the exact solution evaluated at points (x_i, t_j). We consider the following examples:

Example 4.4.3

$$\begin{cases} \dfrac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \dfrac{\partial^2 u(x,t)}{\partial x^2} + \dfrac{\Gamma(4+\alpha)}{6} x^4(2-x)t^3 - 4x^2(6-5x)t^{3+\alpha}, \quad t > 0,\ 0 \le x \le 2, \\ u(x,0) = 0, \\ u(0,t) = u(2,t) = 0. \end{cases}$$

whose analytical solution is $u(x,t) = x^4(2-x)t^{3+\alpha}$.

Example 4.4.4

$$\begin{cases} \dfrac{\pi(x-1)x^4 \csc(\pi\alpha)\cos(x)}{\Gamma(-\alpha)} - x^2 t^\alpha (2x(5x-4)\sin(x) + ((x-5)x(x+4)+12)\cos(x)), \\ \quad t > 0,\ 0 \le x \le 2, \\ u(x,0) = 0, \\ u(0,t) = u(2,t) = 0. \end{cases}$$

whose analytical solution is $u(x,t) = x^4(1-x)t^\alpha \cos(x)$.

The numerical results obtained for the time-fractional diffusion equation (example 4.4.3) on the spaces $V^\alpha_{2,\tau}$ and $V^\alpha_{3,\tau}$ are now presented and the collocation parameters that we have used are listed below:

- For $\alpha = 1/3$ and the first time interval, we consider $c_1 = 0.15$, $c_2 = 0.3$, $c_3 = 0.4$, $c_4 = 0.5$, $c_5 = 0.7$, $c_6 = 0.85$ for $m = 2$. For the remaining intervals we have considered $c_1 = 0.25$, $c_2 = 0.75$ for $m = 2$;
- For $\alpha = 1/2$ and the first time interval, we consider $c_1 = 0.15$, $c_2 = 0.25$, $c_3 = 0.5$, $c_4 = 0.75$ for $m = 2$. For the remaining intervals we have considered $c_1 = 0.25$, $c_2 = 0.75$ for $m = 2$;
- For $\alpha = 2/3$ and the first time interval, we consider $c_1 = 0.15$, $c_2 = 0.3$, $c_3 = 0.5$, $c_4 = 0.7$, $c_5 = 0.85$ for $m = 2$. For the remaining intervals we have considered $c_1 = 0.25$, $c_2 = 0.75$ for $m = 2$;

For each case, the estimates for the time and space rates of convergence were computed and denoted by p and q, respectively.

In table 4.9 we show the numerical results obtained by the described hybrid method and the classical nonpolynomial method on the space V^α_2 (for example 4.4.1) considering three different values of α. As expected we can determine $p \sim 2$ experimentally (not dependent on the order of the fractional derivative) and $q \sim 2$.

We also present the speed-up (SU - ratio between the simulation time of the classical method and the simulation time of the hybrid method), and the maximum and minimum condition number ($\kappa(A) = \|A\|_\infty \left\|A^{-1}\right\|_\infty$) obtained for each simulation. We observe that the new method allows one to obtain the same order of convergence with a less computational effort, with the speed-up increasing with the mesh refinement. Note that is

Table 4.9: Hybrid and nonpolynomial collocation methods on the space V_2^α for example 4.4.3 with three different values of α: values of the maximum of the absolute errors at the mesh points and the experimental orders of convergence p and q related with the stepsizes τ and h, respectively.

Stepsizes			hybrid($\alpha = 2/3$)					
N	N'	h	$\varepsilon_{h,\tau}$	$p = q$	SU	$\kappa(A)_{min}$	$\kappa(A)_{max}$	dim(A)
8	4	0.125	$3.17 \cdot 10^{-1}$	–	45.4	86.7	$1.14 \cdot 10^{+4}$	75/30
16	10	0.0625	$9.59 \cdot 10^{-2}$	1.73	42.8	151.7	$2.60 \cdot 10^{+4}$	155/62
32	22	0.0313	$2.53 \cdot 10^{-2}$	1.92	247.4	281.1	$6.57 \cdot 10^{+4}$	315/126
64	48	0.0156	$6.21 \cdot 10^{-3}$	2.02	142.1	494.8	$1.73 \cdot 10^{+5}$	635/254

nonpolynomial($\alpha = 2/3$)			
N	$\varepsilon_{h,\tau}$	$p = q$	$\kappa(A)_{min}$
8	$2.61 \cdot 10^{-2}$	1.97	$2.93 \cdot 10^{+2}$
16	$6.54 \cdot 10^{-3}$	2.00	$8.19 \cdot 10^{+2}$
32	$1.64 \cdot 10^{-3}$	2.00	$2.20 \cdot 10^{+3}$
64	$4.09 \cdot 10^{-4}$	2.00	$6.64 \cdot 10^{+3}$

