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Stability and convergence of an implicit numerical method for the nonlinear fractional reaction-subdiffusion process

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In this paper, we consider the following nonlinear fractional reaction-subdiffusion process (NFR-SubDP):

$$\frac{\partial u}{\partial t} = {}_0D_t^{1-\gamma}\left[K_\gamma \frac{\partial^2 u}{\partial x^2} + f(u,x,t)\right] + g(u,x,t)$$

wher $f(u,x,t)$ is a linear function of u, the function $g(u,x,t)$ satisfies the Lipschitz condition and ${}_0D_t^{1-\gamma}$ is the Riemann-Liouville time fractional partial derivative of order $1-\gamma$. We propose a new computationally efficient numerical technique to simulate the process. Firstly, the NFR-SubDP is decoupled, which is equivalent to solving a nonlinear fractional reaction-subdiffusion equation (NFR-SubDE). Secondly, we propose an implicit numerical method to approximate the NFR-SubDE. Thirdly, the stability and convergence of the method are discussed using a new energy method. Finally, some numerical examples are presented to show the application of the present technique. This method and supporting theoretical results can also be applied to fractional integro-differential equations.

Keywords: fractional reaction-subdiffusion equation, implicit numerical method, convergence and stability, energy method.

1. Introduction

Various fields of science and engineering deal with dynamical systems that can be described by fractional partial differential equations (FPDE), for example, computational biology (See Yuste & Lindenberg (2001)), physics (See Bisquert (2003); Metzler & Klafter (2000)), chemistry and biochemistry (See Yuste *et al.* (2004)), and hydrological applications (See Liu *et al.* (2004)) due to anomalous diffusion effects in constrained environments. Fractional kinetic equations have proved particularly useful in the context of anomalous slow diffusion (subdiffusion) (See Metzler & Klafter (2000)). Subdiffusive motion is characterized by an asymptotic long-time behavior of the mean square displacement of the form

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

where $0<\gamma<1$ is the anomalous diffusion exponent. Subdiffusive motion is particularly important in the context of complex systems such as glassy and disordered materials, in which pathways are constrained for geometric or energetic reasons. It is also particularly germane to the way in which experiments in low dimensions have to be carried out.

Yuste & Lindenberg (2001) considered coagulation dynamics $A+A\to A$ and $A+A \rightleftharpoons A$ and the annihilation dynamics $A+A\to 0$ for particles moving subdiffusively in one dimension. This scenario combines the ”anomalous kinetics” and ”anomalous diffusion” problems, each of which leads to interesting dynamics separately and to even more interesting dynamics in combination. Yuste & Lindenberg (2002) also considered a combination of these two phenomena and proposed to solve the $A+A$ reaction-subdiffusion problem in one dimension. The situation is more complicated for the $A+B$ problem, because no such exact formulations or solutions have been developed in this case. There is a large literature on the reaction-diffusion problem with different truncation scheme to represent the reaction term, but the literature on the reaction-subdiffusion problem is far more recent and relatively unsettled.

In order to generalize the reaction-diffusion problem to a reaction-subdiffusion problem, we must deal with the subdiffusive motion of the particles. Yuste *et al.* (2004) proposed the following set of reaction-subdiffusion equations:

$$\frac{\partial}{\partial t}a(x,t) = {}_0D_t^{1-\gamma}\{K_\gamma \frac{\partial^2}{\partial x^2}a(x,t)\} - R_\gamma(x,t), \quad (1..2)$$

$$\frac{\partial}{\partial t}b(x,t) = {}_0D_t^{1-\gamma}\{K_\gamma \frac{\partial^2}{\partial x^2}b(x,t)\} - R_\gamma(x,t), \quad (1..3)$$

where K_γ is the generalized diffusion coefficient that appears in Eq. (1..1) and ${}_0D_t^{1-\gamma}v(x,t)$ is the Riemann-Liouville fractional partial derivative of order $1-\gamma$ defined by

$${}_0D_t^{1-\gamma}v(x,t) = \frac{1}{\Gamma(\gamma)}\frac{\partial}{\partial t}\int_0^t \frac{v(x,\eta)}{(t-\eta)^{1-\gamma}}d\eta. \quad (1..4)$$

The reaction term has many different forms. For example, the reaction term $R_\gamma(x,t) = ka(x,t)b(x,t)$ is a linear form of $a(x,t)$ and $b(x,t)$; Seki *et al.* (2003) proposed a reaction-subdiffusion equation that at long times corresponds to choosing a reaction term of the form $R_\gamma(x,t) = k_0D_t^{1-\gamma}a(x,t)b(x,t)$. Cao *et al.* (2006) considered the Michaelis-Menten reaction system with three molecular species and three reaction channels. Suppose now that these chemical reactions are taking place on a one-dimensional membrane of a cell. Then if there are obstacles present on the membrane inhibiting diffusion, the reaction-subdiffusion process is described by the system of fractional differential equations of the form

$$\frac{\partial}{\partial t}a(x,t) = {}_0D_t^{1-\gamma}\{K_\gamma \frac{\partial^2}{\partial x^2}a(x,t) - k_1a(x,t)b(x,t)\} + (k_2+k_3)c(x,t), \quad (1..5)$$

$$\frac{\partial}{\partial t}b(x,t) = {}_0D_t^{1-\gamma}\{K_\gamma \frac{\partial^2}{\partial x^2}b(x,t) - k_1a(x,t)b(x,t)\} + k_2c(x,t), \quad (1..6)$$

$$\frac{\partial}{\partial t}c(x,t) = {}_0D_t^{1-\gamma}\{K_\gamma \frac{\partial^2}{\partial x^2}c(x,t) + k_1a(x,t)b(x,t)\} - (k_2+k_3)c(x,t), \quad (1..7)$$

where $a(x,t), b(x,t), c(x,t)$ denote concentrations, K_γ is the generalized diffusion coefficient, and k_1, k_2, k_3 are the rate coefficients.

