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ABOUT THE CONVERGENCE OF A NUMERICAL SCHEME OF HIGH ORDER TO SOLVE FRACTIONAL REACTION-SUBDIFFUSION EQUATION

Jorge Andrés Julca Avila[1], Aurelio José Parreira[2],
Juan Carlos Zavaleta Aguilar[3 §]

[1,2,3]Department of Mathematics and Statistics
Federal University of São João del-Rei
São João del-Rei, MG, 36307-904, BRAZIL

Abstract: In this work the anomalous diffusion phenomenon with reaction was modeled by Temporal Fractional Partial Differential Equation. The convergence of high order implicit numerical scheme for one-dimension reaction-subdiffusion equation was analyzed. Fort this, we used the Implicit Compact Finite Difference Method for discretization of spacial variable and Backward Finite Difference for temporal variable. For the Riemann-Liouville's temporal fractional derivative we used the Grünwald-Letnikov's discretization. Finally, we proved the convergence order using an example and numerical tests.

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1. Introduction

Phenomena of anomalous diffusion are some of the applications of Fractional Partial Differential Equations (FPDEs), which can be modeled for Continuous Time Random Walk (CTRW). The CTRW are direct generalizations of

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§Correspondence author

classicsal processes of random walks. An anomalous diffusion describes a diffusion process with a non-linear relation with respect to time. Frequently, we have an anomalous diffusion when the mean square displacement of particles is proportional to a power of time variable, i.e.,

$$\langle x^2(t)\rangle \propto t^{\alpha}, \tag{1}$$

where α is the exponent of the anomalous diffusion. For the particular case $\alpha = 1$ we have the classical diffusive motion. For $\alpha > 1$ the motion is super-diffusive and for $0 < \alpha < 1$ the motion is sub-diffusive.

Yuste et al. [12] present a model which describes the diffusion-reaction problem $A + B$ and state that pattern diffuse movement, which describes the evolution of the concentrations $a(x,t)$ and $b(x,t)$ of the particles A and B, respectively, is given by de following *Diffusion-Reaction Equation*

$$a_t = Da_{xx} - Kab \tag{2}$$
$$b_t = Db_{xx} - Kab \tag{3}$$

where D is the diffusion coefficient and K is the biomolecular reaction rate, both assumed constant and equal in each equation.

A subdiffusive motion is characterized by the following asymptotic behavior:

$$\langle x^2(t)\rangle \sim \frac{2K_\gamma}{\Gamma(1+\gamma)}t^{\gamma}, \quad t \to \infty, \tag{4}$$

where $0 < \gamma < 1$ is the exponent of subdiffusion and K_γ is the generalized diffusion coefficient.

The subdiffusive motions occur in complex systems, such as glassy and disordered materials, in which pathways are constrained for geometric or energetic reasons, see e.g. [3]. Chen et al. [4] state some works on anomalous subdiffusion. For example, anomalous subdiffusion of proteins and lipids in membranes observed by fluorescence correlation spectroscopy, anomalous subdiffusion as a measure of cytoplasmic agglomeration in living cells, among others.

The fractional reaction-subdiffusion equations, formulated in [12], are given by

$$a_t = {}_0D_t^{1-\gamma}\Big(K_\gamma a_{xx} - Kab\Big), \tag{5}$$
$$b_t = {}_0D_t^{1-\gamma}\Big(K_\gamma b_{xx} - Kab\Big), \tag{6}$$

where ${}_0D_t^{1-\gamma}$ is the Riemann-Liouville (R-L) operator of order $1-\gamma$. For $0 < \gamma < 1$ a temporal (R-L) fractional derivative of a function $y(t)$ is defined by

$$ {}_0D_t^{1-\gamma} y(t) = \frac{1}{\Gamma(\gamma)} \frac{d}{dt} \int_0^t \frac{y(\tau)}{(t-\tau)^{1-\gamma}} d\tau. \tag{7} $$

Note that the Riemann-Liouville operator is the identity operator, when $\gamma = 1$ and is the classical derivative operator, when $\gamma = 0$.

Decoupling equations (5)-(6), as given in [3], we obtain a *Fractional Reaction-Subdiffusion Equation*,

$$ u_t \quad = \quad {}_0D_t^{1-\gamma}\Big(K_\gamma u_{xx} - Ku\Big) + f, \tag{8} $$

where $u = u(x, y)$ describes the motion of particles of a subdiffusive process with reaction and $f(x, y)$ is a known source term.

Regarding the numerical solution of (8), Chen et al [3] state two classical numerical schemes. The first, is the second-order of convergence in the spacial variable and, the second, considering the bases of finite differences uses Richardson Extrapolation that, through, of a α parameter improves the spacial convergence order. However, it is unclear about the order of convergence of this method.

In this work, we state a high order numerical scheme for (8). The numerical scheme uses compact finite differences for spacial discretization and converge with fourth-order accuracy. The validity of the results is done by an example and several numerical tests for different values of γ.

2. The Model

We state (8) as an initial-boundary value problem. Let $\Omega = (a, b)$, $a \neq b$, $\mathrm{I} = (0, T]$, $T > 0$ be intervals of real numbers. We denote by $\mathrm{Q} = \Omega \times \mathrm{I}$, $\Sigma_a = \{a\} \times \bar{\mathrm{I}}$ and $\Sigma_b = \{b\} \times \bar{\mathrm{I}}$, where Σ_a and Σ_b denote the boundary of Q. An one-dimensional reaction-subdiffusion problem, with initial-boundary condition, consists in finding a function $u : \overline{\mathrm{Q}} \longrightarrow \mathbb{R}$ such that

$$ u_t \quad = \quad {}_0D_t^{1-\gamma}\Big(K_\gamma u_{xx} - Ku\Big) + f \quad \text{in} \quad \mathrm{Q}, \tag{9} $$

$$ u(0) \quad = \quad u_0 \quad \text{on} \quad \Omega, \tag{10} $$

$$ u \quad = \quad \varphi \quad \text{on} \quad \Sigma_a, \tag{11} $$

$$ u \quad = \quad \psi \quad \text{on} \quad \Sigma_b, \tag{12} $$

where K_γ and K take positive values, and $f(x, t)$, $u_0(x)$, $\varphi(t)$ and $\psi(t)$ are sufficiently smooth functions. Therefore, the equations (9)-(12) are our FPDE.

3. Space-Time Discretization

Let the following discrete sets be given:

$$\begin{aligned} \Omega_h &= \{x_i : \ x_i = a + ih, \ i = 1, 2, ..., M-1, \ \ h = (b-a)/M\}, \\ \mathrm{I}^\tau &= \{t_n : \ t_n = n\tau, \ n = 1, 2, ..., N, \ \ \tau = T/N\}, \\ \mathrm{Q}_h^\tau &= \Omega_h \times \mathrm{I}^\tau. \end{aligned}$$

Define a uniform mesh $\mathcal{M}$ by the clausure of set Q_h^τ, i.e.,

$$\mathcal{M} := \overline{\mathrm{Q}_h^\tau} = \mathrm{Q}_h^\tau \cup \partial \mathrm{Q}_h^\tau,$$

where $\partial \mathrm{Q}_h^\tau = \Sigma_a^\tau \cup \Sigma_b^\tau \cup \Omega_h^0$ is a boundary of Q_h^τ and, $\Sigma_a^\tau = \{a\} \times \overline{\mathrm{I}^\tau}$, $\Sigma_b^\tau = \{b\} \times \overline{I^\tau}$ and $\Omega_h^0 = \Omega_h \times \{0\}$, where $\overline{\mathrm{I}^\tau} = \{0\} \cup \mathrm{I}^\tau$. The points $(x_i, t_n) \in \mathcal{M}$ are called nodes of the mesh and, usually denote by (i, n). Let y be a function and consider the notation $y_i^n \equiv y(x_i, t_n)$ and, for a discrete function Y, the following notation, $Y_i^n \equiv Y(i, n)$.

