Finite Difference Methods for the Solution of Fractional Diffusion Equations

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Abstract

Fractional calculus is a mathematical field dealing with integrals and derivatives of arbitrary order. In recent times fractional calculus has found applications in physics, signal-processing, engineering, bio-science, and finance. Anomalous diffusion has received particular interest in the framework of fractional calculus applications. In the time fractional diffusion equation, the standard time derivative is replaced by a fractional order counterpart. Since the analytical solution of fractional differential equations is hard to obtain, finite difference methods in particular became very popular and a large number of schemes has been published very recently. This thesis compares several schemes for both fixed and variable order fractional fractional differential equations and the objective of this summary is to compare different schemes with increasing order of accuracy for the solution of the time fractional diffusion equations. The construction of these schemes is summarized, a numerical example is solved with self-written code and is used to compare the schemes in terms of accuracy and computational cost.
Keywords: Fractional Calculus, Anomalous Diffusion, Fractional Diffusion Equation, Finite Difference Methods, Fractional Derivative, Variable-Order.

1. Introduction

Fractional Calculus is a mathematical field dealing with integrals and derivatives of arbitrary order. Even though the concept dates back to 1695 [1], it was only on the last century that the most impressive achievements were made. Particularly in the last three decades fractional calculus has found applications in physics, signal-processing, engineering, bio-science, and finance [2, 3, 4, 5, 6, 7]. Considering that the analytical solution of fractional differential equations is hard to obtain, numerical methods for their evaluation became understandably attractive. Finite difference methods in particular became very popular and a large number of schemes has been published very recently. Consequently it becomes important to understand how they compare in terms of accuracy, stability and computing times.

Anomalous diffusion see e.g. [3] has received particular interest in the framework of fractional calculus applications. Enjoying non-local properties, fractional integrals and derivatives may describe more accurately anomalous diffusion processes. In fractional diffusion equations, integer order derivatives are replaced by fractional order counterparts, originating what may be considered as three different types of equations: i) time fractional, ii) space fractional and iii) space-time fractional equations. For instance it has been suggested that the probability density function $u(x,t)$ that describes anomalous subdiffusion particles follows the time fractional subdiffusion equation [3, 8, 9, 10]. Naturally, each type of fractional diffusion equation has attracted in its own right a considerable number of works regarding its solution.

Loking at time- fractional diffusion equations, implicit shemes are more favorable than their explicit counterparts, see e.g. [11, 12, 13, 14, 15]. Compact schemes have also attracted many researchers because of the advantadge of keeping the tridiagonal nature, see e.g. [16]. Gao and Sun [17] applied the L1 approximation for the time-fractional derivative and developed a compact finite difference scheme for the fractional sub-diffusion equation. Most of these methods focus on the improvement of the space order accuracy. It is however remarked that other numerical methods have been sought to solve time fractional diffusion equations namely finite element [18] and spectral methods [19, 20]. High order in space and time was sought by Ji and Sun [21] have proposed a high order compact difference scheme able to solve the time fractional diffusion equation with third order accuracy in time. Most recently, Hu and Zhang

[22] have also proposed a second order implicit finite difference method in time for the fractional diffusion equation.

From the brief survey above, there are a multitude of finite difference methods for the approximation of fractional derivatives and their application on schemes for time fractional diffusion equations. The non-local properties of fractional derivatives translate into approximations that have much longer computing times than integer order derivatives. For this reason, the stability criteria of explicit schemes for fractional diffusion equations may lead to prohibitively high computational costs and difficulties in the analysis of the orders of accuracy. As such, this work focuses on implicit schemes that are unconditionally stable. Three different schemes with increasing order of accuracy were selected for time. The main objective of this work is the comparison of these finite difference schemes in terms of accuracy and computational cost.

The compared schemes are: i) the weigted average scheme developed by Yuste [15],with the classic Grünwald-Letnikov Approximation with first order accuracy in time, ii) the recent scheme proposed by Hu and Zhang [22] with second order accuracy and iii) the third-order in time compact finite difference scheme developed by Ji and Sun [21].

This document is organized as follows. On section 2 a brief overview is made of the most important mathematical definitions of fractional integrals and derivatives. In Section 3 approximations for time fractional derivatives are provided. Section 4 will be concerned with finite difference schemes for the constant order time fractional diffusion equation, it begins with the statement of the time fractional diffusion initial boundary-value problem and follows with the construction of the finite difference schemes. A numerical example is provided in section 5 to validate the implementations and to compare the schemes in terms of convergence and computational cost. Concluding remarks are made on chapter 6.

2. Mathematical Preliminaries

In this chapter, the mathematical definitions of fractional integrals and derivatives used throughout this paper are introduced [23].