In this paper, computational techniques for simulating the reaction-subdiffusion process are considered. Firstly, the reaction-subdiffusion process is decoupled, which is equivalent to solving the following nonlinear fractional reaction-subdiffusion equation (NFR-SubDE):

$$\frac{\partial u}{\partial t} = {}_0D_t^{1-\gamma}\left[K_\gamma \frac{\partial^2 u}{\partial x^2} + f(u,x,t)\right] + g(u,x,t), \ \ (x,t) \in \Omega \times [0,T]. \quad (1..8)$$

where $\Omega = [0, L_x]$. We assume that $f(u,x,t)$ is a linear function of u, the function $g(u,x,t)$ satisfies the Lipschitz condition and ${}_0D_t^{1-\gamma}$ is the Riemann-Liouville time fractional partial derivative of order

$1-\gamma$. Some special fractional reaction-diffusion equations of the form (1..8) have been considered (see Bisquert (2003); Cao *et al.* (2006); Chen *et al.* (2007); Henry & Wearne (2000)).

We note that although anomalous diffusion only really makes physical sense in more than two spatial dimensions, the effects of the NFR-SubDE in one spatial dimension are similar to those in higher spatial dimensions. For this reason, we will focus in this paper on one spatial dimension and consider generalizations to higher spatial dimensions in later work.

Some different numerical methods for solving space or time fractional partial differential equations have been proposed. Liu *et al.* (2004) proposed a computational effective method of lines. This method transforms the space fractional partial differential equation into a system of ordinary differential equations that is then solved using backward differentiation formulas. Meerschaert & Tadjeran (2004) developed finite difference approximations for fractional advection-dispersion flow equations. Meerschaert & Tadjeran (2006) examined some practical numerical methods to solve the two-sided space-fractional partial differential equations and discussed stability and convergence of the methods. Tadjeran *et al.* (2006) presented a second order accurate numerical approximation for the fractional diffusion equation. Roop (2006) investigated the computational aspects of the Galerkin approximation using continuous piecewise polynomial basis functions on a regular triangulation of the bounded domain in R^2. Liu *et al.* (2005) derived an analysis of a discrete non-Markovian random walk approximation for the time fractional diffusion equation. Zhuang & Liu (2006) analyzed an implicit difference approximation for the time fractional diffusion equation, and discussed the stability and convergence of the method. Lin & Liu (2007) proposed the high order (2-6) approximations of the fractional ordinary differential equation and discussed the consistency, convergence and stability of these fractional high order methods. Liu *et al.* (2007) discussed an approximation of the Lévy-Feller advection-dispersion process by a random walk and finite difference method. Cao *et al.* (2006) presented a variable coefficient fractional derivative approximation scheme, and used embedding techniques to develop a variable stepsize implementation for solving fractional differential equations. Yu *et al.* (2008) developed a reliable algorithm of the Adomian decomposition method to solve the linear and nonlinear space-time fractional reaction-diffusion equations in the form of a rapidly convergent series with easily computable components, but did not give its theoretical analysis. It is a more difficult task to solve the fractional subdiffusion equation which involves an integro-differential equation. Yuste & Acedo (2005) proposed an explicit finite difference method and a new Von Neumann-type stability analysis for the fractional subdiffusion equation, i.e., the NFR-SubDE without the reaction term. However, they did not give the convergence analysis and pointed out the difficulty of this task when implicit methods are considered. Langlands & Henry (2005) also investigated this problem and proposed an implicit numerical scheme (L1 approximation), and discussed its accuracy and stability. However, the global accuracy of the implicit numerical scheme was not derived and it seems that the unconditional stability for all γ in the range $0<\gamma\leqslant 1$ has not been established. Chen *et al.* (2007) presented a Fourier method for the problem, and they gave the stability analysis and the global accuracy analysis of the difference approximation scheme. Zhuang *et al.* (2008) also proposed new solution and analytical techniques for implicit numerical solution methods. Thus, effective numerical methods and error analyses for NFR-SubDEs are still open problems. The main purpose of this paper is to solve and analyze this problem using a new energy method.

The structure of the paper is as follows. In Section 2, some mathematical preliminaries are introduced. In Section 3, an implicit finite difference method (IFDM) of the NFR-SubDE is proposed. The stability and convergence of the IFDM are discussed in Sections 4 and 5, respectively. Finally, some numerical results are given, which it is found that the theoretical results are in excellent agreement with the numerical results.

2. Mathematical preliminaries

In this section, we introduce some definitions and mathematical notations that will be used in later sections and state their corresponding properties.

Firstly, we give the definition of the temporal fractional integral.

Definition 2..1 (Samko *et al.* (1993)) Let $y(t) \in L^1(a,b)$. The integral

$$I_{a+}^{\gamma} y(t) = \frac{1}{\Gamma(\gamma)} \int_a^t \frac{y(\eta)}{(t-\eta)^{1-\gamma}} d\eta, \quad t > a, \tag{2..1}$$

where $\gamma > 0$, is called the Riemann-Liouville fractional integral of order γ.

In this paper, we refer to $t \in [0,T]$ and $0 < \gamma < 1$. In order to compute $I_{0+}^{\gamma} y(t)$, we begin by discretizing the temporal domain $[0,T]$ by placing a grid over the domain. For convenience, we will use a uniform grid, with grid spacing $\tau = T/n$. If we wish to refer to one of the points in the grid, we call the points $t_k, \ \ k = 0,1,\cdots,n$ where $t_k = k\tau, k = 0,1,\cdots,n$. Hence, for $k = 1,2,\cdots,n$

$$\begin{aligned} I_{0+}^{\gamma} y(t_k) &= \frac{1}{\Gamma(\gamma)} \int_0^{t_k} \frac{y(\eta)}{(t_k-\eta)^{1-\gamma}} d\eta \\ &= \frac{1}{\Gamma(\gamma)} \sum_{j=0}^{k-1} \int_{t_{k-1-j}}^{t_{k-j}} \frac{y(\eta)}{(t_k-\eta)^{1-\gamma}} d\eta. \end{aligned} \tag{2..2}$$

When $t_j \leqslant \eta \leqslant t_{j+1}, j = 0,1,\ldots,k-1$, using

$$y(\eta) = y(t_{j+1}) + \frac{dy(\xi)}{dt}(\eta - t_{j+1}), \quad \eta < \xi < t_{j+1},$$

we obtain

$$|y(\eta) - y(t_{j+1})| \leqslant C_1 \tau.$$

Further, we have

$$|I_{0+}^{\gamma} y(t_k) - \frac{1}{\Gamma(\gamma)} \sum_{j=0}^{k-1} \int_{t_{k-1-j}}^{t_{k-j}} \frac{y(t_{k-j})}{(t_k-\eta)^{1-\gamma}} d\eta| \leqslant C k^{\gamma} \tau^{\gamma+1}. \tag{2..3}$$

Hence, we have (See Oldham & Spanier (1974)) the following lemma.