3.1. Space-Time Discretization

We approach the second-order spatial derivative by second-order finite difference operator and fourth-order compact finite difference operator.

3.1.1. Second Derivative: Second-Order Approximation

For n fixed, the Taylor series about the node (i, n) of the function $y_{i\pm1}^n$, is given by

$$y_{i\pm1}^n = y_i^n \pm h(y_x)_i^n + \frac{1}{2}h^2(y_{xx})_i^n \pm \frac{1}{6}h^3(y_{xxx})_i^n + \mathcal{O}(h^4). \tag{13}$$

From (13),

$$y_{i+1}^n - 2y_i^n + y_{i-1}^n = h^2(y_{xx})_i^n + \mathcal{O}(h^4). \tag{14}$$

Define the second-order central difference operator, δ_x^2, by

$$\delta_x^2 Y_i^n := Y_{i+1}^n - 2Y_i^n + Y_{i-1}^n. \tag{15}$$

Note that this operator uses a three-points stencil. From (14) and (15), we have

$$(y_{xx})_i^n = \frac{1}{h^2}\delta_x^2 Y_i^n + \mathcal{O}(h^2). \tag{16}$$

Thus, $\frac{1}{h^2}\delta_x^2 Y_i^n$ approaches $(y_{xx})_i^n$ with second-order accuracy.

3.1.2. Second Derivative: Fourth-Order Approximation

We describe, quickly, the compact finite difference operators that approximate the second-order spatial derivative. These operators are fourth-order and use three-points stencil. For n fixed, we define, for a first-order derivative, the two main operators of first-order: forward and backward, respectively,

$$\delta_x^+ Y_i^n := Y_{i+1}^n - Y_i^n\,, \qquad \delta_x^- Y_i^n := Y_i^n - Y_{i-1}^n\,, \tag{17}$$

and, the two first-order central difference operators, by

$$\delta_x Y_i^n := Y_{i+1/2}^n - Y_{i-1/2}^n\,, \qquad \delta_x^0 := \delta_x^+ + \delta_x^-\,. \tag{18}$$

From (17) we obtain δ_x^2,

$$\delta_x^2 = \delta_x^+ - \delta_x^- \tag{19}$$

or, also, $\delta_x^2 = \delta_x(\delta_x)$.

From equations (1-60) of [1], we have

$$(y_{xx})_i^n = \left[\frac{2}{h}\sinh^{-1}\frac{\delta_x}{2}\right]^2 y_i^n \tag{20}$$

and, from equations (1-69) and (1-70) of [1],

$$\begin{aligned}
(y_{xx})_i^n &= \left[\frac{2}{h}\mathrm{senh}^{-1}\frac{\delta_x}{2}\right]^2 y_i^n \\
&= \frac{1}{h^2}\left[\delta_x - \frac{1^2}{2^2 3!}\delta_x^3 + \frac{1^2 3^2}{2^4 5!}\delta_x^5 - \frac{1^2 3^2 5^2}{2^6 7!}\delta_x^7 + \ldots\right]^2 y_i^n \\
&= \frac{1}{h^2}\left[\delta_x^2 - \frac{1}{12}\delta_x^4 + \frac{1}{90}\delta_x^6 - \frac{1}{560}\delta_x^8 + \ldots\right] y_i^n.
\end{aligned} \tag{21}$$

On the other hand, we compute

$$\begin{aligned}
\frac{1}{h^2}\left[\frac{\delta_x^2}{1+\frac{1}{12}\delta_x^2}\right] y_i^n &= \frac{1}{h^2}\delta_x^2\left[\frac{1}{1+\frac{1}{12}\delta_x^2}\right] y_i^n \\
&= \frac{1}{h^2}\delta_x^2\left[1 - \frac{1}{12}\delta_x^2 + \frac{1}{144}\delta_x^4 - \frac{1}{1728}\delta_x^6 + \ldots\right] y_i^n \\
&= \frac{1}{h^2}\left[\delta_x^2 - \frac{1}{12}\delta_x^4 + \frac{1}{144}\delta_x^6 - \frac{1}{1728}\delta_x^8 + \ldots\right] y_i^n
\end{aligned} \tag{22}$$

By comparing (21) and (22) we observe that terms are quite similar. Thus, we can consider the following approximation

$$(y_{xx})_i^n \approx \frac{1}{h^2}\left[\frac{\delta_x^2}{1+\frac{1}{12}\delta_x^2}\right]y_i^n \tag{23}$$

or, for some p,

$$(y_{xx})_i^n = \frac{1}{h^2}\left[\frac{\delta_x^2}{1+\frac{1}{12}\delta_x^2}\right]y_i^n + \mathcal{O}(h^p). \tag{24}$$

In order to obtain the truncation error $\mathcal{O}(h^p)$, we multiply (23) by the operator $1+\frac{1}{12}\delta_x^2$. Thus, we have

$$\left[1+\frac{1}{12}\delta_x^2\right](y_{xx})_i^n = \frac{1}{h^2}\delta_x^2 y_i^n + \mathcal{O}(h^p), \tag{25}$$

or

$$\frac{1}{12}(y_{xx})_{i+1}^n + \frac{5}{6}(y_{xx})_i^n + \frac{1}{12}(y_{xx})_{i-1}^n = \frac{1}{h^2}\left[y_{i+1}^n - 2y_i^n + y_{i-1}^n\right] + \mathcal{O}(h^p). \tag{26}$$

In (26) we expand, in a Taylor series about the node (i,n), all functions evaluate at the nodes $(i\pm 1, n)$. The terms on the left hand and right hand, are expanded with truncation error $\mathcal{O}(h^6)$ and $\mathcal{O}(h^8)$, respectively. So,

$$\mathcal{O}(h^p) = \frac{1}{240}h^4(y_{xxxxxx})_i^n + \mathcal{O}(h^6). \tag{27}$$

From (24) and (27), we have

$$(y_{xx})_i^n = \frac{1}{h^2}\left[\frac{\delta_x^2}{1+\frac{1}{12}\delta_x^2}\right]Y_i^n + \frac{1}{240}h^4(y_{xxxxxx})_i^n + \mathcal{O}(h^6). \tag{28}$$

Therefore, $\frac{\delta_x^2}{1+\frac{1}{12}\delta_x^2}$ is the fourth-order compact finite difference operator, for the second-order spatial derivative.

3.2. Temporal Approximation

We will approach the fractional derivative by Grünwald-Letnikov fractional difference operator and, the classical temporal derivative, by backward finite difference operator.