Stepsizes			hybrid($\alpha = 1/2$)					
N	N'	h	$\varepsilon_{h,\tau}$	$p = q$	SU	$\kappa(A)_{min}$	$\kappa(A)_{max}$	dim(A)
8	4	0.125	$4.16 \cdot 10^{-1}$	–	30.1	101.2	744.3	60/30
16	8	0.0625	$1.39 \cdot 10^{-1}$	1.58	32.2	251.1	$2.36 \cdot 10^{32}$	124/62
32	19	0.0313	$3.95 \cdot 10^{-2}$	1.81	54.5	529.1	$5.88 \cdot 10^{+3}$	252/126
64	42	0.0156	$1.03 \cdot 10^{-2}$	1.94	167.8	1144	$1.67 \cdot 10^{+4}$	508/254

nonpolynomial($\alpha = 1/2$)			
N	$\varepsilon_{h,\tau}$	$p = q$	$\kappa(A)_{min}$
8	$2.92 \cdot 10^{-2}$	1.99	$2.27 \cdot 10^{+2}$
16	$7.31 \cdot 10^{-3}$	2.00	$6.84 \cdot 10^{+3}$
32	$1.83 \cdot 10^{-3}$	2.00	$2.04 \cdot 10^{+3}$
64	$4.57 \cdot 10^{-4}$	2.00	$6.08 \cdot 10^{+3}$

Stepsizes			hybrid($\alpha = 1/3$)					
N	N'	h	$\varepsilon_{h,\tau}$	$p = q$	SU	$\kappa(A)_{min}$	$\kappa(A)_{max}$	dim(A)
8	3	0.125	$5.75 \cdot 10^{-1}$	–	116	125.1	$3.26 \cdot 10^{+6}$	90/30
16	6	0.0625	$2.21 \cdot 10^{-1}$	1.38	173	372.6	$1.10 \cdot 10^{+7}$	186/62
32	15	0.0313	$6.90 \cdot 10^{-2}$	1.68	629.4	934.0	$2.72 \cdot 10^{+7}$	378/126
64	32	0.0156	$1.92 \cdot 10^{-2}$	1.85	198.2	2699	$8.88 \cdot 10^{+7}$	762/254
128	71	0.0078	$5.00 \cdot 10^{-3}$	1.94	-	7278	$2.86 \cdot 10^{+8}$	1530/510

nonpolynomial($\alpha = 1/3$)			
N	$\varepsilon_{h,\tau}$	$p = q$	$\kappa(A)_{min}$
8	$3.18 \cdot 10^{-2}$	1.99	$5.81 \cdot 10^{+3}$
16	$8.00 \cdot 10^{-3}$	1.99	$1.66 \cdot 10^{+4}$
32	$2.00 \cdot 10^{-3}$	2.00	$5.07 \cdot 10^{+4}$
64	$5.00 \cdot 10^{-4}$	2.00	$1.67 \cdot 10^{+5}$

some cases we managed to obtain speed-ups of 173x. We may also conclude that SU increases with the dimension of the space V_m^α. Regarding the condition number, we have that $\kappa(A)_{max}$ is the same for both the methods, and, this value is obtained only for the

first iteration in time. For the hybrid method the value of $\kappa(A)$ for the remaining iterations remains constant, and is given by $\kappa(A)_{min}$. For the nonpolynomial method the $\kappa(A)$ decreases along iterations, being its minimum value achieved only in the last iteration. Note that difference between the $\kappa(A)_{min}$ for the two methods, being the condition number really low for the hybrid method. This makes this method more robust, since less significant digits will be lost along the numerical procedure. We also present in this table the dimension of the matrices obtained for the first and remaining time intervals ($\dim(A)$). This is denoted by a/b with $a \times a$ the dimension of the matrix for the first time interval and $b \times b$ the dimension of the matrix for the remaining intervals (for the hybrid method). It should be remarked that $\dim(A) = a \times a$ for the nonpolynomial method (in all time intervals), making this method significantly slower when compared to hybrid method.

We have tested higher orders of convergence by considering the space $V_3^{1/2}$ for example 4.4.3. The results are shown in Table 4.10. We observed an experimental convergence order of $\mathrm{O}(\tau_{max}^m) + \mathrm{O}(h^2)$.

Table 4.10: Hybrid collocation method on the space $V_3^{1/2}$ for example 4.4.3: values of the maximum of the absolute errors at the mesh points and the experimental order of convergence p related with the stepsizes $\tau = (h)^{2/3}$ (m=3), and h.

Stepsizes			hybrid($\alpha = 1/2$) - $V_3^{1/2}$	
N	N'	h	$\varepsilon_{h,\tau}$	p
16	6	0.0156	$2.13 \cdot 10^{-2}$	–
25	11	0.0078	$6.58 \cdot 10^{-3}$	2.55
40	19	0.0039	$1.78 \cdot 10^{-3}$	2.83
64	32	0.00195	$4.60 \cdot 10^{-4}$	2.93

Finally, we performed numerical simulations considering Example 4.4.4, that presents a stronger singularity.

We have considered the space $V_2^{1/2}$ and the results are shown in Table 4.11. Again, we observe the expected convergence rates.