LEMMA 2..1 If $y(t) \in C^1[0,T]$, then

$$I_{0+}^{\gamma} y(t_k) = \frac{\tau^{\gamma}}{\Gamma(\gamma+1)} \sum_{j=0}^{k-1} b_j^{(\gamma)} y(t_{k-j}) + R_{k,\gamma} \tag{2..4}$$

where

$$b_j^{(\gamma)} = (j+1)^{\gamma} - j^{\gamma}, j = 0,1,\cdots,n-1, \tag{2..5}$$

and $|R_{k,\gamma}| \leqslant C t_k^{\gamma} \tau$.

LEMMA 2..2 In (2..5), the coefficients $b_k^{(\gamma)} (k = 0,1,2,\ldots)$ satisfy the following properties:
(i) $b_0^{(\gamma)} = 1$, $b_k^{(\gamma)} > 0$, $k = 0,1,2,\ldots$;
(ii) $b_k^{(\gamma)} > b_{k+1}^{(\gamma)}$, $k = 0,1,2,\ldots$;
(iii) there exists a positive constant $C > 0$, such that $\tau \leqslant C b_k^{(\gamma)} \tau^{\gamma}$, $k = 1,2,\ldots$.

Proof. Let $\psi_1(x)=x^\gamma$ and $\psi_2(x)=(x+1)^\gamma-x^\gamma$. It is easily seen that $\psi_1(x)$ is monotone increasing and $\psi_2(x)$ is monotone decreasing when $x>0$. Thus, (i) and (ii) hold.

As for (iii), using

$$\lim_{n\to\infty}\frac{n^{\gamma-1}}{b_n^{(\gamma)}}=\lim_{n\to\infty}\frac{n^{-1}}{(1+n^{-1})^\gamma-1}=\frac{1}{\gamma},$$

and the result of a convergent sequence is a bounded sequence then there exists a positive constant C_1 such that

$$\frac{n^{\gamma-1}}{b_n^{(\gamma)}}\leqslant C_1,$$

or

$$n^{-1}\leqslant C_1 b_n^{(\gamma)}n^{-\gamma}\leqslant C_1 b_k^{(\gamma)}n^{-\gamma}.$$

Thus, from $\tau=T/n$, the inequality (iii) is obtained. □

LEMMA 2..3 If $y(t)\in C^2[0,T]$, then

$$I_{0+}^\gamma y(t_{k+1})-I_{0+}^\gamma y(t_k)=\frac{\tau^\gamma}{\Gamma(\gamma+1)}\left[y(t_{k+1})+\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)}-b_j^{(\gamma)})y(t_{k-j})\right]+R_{k,\gamma}^{(2)}, \tag{2..6}$$

where $|R_{k,\gamma}^{(2)}|\leqslant Cb_k^{(\gamma)}\tau^{1+\gamma}$.

Proof. For $k=0,1,\ldots,n-1$, we have

$$\begin{aligned} I_{0+}^\gamma y(t_{k+1})-I_{0+}^\gamma y(t_k) &= \tfrac{1}{\Gamma(\gamma)}\left[\int_0^{t_{k+1}}\tfrac{y(\eta)}{(t_{k+1}-\eta)^{1-\gamma}}d\eta-\int_0^{t_k}\tfrac{y(\eta)}{(t_k-\eta)^{1-\gamma}}d\eta\right]\\ &= \tfrac{1}{\Gamma(\gamma)}\left[\int_0^{\tau}\tfrac{y(\eta)}{(t_{k+1}-\eta)^{1-\gamma}}d\eta+\int_0^{t_k}\tfrac{y(\eta+\tau)-y(\eta)}{(t_k-\eta)^{1-\gamma}}d\eta\right]\\ &= \tfrac{1}{\Gamma(\gamma)}\left[\int_0^{\tau}\tfrac{y(\eta)}{(t_{k+1}-\eta)^{1-\gamma}}d\eta+\sum_{j=0}^{k-1}\int_{t_j}^{t_{j+1}}\tfrac{y(\eta+\tau)-y(\eta)}{(t_k-\eta)^{1-\gamma}}d\eta\right]. \end{aligned}$$

If $y(t)\in C^2[0,T]$, then

$$|y(\eta)-y(\tau)|=|y'(\xi)(\eta-\tau)|\leqslant C\tau.$$

When $t_j\leqslant\eta\leqslant t_{j+1}$, we can obtain

$$\begin{aligned} y(\eta+\tau)-y(\eta) &= y(t_{j+2})-y(t_{j+1})+(y'(\varsigma_j+\tau)-y'(\varsigma_j))(\eta-t_{j+1})\\ &= y(t_{j+2})-y(t_{j+1})+y''(\rho_j)\tau(\eta-t_{j+1}). \end{aligned}\tag{2..7}$$

Hence, $|y(\eta+\tau)-y(\eta)-[y(t_{j+2})-y(t_{j+1})]|\leqslant C\tau^2$.

Thus, we get

$$I_{0+}^\gamma y(t_{k+1})-I_{0+}^\gamma y(t_k)=\frac{\tau^\gamma}{\Gamma(\gamma+1)}\left\{b_k^{(\gamma)}y(t_1)+\sum_{j=0}^{k-1}b_{k-j-1}\left[y(t_{j+2})-y(t_{j+1})\right]\right\}+R_{k,\gamma}^{(1)},$$

where $|R_{k,\gamma}^{(1)}|\leqslant Cb_k^{(\gamma)}\tau^{1+\gamma}+C\tau^2 t_k^\gamma$.