3.2.1. Fractional Derivative

According to [8], the α-order Riemann-Liouville fractional derivative, $\alpha > 0$, is equivalent to the α-order Grünwald-Letnikov fractional derivative, defined by

$$ {}_0D_t^\alpha y(t) = \lim_{\tau\to 0} \frac{1}{\tau^\alpha} \sum_{j=0}^{[t/\tau]} \omega_j^\alpha \, y(t - j\tau), \; t \geqslant 0, \tag{29} $$

where $[t/\tau]$ denotes the integer part of t/τ, and ω_j^α are the coefficient of the generating function $\omega(z+\alpha)$, i.e.,

$$ \omega(z+\alpha) = \sum_{j=0}^{\infty} \omega_j^\alpha z^j. \tag{30} $$

Note that (29) can be reformulated as follows

$$ {}_0D_t^\alpha y(t) = \frac{1}{\tau^\alpha} \sum_{j=0}^{[t/\tau]} \omega_j^\alpha \, y(t - j\tau) + \mathcal{O}(\tau^p). \tag{31} $$

According to [6], [11] the truncation error $\mathcal{O}(\tau^p)$ in (31), depends on the choice the ω_j^α. When $\omega(z+\alpha) = (1-z)^\alpha$ we have $\omega_j^\alpha = (-1)^j \binom{\alpha}{j}$ and, consequently, $p = 1$. Thus, the fractional derivative of the discrete function, $y^n \equiv y(t_n)$, is given by

$$ {}_0D_t^\alpha y^n = \frac{1}{\tau^\alpha} \sum_{j=0}^{n} \omega_j^\alpha \, y^{n-j} + \mathcal{O}(\tau), \tag{32} $$

where the coefficients ω_j^α are obtained, recursively, by the following formula:

$$ \omega_0^\alpha = 1, \quad \omega_j^\alpha = \left[1 - \frac{(\alpha+1)}{j}\right] \omega_{j-1}^\alpha, \quad j = 1, 2, ..., n. \tag{33} $$

We define the α-order Grünwald-Letnikov fractional operator, by

$$ {}_0\delta_t^\alpha Y^n := \frac{1}{\tau^\alpha} \sum_{j=0}^{n} \omega_j^\alpha \, Y^{n-j}. \tag{34} $$

Therefore, the Grünwald-Letnikov fractional derivative can be expressed as

$$ {}_0D_t^\alpha y^n = {}_0\delta_t^\alpha Y^n + \mathcal{O}(\tau). \tag{35} $$

3.2.2. First-Order Derivative

For the first-order temporal derivative, we define the first-order backward finite difference operator:

$$\delta_t^- Y_i^n := Y_i^n - Y_i^{n-1}. \tag{36}$$

Thus, the temporal derivative with truncation error $\mathcal{O}(\tau)$ has the form

$$(y_t)_i^n = \frac{1}{\tau}\delta_t^- Y_i^n + \mathcal{O}(\tau). \tag{37}$$

4. Compact Finite Difference Scheme

Substituting the operators: fourth-order compact finite difference, α-order Grünwald-Letnikov fractional and first-order backward finite difference in our FPDE, (9)-(12), we obtain the following Compact Finite Difference (CFD) numerical scheme:

$$\begin{aligned}
\frac{1}{\tau}\delta_t^- U_i^n &= {}_0\delta_t^{1-\gamma}\Bigg(K_\gamma \frac{1}{h^2}\Big[\frac{\delta_x^2}{1+\frac{1}{12}\delta_x^2}\Big]U_i^n - KU_i^n\Bigg) + f_i^n \quad \text{in} \quad Q_h^\tau && (38)\\
U_i^0 &= (u_0)_i \quad \text{on} \quad \Omega_h && (39)\\
U_0^n &= \varphi^n \quad \text{on} \quad \Sigma_a^\tau && (40)\\
U_M^n &= \psi^n \quad \text{on} \quad \Sigma_b^\tau, && (41)
\end{aligned}$$

where U_i^n is a theoretical solution of our numerical scheme at a node $(i,n) \in Q_h^\tau$. The equation (38) is equivalent to

$$\delta_t^- U_i^n = K_\gamma \frac{\tau}{h^2}\Big[1+\frac{1}{12}\delta_x^2\Big]^{-1}\big({}_0\delta_t^{1-\gamma}\big)\delta_x^2 U_i^n - K\tau\, {}_0\delta_t^{1-\gamma} U_i^n + \tau f_i^n \ \text{in} \ Q_h^\tau. \tag{42}$$

Denote

$$\mu_1 = K_\gamma \frac{\tau}{h^2}, \ \mu_2 = K\tau, \ \mu_3 = \frac{1}{\tau^{1-\gamma}}\Big(\mu_1 - \frac{1}{12}\mu_2\Big)$$
$$\mu_4 = \frac{2}{\tau^{1-\gamma}}\Big(\mu_1 + \frac{5}{12}\mu_2\Big), \quad \lambda_j = \omega_j^{1-\gamma}. \tag{43}$$

Thus, (42) is

$$\begin{aligned}
\Big[1+\frac{1}{12}\delta_x^2\Big]\delta_t^- U_i^n &= \mu_1\big({}_0\delta_t^{1-\gamma}\big)\delta_x^2 U_i^n - \mu_2\Big[1+\frac{1}{12}\delta_x^2\Big]{}_0\delta_t^{1-\gamma} U_i^n \\
&+ \tau\Big[1+\frac{1}{12}\delta_x^2\Big]f_i^n \quad \text{in} \quad Q_h^\tau. && (44)
\end{aligned}$$

After some calculations, the CFD numerical scheme (38)-(41), is given by

$$\begin{aligned}(1-12\mu_3)U_{i-1}^n &+ (10+12\mu_4)U_i^n + (1-12\mu_3)U_{i+1}^n = U_{i-1}^{n-1} + 10U_i^{n-1}\\ &+ U_{i+1}^{n-1} + 12\sum_{j=1}^{n}\lambda_j\Big(\mu_3 U_{i-1}^{n-j} - \mu_4 U_i^{n-j} + \mu_3 U_{i+1}^{n-j}\Big)\\ &+ \tau\big(f_{i-1}^n + 10f_i^n + f_{i+1}^n\big) \quad \text{in} \quad Q_h^\tau \qquad (45)\\ U_i^0 &= (u_0)_i \quad \text{on} \quad \Omega_h \qquad (46)\\ U_0^n &= \varphi^n \quad \text{on} \quad \Sigma_a^\tau \qquad (47)\\ U_M^n &= \psi^n \quad \text{on} \quad \Sigma_b^\tau. \qquad (48)\end{aligned}$$

In the last formulation, it is observed that the CFD numerical scheme is implicit, and reduces to an algebraic linear system of dimension $(M-1)\times(M-1)$. This system, in matrix notation, is given by

$$A\mathbf{U}^n = B\mathbf{U}^{n-1} + C\sum_{j=1}^{n}\lambda_j\mathbf{U}^{n-j} + D\mathbf{F}^n + \mathbf{G}_\Sigma^n, \quad \text{in} \quad Q_h^\tau, \qquad (49)$$

where

$$\begin{aligned} A &= \text{tridiag}(1-12\mu_3, 10+12\mu_4, 1-12\mu_3), & B &= \text{tridiag}(1,10,1),\\ C &= 12\,\text{tridiag}(\mu_3, -\mu_4, \mu_3), & D &= \tau B,\end{aligned}$$

are tridiagonal matrices of order $(M-1)\times(M-1)$,

$$\mathbf{U}^n = (U_1^n \ldots U_{M-1}^n)^{\mathrm{T}}, \qquad \mathbf{F}^n = (f_1^n \ldots f_{M-1}^n)^{\mathrm{T}} \qquad (50)$$

are, respectively, the unknown vector and the vector associated to f, of orders $\mathbb{R}^{M-1}$, and

$$\mathbf{G}_\Sigma^n = -(1-12\mu_3)\mathbf{U}_\Sigma^n + \mathbf{U}_\Sigma^{n-1} + 12\mu_3\textstyle\sum_{j=1}^n\lambda_j\mathbf{U}_\Sigma^{n-j} + \tau\mathbf{F}_\Sigma^n,$$

is the boundary vector of order $\mathbb{R}^{M-1}$, where $\mathbf{U}_\Sigma^n = (U_0^n\,0\,0\ldots0\,U_M^n)^{\mathrm{T}}$ and $\mathbf{F}_\Sigma^n = (f_0^n\,0\,0\ldots0\,f_M^n)^{\mathrm{T}}$.