Definition 2.1. The left and right fractional Riemann-Liouville integrals of order $\alpha > 0$ of a given function $f(t)$, $t \in (a, b)$ are defined as

$$ {}^{RL}_{a}D_t^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-s)^{\alpha-1} f(s) ds \tag{2.1} $$

$$ {}^{RL}_{t}D_b^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_t^b (s-t)^{\alpha-1} f(s) ds \tag{2.2} $$

respectively, where $\Gamma(\cdot)$ denotes Euler's gamma function.

Definition 2.2. The left and right Riemann-Liouville derivatives with order $\alpha > 0$ of the function $f(t)$, $t \in (a, b)$ are defined as

$$ {}^{RL}_{a}D_t^{\alpha} f(t) = \frac{d^m}{dt^m}[D_{a,t}^{-(m-\alpha)} f(t)] = \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dt^m} \int_a^t (t-s)^{m-\alpha-1} f(s) ds \tag{2.3} $$

$$ {}^{RL}_{t}D_b^{\alpha} f(t) = (-1)^m \frac{d^m}{dt^m}[D_{t,b}^{-(m-\alpha)} f(t)] = \frac{(-1)^m}{\Gamma(m-\alpha)} \frac{d^m}{dt^m} \int_t^b (s-t)^{m-\alpha-1} f(s) ds \tag{2.4} $$

respectively, where m is a positive integer satisfying $m-1 \leq \alpha < m$ and $\Gamma(\cdot)$ is Euler's gamma function.

Definition 2.3. The left and right Caputo derivatives with order $\alpha > 0$ of the function $f(t)$, $t \in (a, b)$ are defined as

$$ {}^{C}_{a}D_t^{\alpha} f(t) = {}^{RL}_{a}D_t^{-(m-\alpha)}[f^{(m)}(t)] = \frac{1}{\Gamma(m-\alpha)} \int_a^t (t-s)^{m-\alpha-1} f^{(m)}(s) ds \tag{2.5} $$

$$ {}^{C}_{t}D_b^{\alpha} f(t) = \frac{(-1)^m}{\Gamma(m-\alpha)} \int_t^b (s-t)^{m-\alpha-1} f^{(m)}(s) ds \tag{2.6} $$

respectively, where m is a positive integer satisfying $m-1 \leq \alpha < m$ and $\Gamma(\cdot)$ is Euler's gamma function.

Although the definitions of the Riemann-Liouville and of the Caputo derivatives cannot be assumed equal, they do have the following relationship

$$ {}_a^{RL}D_t^{\alpha} f(t) = {}_a^{C}D_t^{\alpha} f(t) + \sum_{k=0}^{m-1} \frac{f^{(k)}(a)(t-a)^{k-\alpha}}{\Gamma(k+1-\alpha)} \tag{2.7} $$

where $m-1 < \alpha < m$ is a positive integer and f^m is integrable on $[a,t]$. On the special case where $f^k(0) = 0$ with $k = 0, 1, 2, \cdots, m-1, m-1 < \alpha < m$ the Riemann-Liouville and Caputo derivatives are equivalent.

3. Finite difference approximations for time fractional derivatives

In this section, the operators here used to approximate fractional time derivatives are used. Throughout the section let $t \in [0,T]$, $\tau = T/N$ so that $t_n = n\tau$ and $\Omega_\tau = \{t_n | 0 \leq n \leq N\}$. Additionally, let $u(t_n) = u_n$.

3.1. The Grünwald-Letnikov Approximation

The Grünwald-Letnikov approximation [15] is one of the most used approximations for time fractional derivatives. If $u(t)$ is suitably smooth, the left Riemann-Liouville derivative can be approximated with first order accuracy by

$$ \left[{}_0^{RL}D_t^{\gamma} u(t)\right]_{t=t_n} = {}^{GL}\delta_t^{\gamma} u_n + O(\tau) \tag{3.1} $$

where the left Grünwald-Letnikov difference operator is given by

$$ {}^{GL}\delta_t^{\gamma} u_n = \frac{1}{\tau^\gamma} \sum_{k=0}^{n} \omega_j^{(\gamma)} u_{n-k} \tag{3.2} $$

The Grünwald-Letnikov wheights $\omega_k^{(\gamma)} = (-1)^k \binom{\gamma}{k}$, with $k \geq 0$, are the coefficients of the power series of the generating function $(1-z)^\gamma = \sum_{k=0}^{\infty} \omega_k^{(\gamma)} z^k$. These weights satisfy the recursive formula

$$ \omega_k^{(\gamma)} = \left(1 - \frac{\gamma+1}{k}\right) \omega_{k-1}^{(\gamma)}, \quad w_0^{(\gamma)} = 1. \tag{3.3} $$