Thanks to Lemma 2..2, we have proved the following result. □

In this paper, we suppose that the space variable x satisfies $x\in\Omega=[0,L_x]$. Similarly, we discretize the space domain by place a grid on the spatial axis with grid spacing h. Also, we introduce the notation

$$x_i=ih,\quad i=0,1,\ldots,m,$$

where $h=L_x/m$.

Definition 2..2 Let

$$\mathbf{v} = (v_1, v_2, \cdots, v_{m-1})^T$$

and

$$\mathbf{w} = (w_1, w_2, \cdots, w_{m-1})^T$$

are the vectors of the real Euclidean space $\mathbf{R}^{m-1}$, we define

$$(\mathbf{v}, \mathbf{w}) = \sum_{j=1}^{m-1} v_j w_j h, \quad \|\mathbf{v}\|_2 = (\mathbf{v}, \mathbf{v})^{\frac{1}{2}} = (\sum_{j=1}^{m-1} v_j^2 h)^{\frac{1}{2}} \tag{2..8}$$

and $\|\mathbf{v}\|_\infty = \max_{1 \leqslant i \leqslant m-1} |v_i|$.

The following conclusions can be obtained easily.

LEMMA 2..4 Let

$$\Delta v_i = v_{i+1} - v_i, \quad \Delta w_i = w_{i+1} - w_i,$$
$$\delta^2 v_i = v_{i+1} - 2v_i + v_{i-1}, \quad \delta^2 w_i = w_{i+1} - 2w_i + w_{i-1},$$

if $v_0 = w_m = 0$, then

$$(\delta^2 \mathbf{v}, \mathbf{w}) = -v_1 w_1 h - (\Delta \mathbf{v}, \Delta \mathbf{w}), \tag{2..9}$$

where

$$\delta^2 \mathbf{v} = (\delta^2 v_1, \delta^2 v_2, \cdots, \delta^2 v_{m-1})^T,$$

$$\Delta \mathbf{v} = (\Delta v_1, \Delta v_2, \cdots, \Delta v_{m-1})^T,$$

$$\Delta \mathbf{w} = (\Delta w_1, \Delta w_2, \cdots, \Delta w_{m-1})^T.$$

LEMMA 2..5 For $v_i, i = 0, 1, \cdots, m$, if $v_0 = v_m = 0$, then

$$\|\mathbf{v}\|_2^2 \leqslant L_x \|\mathbf{v}\|_\infty^2 \leqslant \frac{L_x^2}{2h^2} \left[h|v_1|^2 + \|\Delta \mathbf{v}\|_2^2 \right],$$

where $h = L_x/m$.

Proof. The first inequality is apparent.

As for the second inequality, let $|v_{i_0}| = \max_{1 \leqslant i \leqslant m-1} |v_i|$,

$$v_{i_0} = v_1 + \sum_{j=1}^{i_0-1} \Delta v_j, \quad v_{i_0} = -\sum_{j=i_0}^{m-1} \Delta v_j.$$

Thus, $2|v_{i_0}| \leqslant |v_1| + \sum_{j=1}^{m-1} |\Delta v_j|$.

Using the Cauchy-Schwarz inequality, we have

$$4|v_{i_0}|^2 \leqslant 2m \left[|v_1|^2 + \sum_{j=1}^{m-1} |\Delta v_j|^2 \right] \leqslant \frac{2L_x}{h^2} \left[h|v_1|^2 + \|\Delta \mathbf{v}\|_2^2 \right].$$

Therefore, $\|\mathbf{v}^k\|_\infty^2 \leqslant \frac{L_x}{2h^2} \left[h|v_1|^2 + \|\Delta \mathbf{v}^k\|_2^2 \right]$. □

We consider the following NFR-SubDE:

$$\frac{\partial u}{\partial t} = {}_0D_t^{1-\gamma}\left[K_\gamma \frac{\partial^2 u}{\partial x^2} + f(u,x,t)\right] + g(u,x,t), \quad (x,t) \in \Omega \times [0,T] \tag{2..10}$$

with initial and boundary conditions:

$$u(x,0) = \phi(x), 0 \leqslant x \leqslant L, \tag{2..11}$$

$$u(0,t) = \varphi_1(t),\ \ u(L,t) = \varphi_2(t),\ \ 0 \leqslant t \leqslant T, \tag{2..12}$$

where $0 < \gamma < 1$. In this equation the expression

$${}_0D_t^{1-\gamma} v(x,t) = \frac{\partial}{\partial t} I_{0+}^{\gamma} v(x,t) \tag{2..13}$$

denotes the Riemann-Liouville fractional derivative of order $1-\gamma$.

Suppose that the function $f(u,x,t)$ and $g(u,x,t)$ are smooth enough and $f(u,x,t)$ is monotone decreasing for u. In this paper, we suppose the continuous problem (2..10)-(2..12) has a smooth solution $u(x,t) \in C_{x,t}^{4,2}(\Omega \times [0,T])$.

Definition 2..3 Let $u(x,t)$ be defined on $\Omega \times [0,T]$ and put

$$\begin{aligned} &\Delta_x u(x_i,t_k) = u(x_{i+1},t_k) - u(x_i,t_k), \\ &\delta_x^2 u(x_i,t_k) = u(x_{i+1},t_k) - 2u(x_i,t_k) + u(x_{i-1},t_k). \end{aligned}$$

Similarly, for an array u_i^k, $i = 0,1,\ldots,m$; $k = 0,1,\ldots,n$, we define

$$\Delta_x u_i^k = u_{i+1}^k - u_i^k,\ \ \delta_x^2 u_i^k = u_{i+1}^k - 2u_i^k + u_{i-1}^k.$$

Integrating both sides of the equation (2..10), we have

$$\begin{aligned} u(x_i,t_{k+1}) - u(x_i,t_k) \quad = \quad & I_{0+}^{\gamma}[K_\gamma \tfrac{\partial^2 u(x_i,t_{k+1})}{\partial x^2} + f(u(x_i,t_{k+1}),x_i,t_{k+1})] \\ & - I_{0+}^{\gamma}[K_\gamma \tfrac{\partial^2 u(x_i,t_k)}{\partial x^2} + f(u(x_i,t_k),x_i,t_k)] + \textstyle\int_{t_k}^{t_{k+1}} g(u(x_i,t),x_i,t)dt. \end{aligned}$$