The following theorem ensures the existence and uniqueness of solutions by our numerical scheme.

Theorem 4.1. *The linear system (49), associated with the CFD numerical scheme (38)-(41), has a unique solution.*

Proof. Note that the matrix A is strictly diagonally dominant. Consequently it is nonsingular and thus invertible. Therefore, our numerical scheme has a unique solution. □

5. Consistency, Stability and Convergence of CFD Scheme

5.1. Consistency

We will prove that our numerical scheme is consistent with our FPDE, with fourth-order spatial accuracy and first-order temporal accuracy.

Lemma 5.1. *For each $n = 1, ..., N$. Let y^{n-j} be a bounded function, $0 < \gamma < 1$ and $\lambda_j = \omega_j^{1-\gamma}$. Then,*

$$\left| \sum_{j=0}^{n} \lambda_j y^{n-j} \right| \leqslant C_n, \quad C_n = c_n n^{\gamma-1}, \quad c_n = \max_{j\in\{0,\dots,n\}} \left| y^{n-j} \right|. \tag{51}$$

Proof.

$$\left| \frac{1}{\tau^{1-\gamma}} \sum_{j=0}^{n} \lambda_j y^{n-j} \right| \leqslant c_n \frac{1}{\tau^{1-\gamma}} \sum_{j=0}^{n} \left| \lambda_j \right|, \quad c_n = \max_{j\in\{0,\dots,n\}} \left| y^{n-j} \right|.$$

From (33) we have $\lambda_j < 0$ for all $j = 1, ..., n$. Thus,

$$\left| \frac{1}{\tau^{1-\gamma}} \sum_{j=0}^{n} \lambda_j y^{n-j} \right| \leqslant c_n \left(\frac{2}{\tau^{1-\gamma}} - \frac{1}{\tau^{1-\gamma}} \sum_{j=0}^{n} \lambda_j \right).$$

From (32) and (7): $\frac{1}{\tau^{1-\gamma}} \sum_{j=0}^{n} \lambda_j = \frac{t_n^{\gamma-1}}{\Gamma(\gamma)} + \mathcal{O}(\tau) = \frac{(n\tau)^{\gamma-1}}{\Gamma(\gamma)} + \mathcal{O}(\tau)$. Hence

$$\left| \frac{1}{\tau^{1-\gamma}} \sum_{j=0}^{n} \lambda_j y^{n-j} \right| \leqslant c_n \Big(2\,\tau^{\gamma-1} - \frac{1}{\Gamma(\gamma)} n^{\gamma-1} \tau^{\gamma-1} + c_o \tau \Big).$$

where c_0 is a constant. Thus

$$\left| \frac{1}{\tau^{1-\gamma}} \sum_{j=0}^{n} \lambda_j y^{n-j} \right| \leqslant C_n \tau^{\gamma-1}, \quad C_n = c_n n^{\gamma-1},$$

or

$$\left| \sum_{j=0}^{n} \lambda_j y^{n-j} \right| \leqslant C_n.$$

$\square$

The *local truncation error* of our scheme, at a node (i,n), is given by

$$R_i^n$$

$$= R_i^n(h,\tau) = \frac{1}{\tau}\delta_t^- U_i^n - {}_0\delta_t^{1-\gamma}\left(K_\gamma \frac{1}{h^2}\Big[\frac{\delta_x^2}{1+\frac{1}{12}\delta_x^2}\Big]U_i^n \;-\; KU_i^n\right) \;-\; f_i^n. \quad (52)$$

Theorem 5.1. *Let* $\tau = h^{\frac{\kappa}{1-\gamma}}$, $0<\kappa<4$. *The CFD numerical scheme (38)-(41) is consistent with FPDE (9)-(12), and there exists a constant* $C_{i,n}>0$ *such that,*

$$|R_i^n| \;\leqslant\; C_{i,n}(n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau), \quad (53)$$

for all h,τ *sufficiently small.*

Proof. From (37),

$$\frac{1}{\tau}\delta_t^- U_i^n \;=\; (u_t)_i^n + \mathcal{O}(\tau), \quad (54)$$

from (28) and (35),

$$\begin{aligned}
&{}_0\delta_t^{1-\gamma}\Big(K_\gamma\,\frac{1}{h^2}\Big[\frac{\delta_x^2}{1+\frac{1}{12}\delta_x^2}\Big]U_i^n\Big) \\
&\quad = K_{\gamma}\,{}_0\delta_t^{1-\gamma}\Big((u_{xx})_i^n - \frac{1}{240}h^4(u_{xxxxxx})_i^n + \mathcal{O}(h^6)\Big) \\
&\quad = K_\gamma\Big({}_0D_t^{1-\gamma}(u_{xx})_i^n - \frac{1}{240}h^4\frac{1}{\tau^{1-\gamma}}\sum_{j=0}^{n}\lambda_j(u_{xxxxxx})_i^{n-j} \\
&\quad + \;\; \mathcal{O}(\tau)\Big),
\end{aligned} \quad (55)$$

and from (35)

$${}_0\delta_t^{1-\gamma}\big(KU_i^n\big) \;=\; K\big({}_0D_t^{1-\gamma}u_i^n + \mathcal{O}(\tau)\big). \quad (56)$$

Substituting (54)-(56) in (52),

$$\begin{aligned}
R_i^n \;&=\; (u_t)_i^n + \mathcal{O}(\tau) - K_\gamma\Big({}_0D_t^{1-\gamma}(u_{xx})_i^n - \frac{1}{240}h^4\frac{1}{\tau^{1-\gamma}}\sum_{j=0}^{n}\lambda_j(u_{xxxxxx})_i^{n-j} \\
&+ \;\; \mathcal{O}(\tau)\Big) + K\Big({}_0D_t^{1-\gamma}u_i^n + \mathcal{O}(\tau)\Big) - f_i^n \\
&=\; \frac{K_\gamma}{240}h^4\tau^{\gamma-1}\left(\sum_{j=0}^{n}\lambda_j(u_{xxxxxx})_i^{n-j}\right) + \mathcal{O}(\tau).
\end{aligned} \quad (57)$$