3.2. Third order weighted and shifted Grünwald difference approximation

In [21] Ji and Sun developed a third order accurate weighted and shifted Grünwald difference operator for the Riemann-Liouville derivative, that they used to construct in a compact difference scheme for the time fractional diffusion equation. The construction of this approximation is now summarized. Supposing that $u \in L_1(\mathbb{R}) \cap \mathcal{C}^{\gamma+1}(\mathbb{R})$, the Riemann-Liouville derivative (2.3) evaluated from negative infinity ($a = -\infty$) can be approximated with first order accuracy by

$$ \left[{}_{-\infty}^{RL}D_t^{\gamma} u(t)\right]_{t=t_n} = {}_p\delta_t^{(\gamma)} u_n + O(\tau) \tag{3.4} $$

where ${}_p\delta_t^{(\gamma)}$ is the shifted Grünwald difference operator [24], defined as

$$ {}_p\delta_t^{(\gamma)} u_n = \frac{1}{\tau^\gamma} \sum_{k=0}^{\infty} \omega_k^{(\gamma)} u_{n-(k-p)} \tag{3.5} $$

uniformly for $t \in \mathbb{R}$ as $\tau \to 0$. The integer p corresponds to the number of shifts and as in the Grünwald-Letnikov approximation, the weights $\omega_k^{(\gamma)}$ are the coefficients of the power series of the generating function $(1-z)^\gamma$, given in equation (3.3).

Moreover, if $u(t) \in L_1(\mathbb{R})$, ${}_{-\infty}D_t^{\gamma+3} u(t)$ and its Fourier transform belong to $L_1(\mathbb{R})$, then the operator in (3.5) can be used to construct a third order approximation for ${}_{-\infty}^{RL}D_t^{\gamma} u(t)$

$$ \left[{}_{-\infty}^{RL}D_t^{\gamma} u(t)\right]_{t=t_n} = {}_{p,q,r}\delta_t^{(\gamma)} u_n + O(\tau^3) \tag{3.6} $$

where ${}_{p,q,r}\delta_t^{(\gamma)}$ is a weighted and shifted Grünwald difference operator defined by

$$ {}_{p,q,r}\delta_t^{(\gamma)} u_n = \rho_1 A_p^{(\gamma)} u_n + \rho_2 A_q^{(\gamma)} u_n + \rho_3 A_r^{(\gamma)} u_n \tag{3.7} $$

with shifts p,q and r are defined in [21] as $(p, q, r) = (0, -1, -2)$ and

$$\rho_1 = \frac{12qr - (6q + 6r + 1)\gamma + 3\gamma^2}{12(qr - pq - pr + p^2)}, \quad \rho_2 = \frac{12pr - (6p + 6r + 1)\gamma + 3\gamma^2}{12(pr - pq - qr + q^2)},$$

$$\rho_3 = \frac{12pq - (6p + 6q + 1)\gamma + 3\gamma^2}{12(pq - pr - qr + r^2)}$$

Introducing now,

$$\tilde{u}(t) = \begin{cases} u(t), & t \in [0, T] \\ 0, & t \in [-\infty, 0] \end{cases} \tag{3.8}$$

it naturally occurs that ${}^{RL}_{\ 0}D^{\gamma}_{t}u(t) = {}^{RL}_{-\infty}D^{\gamma}_{t}\tilde{u}(t)$ and therefore ${}^{RL}_{\ 0}D^{\gamma}_{t}u(t)$ can be approximated with third order accuracy by

$$\left[{}^{RL}_{\ 0}D^{\gamma}_{t}u(t)\right]_{t=t_n} = {}^{WS3}\delta^{\gamma}_{t}u_n + +O(\tau^3) \tag{3.9}$$

where the weighted and shifted difference operator ${}^{WS3}\delta^{\gamma}_{t}u(t)$ becomes

$${}^{WS3}\delta^{\gamma}_{t}u_n = \frac{1}{\tau^{\gamma}}\left[\rho_1 \sum_{k=0}^{n} \omega^{(\gamma)}_{k} u_{n-k} + \rho_2 \sum_{k=0}^{n-1} \omega^{(\gamma)}_{k} u_{n-(k+1)} + \rho_3 \sum_{k=0}^{n-2} \omega^{(\gamma)}_{k} u_{n-(k+2)}\right] \tag{3.10}$$

For simplicity, the ${}^{GD3}\delta^{\gamma}_{t}$ operator can be written as

$${}^{GD3}\delta^{\gamma}_{t}u_n = \frac{1}{\tau^{\gamma}} \sum_{k=0}^{n} g^{(\gamma)}_{k} u^{n-k}, \quad n = 2, 3, ..., N \tag{3.11}$$

where

$$\begin{cases} g^{(\gamma)}_0 = \rho_1 \omega^{(\gamma)}_0 \\ g^{(\gamma)}_1 = \rho_1 \omega^{(\gamma)}_1 + \rho_2 \omega^{(\gamma)}_0 \\ g^{(\gamma)}_k = \rho_1 \omega^{(\gamma)}_k + \rho_2 \omega^{(\gamma)}_{k-1} + \rho_3 \omega^{(\gamma)}_{k-2}, \quad k \geq 2 \end{cases} \tag{3.12}$$

In addition to fractional derivatives, integer order derivative will also need to be approximated throughout the coming sections.