Applying Lemma 2..3 and the following formulae:

$$\frac{\partial^2 u(x_i,t_j)}{\partial x^2} = \frac{1}{h^2}\delta_x^2 u(x_i,t_j) - \frac{h^2}{12}\frac{\partial^4 u(\xi_i,t_j)}{\partial x^4},\ \ x_{i-1} \leqslant \xi_i \leqslant x_{i+1}$$

and

$$\int_{t_k}^{t_{k+1}} g(u(x_i,t),x_i,t)dt = \frac{\tau}{2}\left[g(u(x_i,t_{k+1}),x_i,t_{k+1}) + g(u(x_i,t_k),x_i,t_k)\right] + O(\tau^2),$$

where $i = 1,2,\ldots,m-1$; $k = 0,1,\ldots,n-1$, we obtain

$$\begin{aligned} u(x_i,t_{k+1}) \quad = \quad & u(x_i,t_k) + \tfrac{\tau^\gamma}{\Gamma(\gamma+1)}\left[K_\gamma \cdot \tfrac{1}{h^2}\delta_x^2 u(x_i,t_{k+1}) + f(u(x_i,t_{k+1}),x_i,t_{k+1})\right] \\ & + \tfrac{\tau^\gamma}{\Gamma(\gamma+1)}\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})K_\gamma \cdot \tfrac{1}{h^2}\delta_x^2 u(x_i,t_{k-j}) \\ & + \tfrac{\tau^\gamma}{\Gamma(\gamma+1)}\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)}) f(u(x_i,t_{k-j}),x_i,t_{k-j}) \\ & + \tfrac{\tau}{2}\left[g(u(x_i,t_{k+1}),x_i,t_{k+1}) + g(u(x_i,t_k),x_i,t_k)\right] + R_{i,\gamma}^{k+1}, \end{aligned}$$

where $|R_{i,\gamma}^{k+1}| \leqslant Cb_k^{(\gamma)}\tau^{\gamma}(\tau+h^2)$.

Let

$$\mathbf{R}_{\gamma}^{k} = (R_{1,\gamma}^{k}, R_{2,\gamma}^{k}, \cdots, R_{m-1,\gamma}^{k})^{T},$$

and $r_1 = K_{\gamma}\frac{\tau^{\gamma}}{\Gamma(\gamma+1)h^2}$, $r_2 = \frac{\tau^{\gamma}}{\Gamma(\gamma+1)}$, then the above results can be summarized in the following lemma.

LEMMA 2..6

$$\begin{aligned} u(x_i,t_{k+1}) &= u(x_i,t_k) + r_1[\delta_x^2 u(x_i,t_{k+1}) + \sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})\delta_x^2 u(x_i,t_{k-j})] \\ &+ r_2[f(u(x_i,t_{k+1}),x_i,t_{k+1}) + \sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)}) f(u(x_i,t_{k-j}),x_i,t_{k-j})] \\ &+ \frac{\tau}{2}[g(u(x_i,t_{k+1}),x_i,t_{k+1}) + g(u(x_i,t_k),x_i,t_k)] + R_{i,\gamma}^{k+1}, \end{aligned}$$

where

$$\|\mathbf{R}_{\gamma}^{k}\|_2 \leqslant Cb_k^{(\gamma)}\tau^{\gamma}(\tau+h^2).$$

3. An implicit numerical method for the NFR-SubDE and theoretic analysis

Let u_i^k be the numerical approximation to $u(x_i,t_k)$. Applying Lemma 2..6, we can obtain the following fractional implicit difference approximation (FIDA):

$$\begin{aligned} u_i^{k+1} &= u_i^k + r_1\delta_x^2 u_i^{k+1} + r_1\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})\delta_x^2 u_i^{k-j} \\ &+ r_2 f(u_i^{k+1},x_i,t_{k+1}) + r_2\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)}) f(u_i^{k-j},x_i,t_{k-j}) \\ &+ \frac{\tau}{2}\left[g(u_i^{k+1},x_i,t_{k+1}) + g(u_i^k,x_i,t_k)\right], \end{aligned} \qquad (3..1)$$

where $i = 1,2,\ldots,m-1, k = 0,1,2,\ldots,n-1$.

The initial and boundary conditions can be discretized by

$$u_i^0 = \phi(ih),\ \ i = 0,1,2,\ldots,m, \qquad (3..2)$$

$$u_0^k = \varphi_1(k\tau),\ \ u_m^k = \varphi_2(k\tau),\ \ k = 0,1,2,\cdots,n. \qquad (3..3)$$

3.1. *Stability of the FIDA*

We suppose that $\widetilde{u}_i^k$ $(i=0,1,2,\cdots,m;\quad j=0,1,2,\cdots,n)$ is the approximate solution of (3..1), (3..2) and (3..3). The error $\varepsilon_i^k = u_i^k - \widetilde{u}_i^k$ satisfies

$$\begin{aligned}
\varepsilon_i^{k+1} &= \varepsilon_i^k + r_1\delta_x^2\varepsilon_i^{k+1} + r_1\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})\delta_x^2\varepsilon_i^{k-j} \\
&+ r_2\left[f(u_i^{k+1},x_i,t_{k+1}) - f(\widetilde{u}_i^{k+1},x_i,t_{k+1})\right] \\
&+ r_2\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})\left[f(u_i^{k-j},x_i,t_{k-j}) - f(\widetilde{u}_i^{k-j},x_i,t_{k-j})\right] \\
&+ \frac{\tau}{2}\left[g(u_i^{k+1},x_i,t_{k+1}) - g(\widetilde{u}_i^{k+1},x_i,t_{k+1})\right] \\
&+ \frac{\tau}{2}\left[g(u_i^{k},x_i,t_{k}) - g(\widetilde{u}_i^{k},x_i,t_{k})\right] \qquad (3..4)
\end{aligned}$$

and

$$\varepsilon_0^k = 0,\;\; \varepsilon_m^k = 0,\;\; k=0,1,2,\cdots,n. \qquad (3..5)$$

In this paper, we only discuss the case of $f(u,x,t) = -\alpha u + \beta(x,t)$, where $\alpha > 0$ is a constant and $\beta(x,t)$ is independent of u, i.e., $f(u,x,t)$ is a linear function of u, and suppose that the function $g(u,x,t)$ satisfies the Lipschitz condition, i.e.,

$$|g(u_1,x,t) - g(u_2,x,t)| \leqslant L|u_1-u_2|,\;\; \forall u_1,u_2. \qquad (3..6)$$

So,

$$\begin{gathered}
f(u_i^j,x_i,t_j) - f(\widetilde{u}_i^j,x_i,t_j) = -\alpha\varepsilon_i^j, \\
|g(u_i^j,x_i,t_j) - g(\widetilde{u}_i^j,x_i,t_j)| \leqslant L|\varepsilon_i^j|,
\end{gathered}$$

where $i=1,2,\cdots,m-1;\;\; j=1,2,\cdots,n$.