By Lemma 5.1, the term of summation is bounded and, the term $h^4\tau^{\gamma-1} \to 0$, if $h^4 \to 0$ faster than $\tau^{\gamma-1}$. Thus, for $\tau = h^{\frac{\kappa}{1-\gamma}}$, $0 < \kappa < 4$, the truncation error $R_i^n \to 0$ as $h, \tau \to 0$. For each (i, n) fixed, we have from (57) and from constant C_n, in (51), that

$$\begin{aligned} R_i^n &= \mathcal{O}\big(h^4\tau^{\gamma-1}n^{\gamma-1} + \tau\big) = \mathcal{O}\big(h^4\tau^{\gamma-1}n^{\gamma-1} + \tau + h^4 + n^{\gamma-1}\tau^{\gamma}\big) \\ &= \mathcal{O}\Big((n^{\gamma-1}\tau^{\gamma-1} + 1)(h^4 + \tau)\Big), \quad h, \tau \to 0. \end{aligned}$$

Therefore, there exists a positive constant $C_{i,n}$ such that,

$$|R_i^n| \leqslant C_{i,n}(n^{\gamma-1}\tau^{\gamma-1} + 1)(h^4 + \tau)$$

for all h, τ sufficiently small. $\square$

5.2. Stability Analysis

We will analyze the stability of CFD numerical scheme (38)-(41) by means of Fourier Analysis.

The unknown vector $\mathbf{U}^n$, in (50), corresponds to the theoretical solution of numerical scheme. Denote by $\widetilde{\mathbf{U}}^n$ the approximate solution of numerical scheme. The initial condition of numerical scheme is given by $\mathbf{U}^0 = (U_1^0 \dots U_{M-1}^0)^{\mathrm{T}}$ and, $\widetilde{\mathbf{U}}^0$ denotes the initial approximation of the numerical scheme.

The *round-off error* of our numerical scheme is defined by $\rho^n := \mathbf{U}^n - \widetilde{\mathbf{U}}^n$, $n = 1, 2, \dots, N$. We can consider, further, $\rho^n = (\rho_1^n \dots \rho_{M-1}^n)^{\mathrm{T}}$.

Applying $\mathbf{U}^n$ and $\widetilde{\mathbf{U}}^n$ in (49) and subtracting both equations, we obtained the round-off error equation

$$A\rho^n = B\rho^{n-1} + C\sum_{j=1}^{n} \lambda_j \rho^{n-j}\,, \quad \text{in} \quad \mathrm{Q}_h^\tau \tag{58}$$

with initial and boundary conditions

$$\rho^0 = \mathbf{U}^0 - \widetilde{\mathbf{U}}^0 \quad \text{on} \quad \Omega_h \tag{59}$$

$$\rho_0 = 0 \quad \text{on} \quad \Sigma_a^\tau \tag{60}$$

$$\rho_M = 0 \quad \text{on} \quad \Sigma_b^\tau. \tag{61}$$

In order to find the best approximation for the round-off error, we define, for each $n = 1, \dots, N$, the following function $\chi^n : [a, b] \to \mathbb{R}$, by

$$\chi^n(x) = \begin{cases} 0\,, & a \leqslant x \leqslant a + \frac{h}{2} \\ \rho_i^n\,, & x_i - \frac{h}{2} < x < x_i + \frac{h}{2}\,, \quad i = 1, \dots, M-1, \\ 0\,, & b - \frac{h}{2} < x \leqslant b. \end{cases}$$

The expansion Fourier series for this function, is given by

$$\chi^n(x) = \frac{1}{\sqrt{b-a}} \sum_{m=-\infty}^{\infty} c_n(m) e^{i2m\pi(x-a)/(b-a)}, \tag{62}$$

where

$$c_n(m) = \frac{1}{\sqrt{b-a}} \int_a^b e^{-i2m\pi(x-a)/(b-a)} \chi^n(x) dx. \tag{63}$$

Theorem 5.2. *The function χ satisfies the Parseval's Identity*

$$\int_a^b |\chi^n(x)|^2 dx = \sum_{m=-\infty}^{\infty} |c_n(m)|^2.$$

Proof. The proof of this identity can be found at Lemma 1 of [5]. □

The round-off error ρ^n, in the discrete l^2-norm, is given by

$$\|\rho^n\|_{l^2}^2 = \left(\sum_{i=1}^{M-1} h|\rho_i^n|^2 \right) \tag{64}$$

By a simple calculation we can prove that $\|\rho^n\|_{l^2}^2 = \int_a^b |\chi^n(x)|^2 dx$, see equation (13) of [2]. Thus, by Parseval's Identity, we have $\|\rho^n\|_{l^2}^2 = \sum_{m=-\infty}^{\infty} |c_n(m)|^2$.

Based on the above analysis we can suppose that the solution of (58) has the following form

$$\rho_i^n = \frac{1}{\sqrt{b-a}} d_n e^{\mathbf{i}\sigma i h}, \tag{65}$$

where $\sigma = 2\pi/(b-a)$. Substituting (65) in (58), we have

$$d_n A e^{\mathbf{i}\sigma i h} = d_{n-1} B e^{\mathbf{i}\sigma i h} + \left(\sum_{j=1}^{n} \lambda_j d_{n-j} \right) C e^{\mathbf{i}\sigma i h}, \quad \text{in} \quad \mathrm{Q}_h^\tau. \tag{66}$$

The ith equation of the above linear system, is given by

$$\tilde{a} d_n = \tilde{b} d_{n-1} + \tilde{c} \left(\sum_{j=1}^{n} \lambda_j d_{n-j} \right), \tag{67}$$

where

$$\begin{aligned} \tilde{a} &= (1-12\mu_3)e^{-\mathbf{i}\sigma h} + (10+12\mu_4) + (1-12\mu_3)e^{\mathbf{i}\sigma h} \\ &= 4\Big[3 - \sin^2\Big(\frac{\sigma h}{2}\Big)\Big] - 12\Big\{\mu_3\Big[2 - 4\sin^2\Big(\frac{\sigma h}{2}\Big)\Big] - \mu_4\Big\} \end{aligned} \tag{68}$$

$$\tilde{b} \;=\; e^{-\mathbf{i}\sigma h} + 10 + e^{\mathbf{i}\sigma h} \;=\; 4\Big[3 - \sin^2\Big(\frac{\sigma h}{2}\Big)\Big] \tag{69}$$

$$\tilde{c} \;=\; 12\Big(\mu_3 e^{-\mathbf{i}\sigma h} - \mu_4 + \mu_3 e^{\mathbf{i}\sigma h}\Big) \;=\; 12\Big\{\mu_3\Big[2 - 4\sin^2\Big(\frac{\sigma h}{2}\Big)\Big] - \mu_4\Big\}. \tag{70}$$

Note that $\tilde{a}, \tilde{b}$ and $\tilde{c}$ satisfy the following relation

$$\tilde{a} = \tilde{b} - \tilde{c}, \quad b > 0. \tag{71}$$

From (70) we have: $-\tilde{c} = 12\mu_4 - 24\mu_3 + 48\mu_3 \sin^2\Big(\frac{\sigma h}{2}\Big)$ and, from (43), $12\mu_4 - 24\mu_3 > 0$. Thus, $\tilde{c} < 0$ and, therefore, $\tilde{a} > 0$.