Take two positive integers M, N and let $h = (b - a)/M$ and $\tau = T/N$. Define $x_i = ih(0 \leq i \leq M)$, $t_n = n\tau(0 \leq n \leq N)$, $\Omega_h = \{x_i | 0 \leq i \leq M\}$ and $\Omega_\tau = \{t_n | 0 \leq n \leq N\}$. The computational domain $[a, b] \times [0, T]$ is then covered by $\Omega^{\tau}_{h} = \Omega_h \times \Omega_\tau$. Moreover, let $u^n_i = u(x_i, t_n)$.

At time level $n + 1/2$ it holds that

$$\left.\frac{\partial u}{\partial t}\right|_{x_i, t_{n+\frac{1}{2}}} = \delta_t u^{n+\frac{1}{2}}_{i} + O(\tau^2), \quad where \quad \delta_t u^{n+\frac{1}{2}}_{i} = \frac{u^{n+1}_i - u^n_i}{\tau} \tag{3.13}$$

The second order space derivative can be approximated at $x = ih$ with

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i, t_n} = \delta^2_x u^n_i + O(h^2), \quad where \quad \delta^2_x u^n_i = \frac{u^n_{i-1} - 2u^n_i + u^n_{i+1}}{h^2} \tag{3.14}$$

4. Time fractional diffusion equations

4.1. Problem statement

Attention will now be devoted to the development of schemes for time fractional diffusion equations. To this purpose, the two most common forms of these equations are presented. Throughout this section take two positive integers M, N and let $h = (b - a)/M$ and $\tau = T/N$. Define $x_i = ih(0 \leq i \leq M)$, $t_n = n\tau(0 \leq n \leq N)$, $\Omega_h = \{x_i | 0 \leq i \leq M\}$ and $\Omega_\tau = \{t_n | 0 \leq n \leq N\}$. The computational domain $[a, b] \times [0, T]$ is then covered by $\Omega^{\tau}_{h} = \Omega_h \times \Omega_\tau$. Moreover, let $u^n_i = u(x_i, t_n)$.

Equations (4.1)-(4.3) give the first form of time fractional diffusion equations, where the time fractional derivative is of the Riemann-Liouville type. This form of the time fractional diffusion equation is used in the schemes within sections 4.2 and 4.3.

$$\frac{\partial u}{\partial t} = {}^{RL}_{\ 0}D^{1-\gamma}_{t}\left[K_\gamma \frac{\partial^2 u}{\partial x^2}\right] + f(x, t), x \in [a, b], t \in [0, T] \tag{4.1}$$

$$u(0,t)=\phi(t), u(L,t)=\Phi(t), t\in[0,T] \tag{4.2}$$

$$u(x,0)=0, x\in[a,b] \tag{4.3}$$

where K_γ is the diffusion coefficient and ${}^{RL}_{0}D_t^{1-\gamma}$ is the Riemann-Liouville derivative of order $(1-\gamma)$ of function u as defined in section 2.

Alternatively, the Caputo fractional derivative can be used, in which case the initial-boundary value problem of the form (4.4)-(4.6). Time fractional derivatives of the Caputo type will be used on the scheme of section 4.4.

$${}^C_0D_t^\gamma u(x,t)=K_\gamma\frac{\partial^2 u(x,t)}{\partial x^2}+F(x,t), x\in[0,L], t\in[0,T] \tag{4.4}$$

$$u(0,t)=\phi(t), u(L,t)=\Phi(t), t\in[0,T] \tag{4.5}$$

$$u(x,0)=w(x), x\in[a,b] \tag{4.6}$$

once again, K_γ is the diffusion coefficient and ${}^C_0D_t^\gamma$ is the Caputo derivative with order γ of the function as defined in section 2.

The conversion between these two forms can be made in a straightforward manner when $u(x,t=0)=0$.

4.2. First order finite difference scheme

The first scheme here shown for the time fractional diffusion equation was developed by Yuste in [15], to which a source term was added.