Table 4.11: Hybrid collocation method on the space $V_3^{1/2}$ for example 4.4.4: values of the maximum of the absolute errors at the mesh points and the experimental order of convergence p related with the stepsizes $\tau = (h)^{2/3}$ (m=3), and h.

hybrid($\alpha = 1/2$) - $V_2^{1/2}$				
N	N'	h	$\varepsilon_{h,\tau}$	$p = q$
8	4	0.0625	$1.75 \cdot 10^{-3}$	–
16	8	0.0313	$4.17 \cdot 10^{-4}$	2.01
32	19	0.0156	$1.04 \cdot 10^{-4}$	2.00
64	42	0.00785	$2.60 \cdot 10^{-5}$	2.00

4.4.2.2 Conclusions

In this work we have a derived a hybrid numerical method that can deal with both smooth and nonsmooth solutions of the Time-Fractional-Diffusion-Equation. The method uses a nonpolynomial collocation method in the first time interval and a polynomial collocation method in the remaining intervals. By using the hybrid method we managed to obtain numerical solutions that are 173x faster than the ones obtained with the nonpolynomial

collocation method. The numerical method is robust and also allows one to choose the degree of accuracy intended to solve the fractional differential equation by setting a different number of collocation points. We performed numerical tests and observed an experimental convergence order of $\mathrm{O}(\tau_{max}^{m}) + \mathrm{O}(h^2)$.

5.1 Main Conclusions and Discussion

In this work we have tackled three main problems often encountered in applications of fractional calculus and numerical methods used to solve fractional differential equations. These are:

1. The existing gap between Engineering and Mathematics that resulted in a not so fundamented substitution of classical derivatives by their fractional counterpart, creating models that allow a better description of real world phenomena, but, that at the same time change the dimensions of the parameters involved;

2. The hereditary properties of the fractional operators that result in slow computations;

3. The dependency of the convergence of the numerical methods for fractional differential equations on the order of the fractional derivative and the nonexistence of fast and robust methods that can deal with the potential singularities of the solution of fractional differential equations.

Item 1: We have presented a fundamental explanation on the use of fractional derivatives to model anomalous diffusion. A numerical method was devised to solve a general fractional diffusion equation equation, which was proved to be stable and convergent. The method can deal with the Neumann boundary conditions and the variation of the thermal diffusivity in space (we prove its convergence (convergence order of $O(\Delta x^2 + \Delta t^{2-\alpha})$, $0 < \alpha < 1$) and stability). As an example of what is often done in the litterature, we substituted in the bioheat equation the classical time derivative by a fractional derivative. This lead to the *creation* of a new parameter that should be temperature dependent. We managed to obtain a better fit of experimental results, but, this conclusion should be explained with care. There is no doubt that the fractional derivative may improve the quality of the model, but we have added a new modeling parameter, and therefore, we can not say this is a better model when compared to the classical one. The typical substitution of the classical derivative by a fractional derivative should be performed with care. First: there should be a physical

reason for this substitution, and, second: the units of the parameters used in the equations are changed in the presence of the fractional derivative, therefore we can not used them as regular properties. Regarding the numerical method, it should be highlighted the fact that when deriving the proofs of convergence and stability we have assumed certain regularity properties of the solution that may not be verified in reality. In this cases we are expecting the order of the method to decrease.

The error analysis assumes a certain regularity of the solution, that is not always verified. This fact was explored and numerical tests were performed in order to evaluate how the method behaves with highly singular solutions.

Item 2: We have developed a new numerical method for the solution of distributed order time-fractional diffusion equations, based on the approximation of the solution by a Chebyshev truncated double series, and the subsequent collocation of the resulting discretised system of equations at suitable collocation points. We reviewed the existing papers on the numerical solution for this type of equations, and, we also present for the first time a detailed error analysis for the proposed numerical method.

The error analysis assumes a certain regularity of the solution, that is not always verified. This fact was explored and numerical tests were performed in order to evaluate how the method behaves with highly singular solutions. It was always observed convergence, and the numerical method proved to be faster than the traditional finite difference approach.

Item 3: We have improved the accuracy and robustness of numerical methods for the Time-Fractional diffusion equation. A new numerical method has been developed for the solution of the time-fractional diffusion equation that consists of the method of lines combined with a non-polynomial collocation method. The method presented here may be easily extended to other type of fractional PDEs, to problems with different boundary conditions and to equations with higher space dimension. We proved that the order of convergence of the time approximation is optimal.

Finally, we have derived the most important contribution of this thesis: an hybrid method consisting of a combination of a non-polynomial approximation on the first interval of the time discretisation and a polynomial approximation on the remaining time discretisation intervals. This resulted in a much faster numerical method that can deal with the potential singularities of the solution.

We may therefore conclude that the objectives of this work were achieved. In the future, the numerical methods can be improved and extended to different types of fractional differential equations. Also, the creation of different fractional operators that have the *memory* properties but that are less computational demanding should be explored.

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Colophon

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