From (67), we have

$$d_n = \frac{\tilde{b}}{\tilde{b} - \tilde{c}} d_{n-1} + \frac{\tilde{c}}{\tilde{b} - \tilde{c}} \Bigg(\sum_{j=1}^{n} \lambda_j d_{n-j}\Bigg). \tag{72}$$

If $\tilde{c} < 0$, we have the following recursive formula,

$$|d_n| \leqslant \frac{\tilde{b}}{\tilde{b} - \tilde{c}} |d_{n-1}| - \frac{\tilde{c}}{\tilde{b} - \tilde{c}} \Bigg(\sum_{j=1}^{n} |\lambda_j||d_{n-j}|\Bigg), \quad n = 1, ..., N. \tag{73}$$

Lemma 5.2. *The coefficients* λ_j $(j = 0, 1, 2, ...)$ *satisfy*
(1) $\lambda_0 = 1, \quad \lambda_1 = \gamma - 1$ *and* $\lambda_j < 0, \ j = 1, 2, ...$
(2) $\sum_{j=0}^{\infty} \lambda_j = 0$ *and* $\forall n \in \mathbb{N}^*, \ -\sum_{j=1}^{n} \lambda_j < 1.$

Proof. A proof this lemma can be found at Lemma 2.1 of [4]. □

For the case $n = 1$, the recursive formula, we provide

$$|d_1| \;\leqslant\; \frac{\tilde{b}}{\tilde{b} - \tilde{c}} |d_0| - \frac{\tilde{c}}{\tilde{b} - \tilde{c}} |\lambda_1||d_0| = \Big(\frac{\tilde{b}}{\tilde{b} - \tilde{c}} + \lambda_1 \frac{\tilde{c}}{\tilde{b} - \tilde{c}}\Big)|d_0|.$$

By the part (1) of the Lemma 5.2,

$$|d_1| \leqslant |d_0|. \tag{74}$$

Lemma 5.3. *Let* d_n *be the coefficient of (65) and* $\tilde{c} < 0$*. Then,*

$$|d_n| \leqslant |d_0|, \quad \forall n \in \mathbb{N}^*. \tag{75}$$

Proof. We will use the Second principle of mathematical induction.

For $n = 1$ this was already proved in (74).

For all $n \in \mathbb{N}^*$, $1 \leqslant k \leqslant n-1$, suppose $|d_k| \leqslant |d_0|$. Then, (73) imply

$$|d_n| \leqslant \left[\frac{\tilde{b}}{\tilde{b}-\tilde{c}} - \frac{\tilde{c}}{\tilde{b}-\tilde{c}}\Big(\sum_{j=1}^{n}|\lambda_j|\Big)\right]|d_0| = \left[\frac{\tilde{b}}{\tilde{b}-\tilde{c}} - \frac{\tilde{c}}{\tilde{b}-\tilde{c}}\Big(-\sum_{j=1}^{n}\lambda_j\Big)\right]|d_0|. \quad (76)$$

By the second expression, of part (2) of Lemma 5.2, we conclude that $|d_n| \leqslant |d_0|$, $\forall n \in \mathbb{N}^*$. □

Theorem 5.3. *The CFD numerical scheme (38)-(41) is unconditionally stable.*

Proof. Applying (64), (65) and Lemma 5.3, we have

$$\begin{aligned} \|\mathbf{U}^n - \widetilde{\mathbf{U}}^n\|_{l^2}^2 &= \|\rho^n\|_{l^2}^2 = \left(\sum_{i=1}^{M-1} h|\rho_i^n|^2\right) = \left(\sum_{i=1}^{M-1} h\Big|\frac{1}{\sqrt{b-a}}e^{\mathbf{i}\sigma ih}\Big|^2\right)|d_n|^2 \\ &\leqslant \left(\sum_{i=1}^{M-1} h\Big|\frac{1}{\sqrt{b-a}}e^{\mathbf{i}\sigma ih}\Big|^2\right)|d_0|^2 = \|\rho^0\|_{l^2}^2 = \|\mathbf{U}^0 - \widetilde{\mathbf{U}}^0\|_{l^2}^2 \end{aligned}$$

This completes the proof. □

5.3. Convergence Analysis

A result analogous to the Lax Equivalence Theorem, in fractional integration, is given in [6], which expresses that a numerical method is of p-order convergent if, and only if, is consistent and stable, of p-order. In our case it was already shown that the CFD numerical scheme is consistent with $(n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau)$-order accuracy and unconditionally stable. Now we will show that is convergent with $(h^4+\tau)$-order accuracy.

In this section, we will use the inner product and norm on l^2 space and we will denote them by $(\,\cdot\,)$ and $\|\cdot\|$, respectively.

Before enunciate the convergence theorem first we consider the following results.

Lemma 5.4. *Let $S \in L(\mathbb{R}^n)$ be a symmetric matrix with eigenvalues $\omega_1 \leqslant \omega_2 \leqslant ... \leqslant \omega_n$. Then,*

$$\omega_1\mathbf{x}^{\mathbf{T}}\mathbf{x} \leqslant \mathbf{x}^{\mathbf{T}}S\mathbf{x} \leqslant \omega_n\mathbf{x}^{\mathbf{T}}\mathbf{x}, \quad \forall \mathbf{x} \in \mathbb{R}^n. \quad (77)$$

Proof. The proof of this lemma can be found in [7], p. 21. $\square$

Lemma 5.5. *Let $S \in L(\mathbb{R}^n)$ be a symmetric matrix and $\omega_{\max}(S)$ be the maximal eigenvalue of S. Then, for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$,*

$$\left|\left(S\mathbf{x}, \mathbf{y}\right)\right| \leqslant |\omega_{\max}(S)| \, \|\mathbf{x}\| \|\mathbf{y}\|. \tag{78}$$

Proof.

$$\left|\left(S\mathbf{x}, \mathbf{y}\right)\right| \leqslant \|S\mathbf{x}\| \|\mathbf{y}\| \leqslant \|S\| \|\mathbf{x}\| \|\mathbf{y}\|.$$

In the l^2 space, $\|S\| = \max_{\|z\|=1} \|S\mathbf{z}\| = \rho\left(SS^{\mathbf{T}}\right)^{1/2} = \rho(S) = |\omega_{\max}(S)|$, where $\rho(S)$ is the *resolvent* of S.

$\square$

Lemma 5.6. *Let $a, b, c \in \mathbb{R}$ with $ac \geqslant 0$. Then, the eigenvalues of tridiagonal matrix, $S = \mathrm{tridiag}(a, b, c)$, of order $M - 1 \times M - 1$, are given by*

$$\omega_i(S) \quad = \quad b + 2\sqrt{ac} \cos\left(\frac{i\pi}{M}\right), \quad 1 \leqslant i \leqslant M - 1. \tag{79}$$

Proof. The idea of the proof of this lemma can be found in equation (2.2.40) of [10]. $\square$

In the following, we will enunciate a part of Gronwall Lemma.