Lets consider, equation (4.1) at the off-lattice point $(x_i, t_{n+\frac{1}{2}})$

$$\frac{\partial}{\partial t}u_i^{n+1/2}=K_\gamma\,{}^{RL}_{0}D_t^{(1-\gamma)}\left(\frac{\partial^2}{\partial x^2}u_i^{n+1/2}\right)+f_i^{n+1/2}=0 \tag{4.7}$$

The integer order time and space derivatives in this equation are now replaced by the three-point centred operator (3.13), for the first order time derivative and a weighted average of the three-point centred finite difference operator in (3.14), evaluated at times t_n and t_{n+1}. Furthermore, the Riemman-Liouville derivative is substituted by the Grünwald-Letnikov difference operator defined in (3.2).

$$\delta_t u_i^{n+1/2}-\left[\theta K_\gamma\delta_t^{1-\gamma}\delta_x^2u_i^n+(1-\theta)K_\gamma\delta_t^{1-\gamma}\delta_x^2u_i^{n+\frac{1}{2}}+\theta f_i^n+(1-\theta)f_i^{n+1}\right]=T_j^{n+1/2} \tag{4.8}$$

Neglecting the truncation error and expanding the difference operators using equations (3.13), (3.14) and (3.2) a computable finite difference scheme is achieved

$$-\tilde{S}u_{j-1}^{n+1}+(1+2\tilde{S})u_j^{n+1}-\tilde{S}u_j^{n+1}=R \tag{4.9}$$

where

$$\tilde{S}=(1-\theta)\omega_0^{(1-\gamma)}S,\quad S=K_\gamma\frac{(\tau)^\gamma}{(h)^2} \tag{4.10}$$

and

$$R=u_j^n+S\sum_{k=0}^{n}\left[(1-\theta)\omega_{k+1}^{(1-\gamma)}+\theta\omega_k^{(1-\gamma)}\right]\left[u_{j-1}^{n-k}-2u_j^{n-k}+u_{j+1}^{n-k}\right]+\tau^\gamma\left[\theta f_i^n+(1-\theta f_i^{n+1}\right]. \tag{4.11}$$

Though the scheme is in general implicit, some particular cases are to be pointed out. If $\theta=1$ the scheme is fully explicit while for $\theta=0$ the scheme is fully explicit. For $\theta=1/2$, a Crank-Nicholson type scheme is achieved.

$$\frac{1}{S}\geq\frac{1}{S_\times}\equiv 2(2\theta-1)W(-1,1-\gamma) \tag{4.12}$$

where $W(z,\gamma)$ is the generating function of the coefficients, in this case$W(z,\gamma)=(1-z)^\gamma$.

4.3. Second order implicit finite difference scheme

In [22] Hu and Zhang develop, through an integration method, a second order difference scheme for the time fractional diffusion equation. A detailed description of this method can be found within the thesis.

4.4. Third order compact finite difference scheme

The final scheme here presented for time fractional diffusion equations was developed by Ji and Sun in [21]. This high-order compact difference scheme uses the third order accurate time weighted and shifted Grünwald difference operator for time discretization defined in (3.10). For the spacial direction, a compact technique is employed. Even though Ji and Sun derive an approximation for the Riemann-Liouville derivatives, they then focus on the particular cases where there is equivalence between the Riemann-Liouville and Caputo forms of the time fractional diffusion problem, developing a scheme for the Caputo form of the time fractional initial-boundary value problem in equations (4.4)-(4.6). Before proceeding further with the discretization there are two lemmas in [21] which are fundamental to the development of the scheme that will now be stated.

Lemma 4.1. If u(0)=0, then it holds that ${}_0D_t^{-\gamma}({}_0^CD_t^{\gamma}u(t)) = u(t)$ for $0 < \gamma < 1$.

Lemma 4.2. Define $\theta(s) = (1-s)^3 = [5 - 3(1-s)^2]$. if $g(x) \in C^6[a,b]$,$h = (b-a)/M$, $x_i = a + ih(0 \leq i \leq M)$ it holds that

$$\frac{1}{12}[g''(x_{i-1}) + 10g''(x_i) + g''(x_{i+1})] = \frac{g(x_{i-1} - 2g(x_i) + g(x_{i+1})}{h^2} + \mathcal{O}(h^4), \quad 1 \leq i \leq M-1 \tag{4.13}$$

In addition, let an average operator be defined as

$$\mathcal{A}u_i^n = \begin{cases} \frac{1}{12}(u_{i-1}^n + 10u_i^n + u_{i+1}^n) = (I + \frac{h^2}{12}\delta_x^2)u_i^n, & 1 \leq i \leq M-1 \\ u_i^n, \quad i = 0 \quad \text{or} \quad M \end{cases} \tag{4.14}$$

Looking at the structure of the time weighted and shifted Grünwald difference operator in (3.10), it can be seen that the discretization of the first time level for equation (4.4) needs to be considered separately from the second to the Nth time levels. It will be further assumed that $u(x,t) \in C_{x,t}^{6,5}([a,b] \times [0,T])$ and $\frac{\partial^k u(x,0)}{\partial t^k} = 0$ for $k = 0, 1, ..., 5$, which allows for ${}_0^CD_t^{\gamma}u(x_i,t_n) = {}_0^{RL}D_t^{\gamma}u(x_i,t_n))$.