Therefore, Eq. (3..4) can be rewritten as

$$\begin{aligned}
\varepsilon_i^{k+1} &= \varepsilon_i^k + r_1\delta_x^2\varepsilon_i^{k+1} + r_1\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})\delta_x^2\varepsilon_i^{k-j} \\
&\quad -\alpha r_2\left[\varepsilon_i^{k+1} + \sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})\varepsilon_i^{k-j}\right] \\
&\quad +\frac{\tau}{2}\left[g(u_i^{k+1},x_i,t_{k+1}) - g(\widetilde{u}_i^{k+1},x_i,t_{k+1})\right] \\
&\quad +\frac{\tau}{2}\left[g(u_i^{k},x_i,t_{k}) - g(\widetilde{u}_i^{k},x_i,t_{k})\right]. \qquad (3..7)
\end{aligned}$$

Multiplying (3..7) by $h\varepsilon_i^{k+1}$ and summing up for i from 1 to $m-1$, we obtain

$$\begin{aligned}
\|\mathbf{E}^{k+1}\|_2^2 &= (\mathbf{E}^{k+1},\mathbf{E}^k)+r_1(\delta_x^2\mathbf{E}^{k+1},\mathbf{E}^{k+1})+r_1\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)}-b_j^{(\gamma)})(\delta_x^2\mathbf{E}^{k-j},\mathbf{E}^{k+1})\\
&\quad -\alpha r_2(\mathbf{E}^{k+1},\mathbf{E}^{k+1})+\alpha r_2\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})(\mathbf{E}^{k-j},\mathbf{E}^{k+1})\\
&\quad +\frac{\tau}{2}\sum_{i=1}^{m-1}\left[g(u_i^{k+1},x_i,t_{k+1})-g(\tilde{u}_i^{k+1},x_i,t_{k+1})\right]\varepsilon_i^{k+1}h\\
&\quad +\frac{\tau}{2}\sum_{i=1}^{m-1}\left[g(u_i^{k},x_i,t_{k})-g(\tilde{u}_i^{k},x_i,t_{k})\right]\varepsilon_i^{k+1}h. \qquad (3..8)
\end{aligned}$$

Thanks to Lemma 2..4 and the inequality

$$(\mathbf{E}^j,\mathbf{E}^{k+1})\leqslant\frac{1}{2}\left[\|\mathbf{E}^j\|_2^2+\|\mathbf{E}^{k+1}\|_2^2\right],$$

where $j=1,2,\cdots,k+1$, we obtain

$$\begin{aligned}
\|\mathbf{E}^{k+1}\|_2^2 \leqslant\; & \tfrac{1}{2}\left[\|\mathbf{E}^{k+1}\|_2^2+\|\mathbf{E}^k\|_2^2\right]-r_1[(\varepsilon_1^{k+1})^2h+\|\Delta_x\mathbf{E}^{k+1}\|_2^2]\\
&+r_1\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)}-b_j^{(\gamma)})[-\varepsilon_1^{k-j}\varepsilon_1^{k+1}h-(\Delta_x\mathbf{E}^{k-j},\Delta_x\mathbf{E}^{k+1})]\\
&-\alpha r_2\|\mathbf{E}^{k+1}\|_2^2+\tfrac{\alpha r_2}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})\left[\|\mathbf{E}^{k-j}\|_2^2+\|\mathbf{E}^{k+1}\|_2^2\right]\\
&+\tfrac{\tau}{2}L\|\mathbf{E}^{k+1}\|_2^2+\tfrac{\tau}{4}L(\|\mathbf{E}^{k+1}\|_2^2+\|\mathbf{E}^k\|_2^2).
\end{aligned}$$

Note that

$$\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})=b_0^{(\gamma)}-b_k^{(\gamma)}=1-b_k^{(\gamma)}$$

and

$$\varepsilon_1^{k-j}\varepsilon_1^{k+1}\leqslant\frac{1}{2}\left[|\varepsilon_1^{k-j}|^2+|\varepsilon_1^{k+1}|^2\right].$$

We then have

$$\begin{aligned}\|\mathbf{E}^{k+1}\|_2^2 \leqslant\ & \frac{1}{2}[\|\mathbf{E}^{k+1}\|_2^2+\|\mathbf{E}^{k}\|_2^2]-\frac{r_1}{2}(1+b_k^{(\gamma)})[|\varepsilon_1^{k+1}|^2h+\|\Delta_x\mathbf{E}^{k+1}\|_2^2]\\ &+\frac{r_1}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})(|\varepsilon_1^{k-j}|^2h+\|\Delta_x\mathbf{E}^{k-j}\|_2^2)\\ &-\frac{\alpha r_2}{2}(1+b_k^{(\gamma)})\|\mathbf{E}^{k+1}\|_2^2+\frac{\alpha}{2}r_2\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})\|\mathbf{E}^{k-j}\|_2^2\\ &+\frac{\tau}{4}L\|\mathbf{E}^{k}\|_2^2+\frac{3\tau}{4}L\|\mathbf{E}^{k+1}\|_2^2\\ \leqslant\ & \frac{1}{2}[\|\mathbf{E}^{k+1}\|_2^2+\|\mathbf{E}^{k}\|_2^2]-\frac{r_1}{2}[|\varepsilon_1^{k+1}|^2h+\|\Delta_x\mathbf{E}^{k+1}\|_2^2]\\ &+\frac{r_1}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})(|\varepsilon_1^{k-j}|^2h+\|\Delta_x\mathbf{E}^{k-j}\|_2^2)\\ &-\frac{\alpha r_2}{2}\|\mathbf{E}^{k+1}\|_2^2+\frac{\alpha}{2}r_2\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})\|\mathbf{E}^{k-j}\|_2^2\\ &+\frac{\tau}{4}L\|\mathbf{E}^{k}\|_2^2+\frac{3\tau}{4}L\|\mathbf{E}^{k+1}\|_2^2.\end{aligned}$$