Lemma 5.7. *Suppose that (k_n) and (p_n) are non-negative sequences, and the sequence (ϕ_n) satisfies*

$$\begin{cases} \phi_0 & \leqslant \quad g_0, \\ \phi_n & \leqslant \quad g_0 + \sum_{l=0}^{n-1} p_l + \sum_{l=0}^{n-1} k_l \phi_l, \quad n \geqslant 1, \end{cases} \tag{80}$$

where $g_0 \geqslant 0$. Then, ϕ_n satisfies

$$\phi_n \quad \leqslant \quad \left(g_0 + \sum_{l=0}^{n-1} p_l\right) \exp\left(\sum_{l=0}^{n-1} k_l\right), \quad n \geqslant 1. \tag{81}$$

Proof. A proof of this lemma can be found in [9], p. 14. □

From (53) we have

$$|R_i^n| \leqslant \mathcal{C}(n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau), \quad \mathcal{C} = \max_{(i,n)\in Q_h^n} \mathcal{C}_{i,n}. \tag{82}$$

For all $n = 1, 2, ..., N$ we will denote $\mathbf{R}^n = (R_1^n \, ... \, R_{M-1}^n)^{\mathbf{T}}$. From (78),

$$\|\mathbf{R}^n\|_2 = \left(\sum_{i=1}^{M-1} |R_i^n|^2\right)^{1/2} \leqslant \mathcal{C}_1(n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau), \; \mathcal{C}_1 = \sqrt{\mathcal{C}(M-1)}. \tag{83}$$

For each node $(i, n) \in Q_h^n$, we define the error

$$e_i^n = u_i^n - U_i^n, \tag{84}$$

where u_i^n is the exact solution of the FPDE (9)-(12) at node (i, n). For each $n = 0, 1, ..., N$ we denote the error by $\mathbf{e}^n = (e_1^n \, ... \, e_{M-1}^n)^{\mathbf{T}}$ and the exact solution of the FPDE by $\mathbf{u}^n = (u_1^n \, ... \, u_{M-1}^n)^{\mathbf{T}}$. Thus, from (84) we have that $\mathbf{e}^n = \mathbf{u}^n - \mathbf{U}^n$ for all $n = 0, 1, ..., N$. Applying $\mathbf{u}^n$ and $\mathbf{U}^n$ in (49) and immediately subtracting both equations, we have the error equation

$$A\mathbf{e}^n = B\mathbf{e}^{n-1} + C\sum_{j=1}^{n} \lambda_j \mathbf{e}^{n-j} + D\mathbf{R}^n \,, \quad \text{in} \quad \mathrm{Q}_h^\tau, \tag{85}$$

with initial condition

$$\mathbf{e}^0 = 0 \;\; \text{on} \quad \Omega_h. \tag{86}$$

By considering the scalar product of (85) and $\mathbf{e}^n$, we have

$$\Big(A\mathbf{e}^n, \mathbf{e}^n\Big) = \Big(B\mathbf{e}^{n-1}, \mathbf{e}^n\Big) + \sum_{j=1}^{n} \lambda_j \Big(C\mathbf{e}^{n-j}, \mathbf{e}^n\Big) + \Big(D\mathbf{R}^n, \mathbf{e}^n\Big). \tag{87}$$

Applying the Triangular Inequality to (87),

$$\Big|\Big(A\mathbf{e}^n, \mathbf{e}^n\Big)\Big| \leqslant \Big|\Big(B\mathbf{e}^{n-1}, \mathbf{e}^n\Big)\Big| + \sum_{j=1}^{n} |\lambda_j| \Big|\Big(C\mathbf{e}^{n-j}, \mathbf{e}^n\Big)\Big| + \Big|\Big(D\mathbf{R}^n, \mathbf{e}^n\Big)\Big|. \tag{88}$$

By the symmetry of the matrix A, we can apply Lemma 5.4 at the first term of (88). Thus,

$$\Big|\Big(A\mathbf{e}^n, \mathbf{e}^n\Big)\Big| \geqslant |\omega_{\min}(A)| \, \|\mathbf{e}^n\|^2. \tag{89}$$

Using the symmetry of the matrices B, C and D, and Lemma 5.5,

$$\begin{aligned} \left|\Big(B\mathbf{e}^{n-1}, \mathbf{e}^{n}\Big)\right| &\leqslant |\omega_{\max}(B)|\, \|\mathbf{e}^{n-1}\|\, \|\mathbf{e}^{n}\| \quad , \\ \left|\Big(C\mathbf{e}^{n-1}, \mathbf{e}^{n}\Big)\right| &\leqslant |\omega_{\max}(C)|\, \|\mathbf{e}^{n-j}\|\, \|\mathbf{e}^{n}\| \quad , \\ \left|\Big(D\mathbf{R}^{n}, \mathbf{e}^{n}\Big)\right| &\leqslant |\omega_{\max}(D)|\, \|\mathbf{R}^{n}\|\, \|\mathbf{e}^{n}\|. \end{aligned} \tag{90}$$

Substituting (89) and (90) in (88) and, simplifying,

$$\begin{aligned} |\omega_{\min}(A)|\, \|\mathbf{e}^{n}\| \;&\leqslant\; |\omega_{\max}(B)|\, \|\mathbf{e}^{n-1}\| + |\omega_{\max}(C)| \sum_{j=1}^{n} |\lambda_j|\, \|\mathbf{e}^{n-j}\| \\ &+\; |\omega_{\max}(D)|\, \|\mathbf{R}^{n}\|. \end{aligned} \tag{91}$$

Using Lemma 5.6 we can calculate the eigenvalues of the matrices in (91). Thus

$$\begin{aligned} |\omega_{\min}(A)| &= 12 + \frac{12\mu_2}{\tau^{1-\gamma}} \quad , \quad |\omega_{\max}(B)| = 12, \\ |\omega_{\max}(C)| &= \frac{48\mu_1}{\tau^{1-\gamma}} + \frac{8\mu_2}{\tau^{1-\gamma}} \quad , \quad |\omega_{\max}(D)| = 12\tau. \end{aligned} \tag{92}$$

Substituting (92) in (91),

$$\begin{aligned} \|\mathbf{e}^{n}\| \;&\leqslant\; \frac{1}{1 + \dfrac{\mu_2}{\tau^{1-\gamma}}} \|\mathbf{e}^{n-1}\| + \frac{\dfrac{1}{\tau^{1-\gamma}}\Big(4\mu_1 + \dfrac{2}{3}\mu_2\Big)}{1 + \dfrac{\mu_2}{\tau^{1-\gamma}}} \sum_{j=1}^{n} |\lambda_j|\, \|\mathbf{e}^{n-j}\| \\ &+\; \frac{\tau}{1 + \dfrac{\mu_2}{\tau^{1-\gamma}}} \|\mathbf{R}^{n}\|, \end{aligned} \tag{93}$$

or

$$\|\mathbf{e}^{n}\| \;\leqslant\; \|\mathbf{e}^{n-1}\| + \tau^{\gamma-1}\Big(4\mu_1 + \frac{2}{3}\mu_2\Big) \sum_{j=1}^{n} |\lambda_j|\, \|\mathbf{e}^{n-j}\| + \tau \|\mathbf{R}^{n}\|. \tag{94}$$

By the hypothesis of Theorem 5.1

$$\|\mathbf{e}^{n}\| \;\leqslant\; \|\mathbf{e}^{n-1}\| + h^{-\kappa}\Big(4\mu_1 + \frac{2}{3}\mu_2\Big) \sum_{j=1}^{n} |\lambda_j|\, \|\mathbf{e}^{n-j}\| + \tau \|\mathbf{R}^{n}\|, \tag{95}$$

or equivalently

$$\|\mathbf{e}^{n}\| \leqslant \|\mathbf{e}^{n-1}\| + \mathcal{C}_2 \sum_{j=1}^{n} |\lambda_j|\, \|\mathbf{e}^{n-j}\| + \tau \|\mathbf{R}^{n}\|,\ \mathcal{C}_2 = \Big(\frac{b-a}{M}\Big)^{-\kappa}\Big(4\mu_1 + \frac{2}{3}\mu_2\Big). \tag{96}$$

With this result we can now state the convergence theorem.