The discretization for time levels with $2 \leq n \leq N$ will be first considered. At grid point (x_i, t_n) equation 4.4 gives

$${}_0^CD_t^{\gamma}u_i^n = K_\gamma \frac{\partial^2 u_i^n}{\partial x^2} + f_i^n, \quad 0 \leq i \leq M, \quad 2 \leq n \leq N \tag{4.15}$$

If the weighted and shifted Grünwald difference operator is chosen to approximate ${}_0^CD_t^{\gamma}u(x_i,t_n)$, followed by the application of the average operator $\mathcal{A}$ to both sides of the equation and using Lemma 4.2 will lead to

$$\frac{1}{\tau^\gamma}\sum_{k=0}^{n} g_k^{(\gamma)}\mathcal{A}u_i^{n-k} = K_\gamma\delta_x^2u_i^n + \mathcal{A}f_i^n + R_i^n, 1 \leq i \leq M-1, 2 \leq n \leq N \tag{4.16}$$

where

$$|R_i^n| \leq C_1(\tau^3 + h^4), 1 \leq i \leq M-1, 2 \leq n \leq N \tag{4.17}$$

To obtain the discretization at the first time step, the Riemann-Liouville integral operator ${}_0^{RL}D_t^{-\gamma}$ is applied on both sides of equation (4.4). Making use of lemma 4.1 one obtains

$$u(x,t_1) = \frac{K_\gamma}{\Gamma(\gamma)}\int_0^{t_1}\frac{u_{xx}(x,\xi)}{(t_1-\xi)^{1-\gamma}}d\xi + F(x,t_1) \tag{4.18}$$

using $u_{xx}(x,0)$, $u_{xxt}(x,0)$ and $u_{xx}(x,t_1)$ to make an Hermite interpolation of $u_{xx}(x,\xi)$ on the interval $[0,t_1]$, it follows that

$$P(x,\xi) = u_{xx}(x,0) + u_{xxt}(x,0)(\xi - 0) + \frac{u_{xx}(x,t_1) - u_{xx}(x,0) - \tau u_{xxt}(x,0)}{\tau^2}(\xi - 0)^2 \tag{4.19}$$

If $u(x,0) = 0$ and $u_t(x,0) = 0$ one obtains

$$u(x,t_1) \approx u(x,t_1) = \frac{K_\gamma}{\Gamma(\gamma)}\int_0^{t_1}\frac{P(x,\xi)}{(t_1-\xi)^{1-\gamma}}d\xi + F(x,t_1) = \frac{2K_\gamma}{\Gamma(\gamma+3)}\tau^\gamma u_{xx}(x,t_1) + F(x,t_1) \tag{4.20}$$

where $F(x,t) ={}_0^{RL} D^{-\gamma}f(x,t)$

Once again, applying the space average operator $\mathcal{A}$ and using Lemma 4.2 gives

$$\frac{1}{\tau^\gamma}\mathcal{A}u_i^1 = \frac{2K_\gamma}{\Gamma(\gamma+3)}\delta_x^2 u_i^1 + \frac{1}{\tau^\gamma}\mathcal{A}F(x_i,t_1) + R_i^1, 1 \le i \le M-1 \tag{4.21}$$

where

$$|R_i^1| \le C_3(\tau^3 + h^4), 1 \le i \le M-1 \tag{4.22}$$

Finally, omitting the error terms R_i^n and replacing u_i^n with the numerical approximation U_i^n the final scheme is

$$\frac{1}{\tau^\gamma}\sum_{k=0}^{n} g_k^{(\gamma)}\mathcal{A}U_i^{n-k} = K_\gamma \delta_x^2 U_i^n + \mathcal{A}f_i^n, 1 \le i \le M-1, 2 \le n \le N \tag{4.23}$$

$$\frac{1}{\tau^\gamma}\mathcal{A}U_i^1 = \frac{2K_\gamma}{\Gamma(\gamma+3)}\delta_x^2 U_i^1 + \frac{1}{\tau^\gamma}\mathcal{A}F(x_i,t_1), 1 \le i \le M-1 \tag{4.24}$$

Equations (4.23) and (4.24) are systems of linear diagonally dominant equations, having a unique solution and easily solved. Having discretized the scheme and provided an error estimation Ji and Sun proceed with the stability and convergence analysis of the scheme concluding that the difference scheme is unconditionally stable to for all $\gamma \in [0, \gamma*]$, with $\gamma* = 0.9569347$. Furthermore if $e_i^n = u(x_i,t_n) - u_i^n$, when $N\tau \le T$ it holds that

$$\tau \sum_{m=1}^{N} \|e^m\|_\infty \le= \frac{b-a}{2}\sqrt[2]{C_4 T(c_1^2 T + C_3^2)}(\tau^3 + h^4). \tag{4.25}$$