Also

$$\begin{aligned}&\|\mathbf{E}^{k+1}\|_2^2+r_1\sum_{j=0}^{k}b_j^{(\gamma)}\left[|\varepsilon_1^{k+1-j}|^2h+\|\Delta_x\mathbf{E}^{k+1-j}\|_2^2\right]+\alpha r_2\sum_{j=0}^{k}b_j^{(\gamma)}\|\mathbf{E}^{k+1-j}\|_2^2\\ &\leqslant \|\mathbf{E}^{k}\|_2^2+r_1\sum_{j=0}^{k-1}b_j^{(\gamma)}\left[|\varepsilon_1^{k-j}|^2h+\|\Delta_x\mathbf{E}^{k-j}\|_2^2\right]+\alpha r_2\sum_{j=0}^{k-1}b_j^{(\gamma)}\|\mathbf{E}^{k-j}\|_2^2\\ &+\tfrac{\tau}{2}L\|\mathbf{E}^{k}\|_2^2+\tfrac{3\tau}{2}L\|\mathbf{E}^{k+1}\|_2^2.\end{aligned}$$

Define

$$\rho_k=\|\mathbf{E}^{k}\|_2^2+r_1\sum_{j=0}^{k-1}b_j^{(\gamma)}\left[|\varepsilon_1^{k-j}|^2h+\|\Delta_x\mathbf{E}^{k-j}\|_2^2\right]+\alpha r_2\sum_{j=0}^{k-1}b_j^{(\gamma)}\|\mathbf{E}^{k-j}\|_2^2.$$

Supposing that $\tau<\frac{2}{3L}$, we have

$$(1-\frac{3}{2}L\tau)\rho_{k+1}\leqslant(1+\frac{1}{2}L\tau)\rho_k.$$

Thus,

$$\rho_k\leqslant\left(\frac{1+\frac{1}{2}L\tau}{1-\frac{3}{2}L\tau}\right)^{k-1}\rho_1\leqslant\left(\frac{1+\frac{1}{2}L\tau}{1-\frac{3}{2}L\tau}\right)^{n}\rho_1$$

Note that $n=T/\tau$, and

$$\lim_{n\to\infty}\left(\frac{1+\frac{1}{2}L\tau}{1-\frac{3}{2}L\tau}\right)^{n}=\lim_{n\to\infty}\left(\frac{1+\frac{1}{2n}LT}{1-\frac{3}{2n}LT}\right)^{n}=\frac{e^{\frac{1}{2}LT}}{e^{-\frac{3}{2}LT}}=e^{2LT},$$

so, there is a positive constant $C_1 > 0$, such that $\left(\frac{1+\frac{1}{2}L\tau}{1-\frac{3}{2}L\tau}\right)^n \leqslant C_1$, thereby,

$$\|\mathbf{E}^k\|_2^2 \leqslant \rho_k \leqslant C_1\rho_1.$$

Again, from (3..4), we have

$$\varepsilon_i^1 = \varepsilon_i^0 + r_1\delta_x^2\varepsilon_i^1 - \alpha r_2\varepsilon_i^1 + \frac{\tau}{2}\left[g(u_i^1,x_i,t_1) - g(\widetilde{u}_i^1,x_i,t_1)\right] + \frac{\tau}{2}\left[g(u_i^0,x_i,t_0) - g(\widetilde{u}_i^0,x_i,t_0)\right].$$

Similarly, we have

$$\begin{aligned}\|\mathbf{E}^1\|_2^2 &\leqslant \tfrac{1}{2}\left[\|\mathbf{E}^0\|_2^2 + \|\mathbf{E}^1\|_2^2\right] - r_1\left[(\varepsilon_1^1)^2h + \|\Delta_x\mathbf{E}^1\|_2^2\right] \\ &\quad -\alpha r_2\|\mathbf{E}^1\|_2^2 + \tfrac{\tau}{2}L\left[\|\mathbf{E}^1\|_2^2 + \|\mathbf{E}^0\|_2^2\right] \\ &\leqslant \tfrac{1}{2}\left[\|\mathbf{E}^0\|_2^2 + \|\mathbf{E}^1\|_2^2\right] - \tfrac{r_1}{2}\left[(\varepsilon_1^1)^2h + \|\Delta_x\mathbf{E}^1\|_2^2\right] \\ &\quad -\tfrac{1}{2}\alpha r_2\|\mathbf{E}^1\|_2^2 + \tfrac{\tau}{2}L\left[\|\mathbf{E}^1\|_2^2 + \|\mathbf{E}^0\|_2^2\right].\end{aligned}$$

So, $\rho_1 \leqslant (1+\tau L)\|\mathbf{E}^0\|_2^2 + \tau L\rho_1$. From $\tau L \leqslant 2/3$, we have

$$\rho_1 \leqslant \frac{1+\tau L}{1-\tau L}\|\mathbf{E}^0\|_2^2 \leqslant \frac{1+\frac{2}{3}}{1-\frac{2}{3}}\|\mathbf{E}^0\|_2^2 = 5\|\mathbf{E}^0\|_2^2,$$

i. e.,

$$\|\mathbf{E}^k\|_2^2 \leqslant C\|\mathbf{E}^0\|_2^2,$$

where $C = 5C_1$.

Furthermore, the following theorem of stability can be obtained.

THEOREM 3..1 The FIDA defined by (3..1) is unconditionally stable.

3.2. *Convergence of the FIDA*

In this section, the convergence analysis of the FIDA is discussed. Let $u(x_i,t_k)$ $(i = 1,2,\ldots,m-1;\ \ k = 1,2,\ldots,n)$ be the exact solution of the NFR-SubDE (2..10) - (2..12) at mesh point (x_i,t_k).