Theorem 5.4. *The CFD numerical scheme (38)-(41) is convergent and there exists a positive constant* $\mathbf{C}$*, such that,*

$$\|\boldsymbol{e}^n\| \leqslant \mathbf{C}\big(h^4+\tau\big), \quad \forall i=1,...,N. \tag{97}$$

Proof. Applying (83) in (96), we have

$$\|\mathbf{e}^n\| \leqslant \|\mathbf{e}^{n-1}\| + \mathcal{C}_2 \sum_{j=1}^{n} |\lambda_j|\, \|\mathbf{e}^{n-j}\| + \tau \mathcal{C}_1 (n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau), \tag{98}$$

or, equivalently

$$\|\mathbf{e}^n\| \leqslant \big(1+\mathcal{C}_2|\lambda_1|\big)\|\mathbf{e}^{n-1}\| + \mathcal{C}_2 \sum_{j=2}^{n} |\lambda_j|\, \|\mathbf{e}^{n-j}\| + \tau \mathcal{C}_1 (n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau). \tag{99}$$

Set $\mathcal{C}_3 = 1+\mathcal{C}_2$, we have

$$\begin{aligned}
\|\mathbf{e}^n\| &\leqslant \tau \mathcal{C}_1 (n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau) + \sum_{j=1}^{n} |\mathcal{C}_3\lambda_j|\, \|\mathbf{e}^{n-j}\| \\
&\leqslant \frac{1}{n}\sum_{l=0}^{n-1} \tau \mathcal{C}_1 \big(n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau) + \sum_{j=1}^{n} |\mathcal{C}_3\lambda_j|\, \|\mathbf{e}^{n-j}\| \\
&\leqslant g_0 + \sum_{l=0}^{n-1} p_l + \sum_{j=1}^{n} |\mathcal{C}_3\lambda_j|\, \|\mathbf{e}^{n-j}\|, \qquad (100)
\end{aligned}$$

where $g_0 = \|\mathbf{e}^0\| = 0$, $p_l = \tau\mathcal{C}_1\big(n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau)$. The equation (100) is equivalent to

$$\|\mathbf{e}^n\| \leqslant g_0 + \sum_{l=0}^{n-1} p_l + \sum_{l=0}^{n-1} k_l\, \|\mathbf{e}^l\|, \tag{101}$$

where $k_l = |\mathcal{C}_3\lambda_{n-l}|$. Now, applying Lemma 5.7, we have

$$\begin{aligned}
\|\mathbf{e}^n\| &\leqslant \left(g_0 + \sum_{l=0}^{n-1} p_l\right) \exp\left(\sum_{l=0}^{n-1} k_l\right) \qquad (102) \\
&= n\tau\mathcal{C}_1\mathcal{C}_3\big(n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau)\exp\left(\sum_{j=1}^{n-1}|\lambda_j|\right) \\
&< n\tau e\,\mathcal{C}_1\mathcal{C}_3\big(n^{\gamma-1}\tau^{\gamma-1}+1)(h^4+\tau) \qquad (103) \\
&\leqslant (T^\gamma + T)e\,\mathcal{C}_1\mathcal{C}_3\big(h^4+\tau\big). \qquad (104)
\end{aligned}$$

Hence, there exists a constant $\mathbf{C} = (T^\gamma + T)e\,\mathcal{C}_1\mathcal{C}_3 > 0$, such that, for all $n = 1, ..., N$,

$$\|\mathbf{e}^n\| \leqslant \mathbf{C}\big(h^4 + \tau\big). \tag{105}$$

This completes the proof. $\square$

6. Numerical Results

In this section, we will verify the order of convergence of our numerical scheme, by means of one example and several tests.

Example 1. *Consider the following FPDE, given in [3]:*

$$\begin{aligned} u_t &= {}_0D_t^{1-\gamma}\big(u_{xx} - u\big) + (1+\gamma)e^x t^\gamma \quad in \quad Q \\ u(0) &= 0 \qquad on \quad \Omega \\ u &= t^{1+\gamma} \quad on \quad \Sigma_0 \\ u &= et^{1+\gamma} \quad on \quad \Sigma_1, \end{aligned}$$

where $\mathbf{Q} = (0,1) \times (0,1]$, $\Omega = (0,1)$, $\Sigma_0 = \{0\} \times [0,1]$ *and* $\Sigma_1 = \{1\} \times [0,1]$. *The exact solution is given by* $u(x,t) = e^x t^{1+\gamma}$ *and, maximum error, by*

$$\|\mathbf{e}\|_{l^\infty} = \max_{1\leqslant i\leqslant M-1,\ 1\leqslant n\leqslant N} |u_i^n - U_i^n|. \tag{106}$$

In order to test the order of convergence of our numerical scheme, we consider the following experimental formula, see [5],

$$\mathbf{order}(h,\tau) = \log_2 \frac{\|\mathbf{e}(2h, 16\tau)\|_{l^\infty}}{\|\mathbf{e}(h,\tau)\|_{l^\infty}}. \tag{107}$$

Thus, we take as reference the discretization $h = \tau = 1/4$ *and, we calculate the maximum error. Then, we consider the discretization* $h = 1/8, \tau = 1/64$ *and, we calculate the maximum error. The order of convergence for this last discretization, is given by*

$$\log_2\big(\|\mathbf{e}(1/4, 1/4)\|_{l^\infty} / \|\mathbf{e}(1/8, 1/64)\|_{l^\infty}\big).$$

For $h = 1/16, \tau = 1/1024$, *the order of convergence, is given by*

$$\log_2\big(\|\mathbf{e}(1/8, 1/64)\|_{l^\infty} / \|\mathbf{e}(1/16, 1/1024)\|_{l^\infty}\big).$$

In Table 1, we show the error and order of convergence of our numerical scheme for different values of γ. It is observed that for all of values of γ the spatial convergence is fourth-order. Thus we have improved the order of convergence of 2 to 4, obtained by Chen et al [3].

γ	h	τ	$\|\mathbf{e}\|_{l^\infty}$	**order**
	1/4	1/4	0.8460e -2	-
0.2	1/8	1/64	0.4881e -3	4.1155
	1/16	1/1024	0.2724e -4	4.1631
	1/4	1/4	0.1634e -1	-
0.4	1/8	1/64	0.7903e -3	4.3695
	1/16	1/1024	0.3373e -4	4.5501
	1/4	1/4	0.2343e -1	-
0.6	1/8	1/64	0.9904e -3	4.5642
	1/16	1/1024	0.3801e -4	4.7037
	1/4	1/4	0.3075e -1	-
0.8	1/8	1/64	0.1447e -2	4.4088
	1/16	1/1024	0.6448e -4	4.4885

Table 1: Error and order of convergence of CFD numerical scheme.

7. Conclusion

We applied the Implicit Compaq Finite Difference numerical scheme for Fractional Partial Differential Equation (Reaction-Subdiffusion Equation) and was demonstrated that this numerical scheme is unconditionally stable and converges with fourth-order accuracy for spatial variable. Finally, the numerical result presented is coherent with our theoretical analysis.

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