5. Numerical example

In this section numerical, the behaviour of the selected schemes for the time fractional diffusion equations is studied. A comparison of the schemes is made, confronting the solutions of the same problem given by different schemes, in terms of convergence order, error and computational cost. Consider the following time fractional diffusion equation of the form (4.1)-(4.3)

$$\frac{\partial u}{\partial t} = {}^{RL}_{0}D_t^{1-\gamma}\left[K\frac{\partial^2 u}{\partial x^2}\right] + f(x,t), \quad x \in [0,L], \quad t \in [0,T] \tag{5.1}$$

$$u(x, t=0) = 0, \quad x \in [0,L] \tag{5.2}$$

$$u(x=0,t) = 0, \quad U(x=L,t) = t^{4-\gamma}\sin(1), \quad t \in [0,t] \tag{5.3}$$

where $K = 1$, $L = 1$, $T = 1$ and source term $f(x,t)$ is given by

$$f(x,t) = \sin(x)\left[(4-\gamma)t^{3-\gamma}\frac{\Gamma(5-\gamma)t^3}{6}\right] \tag{5.4}$$

The exact solution of the problem is $u(x,t) = t^{4-\gamma}\sin(x)$.Since $u(x,t=0) = 0$, equation (5.1) can easily be converted to the form of equation (4.4) form by means of the procedure described in section 4.1.

Table 5.1 lists the results of the time convergence analysis of the three schemes that were analysed. For each scheme three different fractional orders ($\gamma = 0.2$, $\gamma = 0.5$ and $\gamma = 0.8$) were considered and the $L^\infty_{h,\tau}$ error was registered with the refinement of the time interval, allowing the computation of the convergence order. The $L^\infty_{h,\tau}$ error is defined as follows

$$L^\infty_{h,\tau} = \max|U_i^n - u_i^n|, \quad 0 \le i \le M, \quad 0 \le n \le N \tag{5.5}$$

Where u_i^n is the exact and U_i^n the numerical solution of problem (5.1)-(5.3), with the mesh step-sizes h and τ at the grid point (x_i,t_n). If $h \ll \tau^{a/b}$ the order of convergence EOC in time of an error $E(h,\tau)$ may be calculated by

$$EOC = log_{\frac{\tau_1}{\tau_2}}\left(\frac{E(h,\tau_1)}{E(h,\tau_2)}\right) \tag{5.6}$$

The time step was kept at value $h = 1/2000$, guaranteeing that in every test case the contribution of the space truncation error to the solution is minimal when compared with the time contribution. Te first, second and third order schemes were shown, in the previous sections, to have errors $\mathcal{O}(\tau + h^2)$, $\mathcal{O}(\tau^2 + h^2)$

Table 5.1: L^∞ error and its order of convergence with decrease of the temporal step size, for the presented schemes for the time fractional diffusion equation. The results were taken with $h = 1/2000$.

	$1/\tau$	$\gamma = 0.2$ $L^\infty_{h,\tau}$	EOC	$\gamma = 0.5$ $L^\infty_{h,\tau}$	EOC	$\gamma = 0.8$ $L^\infty_{h,\tau}$	EOC
$1^{st}Order$	8	2.696E-02	-	2.438E-02	-	2.162E-02	-
	16	1.327E-02	1.02	1.223E-02	1.00	1.100E-02	0.97
	32	6.581E-03	1.01	6.123E-03	1.00	5.550E-03	0.99
	64	3.277E-03	1.01	3.064E-03	1.00	2.787E-03	0.99
	128	1.635E-03	1.00	1.533E-03	1.00	1.397E-03	1.00
	256	8.168E-04	1.00	7.664E-04	1.00	6.991E-04	1.00
	512	4.082E-04	1.00	3.832E-04	1.00	3.497E-04	1.00
$2^{nd}Order$	8	1.223E-03	-	8.840E-04	-	8.613E-04	-
	16	2.939E-04	2.06	2.156E-04	2.04	2.101E-04	2.04
	32	7.097E-05	2.05	5.301E-05	2.02	5.164E-05	2.02
	64	1.721E-05	2.04	1.310E-05	2.02	1.276E-05	2.02
	128	4.187E-06	2.04	3.248E-06	2.01	3.164E-06	2.01
	256	1.022E-06	2.03	8.079E-07	2.01	7.871E-07	2.01
	512	2.510E-07	2.03	2.019E-07	2.00	1.967E-07	2.00
$3^{rd}Order$	8	5.792E-05	-	1.164E-04	-	2.053E-04	-
	16	7.518E-06	2.95	1.461E-05	2.99	3.357E-05	2.61
	32	9.568E-07	2.97	1.829E-06	3.00	4.982E-06	2.75
	64	1.207E-07	2.99	2.288E-07	3.00	7.362E-07	2.76
	128	1.517E-08	2.99	2.863E-08	3.00	1.007E-07	2.87
	256	1.926E-09	2.98	3.608E-09	2.99	1.337E-08	2.91
	512	2.691E-10	2.84	4.915E-10	2.88	1.772E-09	2.92

and $\mathcal{O}(\tau^3 + h^4)$, respectively and any $h \leq \tau$ will result for the three cases in a smaller contribution of the space error.

The results for the first order scheme, listed in the table correspond to $\theta = 0$, the fully implicit situation. Other values of θ were tested namely $\theta = 1/2$, but use of first order weights in the computation of the time fractional derivative prevents that higher than first order convergence is achieved. Consequently the results with other θ values display similar results. The first order scheme clearly shows the expected first order of convergence,with the halving of the maximum error with the halving of the time step. Moreover, a slight error decrease can be seen with the increase in γ, all within the same order of magnitude.

The second order scheme follows also the theoretical second order predictions for error convergence. This scheme naturally allows a significant reduction of the maximum error when compared with the first order scheme. A slight error decrease with the increase of γ is also observed in this case.

The third order scheme, even if it can be said that it behaves according to the theoretical results, shows a need for smaller time steps to reach asymptotic convergence in the case of $\gamma = 0.8$. On the other hand, the results for $\gamma = 0.2$ and $\gamma = 0.5$ show third order convergence even with the coarse grids. Contrary to the two previous schemes, a slight increase in the error is observed with the increase γ. Naturally, the maximum errors observed are orders of magnitude smaller than with the two previous schemes.

Table 5.2 lists the computing times of each of the solutions used to produce the results of Table 5.1 with ($\gamma = 0.5$) and no significant differences were observed for other γ values. The results on Table 5.1 show that the time of computation is decreasing with the order of the scheme partly because the computation of time fractional derivatives involves all previous time steps, regardless of the order of the scheme the number of time steps involved will be the same. It was seen that this decrease is mainly due to the computing times of the right side matrix, when building the scheme. The matrix associated with the implicit time step showed similar spectral radius for every scheme and the times for the solution of the system of equations at each time step also revealed to be identical. The first order scheme requires the computation of the weighted average of the time fractional derivative of the space derivative in two time steps, while the second order scheme evaluates the fractional derivative at only one time step, thus explaining the observed drop in computing time. The third order scheme also reveals a considerable decrease of computing times with respect to the second order schemes that may be related with the solution of the fractional diffusion equation in the Caputo form.

These results indicate that high order schemes for the solution of the time fractional diffusion equation are the best choice and the ability of reaching the same order of magnitude with less time steps is an enormous advantage, with significant reduction of computing times.

Table 5.2: Time of computation for each scheme for each of the presented schemes. The results correspond to a constant space step $h = 1/2000$.

	Time Of Computation (s)		
$1/\tau$	$1^{st}Order$	$2^{nd}Order$	$3^{rd}Order$
8	0.095	0.090	0.332
16	0.105	0.093	0.363
32	0.149	0.116	0.367
64	0.288	0.225	0.400
128	0.949	0.672	0.636
256	3.390	2.331	1.287
512	14.125	9.124	4.209

6. Conclusions

Three schemes for the time fractional diffusion equation were presented, and compared in terms of accuracy and computing time through numerical examples. All the schemes have shown to follow the theoretical predictions of their order of convergence. It was seen that weighted and shifted methods increase greatly increase computing times by considering two time levels in the time fractional derivative and that high order schemes for the solution of the time fractional diffusion equation are the best choice and the ability of reaching the same order of magnitude with less time steps is an enormous advantage, with significant reduction of computing times.

This work is part of a thesis where a similar comparison was also made for space and time-space fractional diffusion equations. An analysis was also made regarding the variable order effects in the modelling of a sub-diffusive system. This thesis presents an important effort in the building of a road between fractional calculus and it's engineering applications. A total of nine finite difference schemes are implemented and compared within three different types of fractional diffusion equations, providing the tools and knowledge to properly apply finite differences in the solution of fractional partial differential equations. An intuitive grasp on how the order of the time fractional derivative impacts the solution of a sub-diffusive system was also achieved, both for the constant and variable order cases, greatly increasing the odds of a successful application. The mastery of a numerical solution method and the understanding of the effects of constant and variable order have gathered necessary conditions and sufficient conditions to proceed with a real world application.

There is plenty future work to be done in the realm of fractional calculus. Schemes regarding other types of equation can be solved and the problem can be extended to the two-dimensional case. A higher order scheme in time and space should also be developed for the time-space fractional diffusion equation. Regarding variable order diffusion equations, a higher order scheme could also be implemented and the analysis of the order effects could be extended to the space derivative or to the fractional diffusion-wave equation. As the purpose of this work is also paving the way to future engineering applications one could now start by a simple study of diffusion, for instance in porous media, using the results obtained with a commercial software to do a parametric study of the order of the derivative in the diffusion equation. s

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