Define $\eta_i^k = u(x_i,t_k) - u_i^k$, $(i = 1,2,\ldots,m-1;\ \ k = 1,2,\ldots,n)$ and $\mathbf{Y}^k = (\eta_1^k,\eta_2^k,\cdots,\eta_{m-1}^k)^T$. Using $u_i^k = u(x_i,t_k) - \eta_i^k$, substitution into (3..1) leads to

$$\begin{aligned}\eta_i^{k+1} &= \eta_i^k + r_1\delta_x^2\eta_i^{k+1} + r_1\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})\delta_x^2\eta_i^{k-j} \\ &\quad + r_2\left[f(u(x_i,t_{k+1}),x_i,t_{k+1}) - f(u_i^{k+1},x_i,t_{k+1})\right] \\ &\quad + r_2\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})\left[f(u(x_i,t_{k-j}),x_i,t_{k-j}) - f(u_i^{k-j},x_i,t_{k-j})\right] \\ &\quad + \frac{\tau}{2}\left[g(u(x_i,t_{k+1}),x_i,t_{k+1}) - g(u_i^{k+1},x_i,t_{k+1})\right] \\ &\quad + \frac{\tau}{2}\left[g(u(x_i,t_k),x_i,t_k) - g(u_i^k,x_i,t_k)\right] + R_{i,\gamma}^{k+1} \qquad (3..9)\end{aligned}$$

and

$$\eta_i^0 = 0, \ \ i = 0,1,2,\cdots,m, \tag{3..10}$$

$$\eta_0^k = 0, \ \ \eta_m^k = 0, \ \ k = 0,1,2,\cdots,n. \tag{3..11}$$

Similarly, we can obtain

$$\begin{aligned}
\|\mathbf{Y}^{k+1}\|_2^2 \ = \ & (\mathbf{Y}^{k+1},\mathbf{Y}^k) + r_1(\delta_x^2\mathbf{Y}^{k+1},\mathbf{Y}^{k+1}) + r_1\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})(\delta_x^2\mathbf{Y}^{k-j},\mathbf{Y}^{k+1}) \\
& -\alpha r_2(\mathbf{Y}^{k+1},\mathbf{Y}^{k+1}) + \alpha r_2\sum_{j=0}^{k-1}(b_j^{(\gamma)} - b_{j+1}^{(\gamma)})(\mathbf{Y}^{k-j},\mathbf{Y}^{k+1}) \\
& +\frac{\tau}{2}\sum_{i=1}^{m-1}\left[g(u_i^{k+1},x_i,t_{k+1}) - g(\tilde{u}_i^{k+1},x_i,t_{k+1})\right]\eta_i^{k+1}h \\
& +\frac{\tau}{2}\sum_{i=1}^{m-1}\left[g(u_i^{k},x_i,t_{k}) - g(\tilde{u}_i^{k},x_i,t_{k})\right]\eta_i^{k+1}h \\
& +(\mathbf{R}_\gamma^{k+1},\mathbf{Y}^{k+1}).
\end{aligned} \tag{3..12}$$

Thanks to Lemma 2..4 and the inequalities

$$|(\mathbf{Y}^j,\mathbf{Y}^{k+1})| \leqslant \frac{1}{2}\left[\|\mathbf{Y}^j\|_2^2 + \|\mathbf{Y}^{k+1}\|_2^2\right],$$

$$|(\mathbf{R}_\gamma^{k+1},\mathbf{Y}^{k+1})| \leqslant \frac{r_1h^2b_k^{(\gamma)}}{L_x^2}\|\mathbf{Y}^{k+1}\|_2^2 + \frac{L_x^2}{4r_1h^2b_k^{(\gamma)}}\|\mathbf{R}_\gamma^{k+1}\|_2^2,$$

we obtain

$$\begin{aligned}
\|\mathbf{Y}^{k+1}\|_2^2 \ \leqslant \ & \tfrac{1}{2}\left[\|\mathbf{Y}^{k+1}\|_2^2 + \|\mathbf{Y}^k\|_2^2\right] - r_1[(\eta_1^{k+1})^2h + \|\Delta_x\mathbf{Y}^{k+1}\|_2^2] \\
& + r_1\sum_{j=0}^{k-1}(b_{j+1}^{(\gamma)} - b_j^{(\gamma)})[-\eta_1^{k-j}\eta_1^{k+1}h - (\Delta_x\mathbf{Y}^{k-j},\Delta_x\mathbf{Y}^{k+1})] \\
& -\alpha r_2\|\mathbf{Y}^{k+1}\|_2^2 + \tfrac{\alpha r_2}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma)} - b_{j+1}^{(\gamma)})\left[\|\mathbf{Y}^{k-j}\|_2^2 + \|\mathbf{Y}^{k+1}\|_2^2\right] \\
& + \tfrac{\tau}{4}L(\|\mathbf{Y}^{k+1}\|_2^2 + \|\mathbf{Y}^k\|_2^2) + \tfrac{\tau}{2}L\|\mathbf{Y}^{k+1}\|_2^2 \\
& + \tfrac{r_1h^2b_k^{(\gamma)}}{L_x^2}\|\mathbf{Y}^{k+1}\|_2^2 + \tfrac{L_x^2}{4r_1h^2b_k^{(\gamma)}}\|\mathbf{R}_\gamma^{k+1}\|_2^2.
\end{aligned}$$

Note that

$$\sum_{j=0}^{k-1}(b_j^{(\gamma)} - b_{j+1}^{(\gamma)}) = b_0^{(\gamma)} - b_k^{(\gamma)} = 1 - b_k^{(\gamma)}$$

and

$$|\eta_1^{k-j}\eta_1^{k+1}| \leqslant \frac{1}{2}\left[|\eta_1^{k-j}|^2 + |\eta_1^{k+1}|^2\right].$$

We have

$$\begin{aligned}\|\mathbf{Y}^{k+1}\|_2^2 \leqslant\ & \tfrac{1}{2}[\|\mathbf{Y}^{k+1}\|_2^2+\|\mathbf{Y}^k\|_2^2]-\tfrac{r_1}{2}(1+b_k^{(\gamma)})[|\eta_1^{k+1}|^2h+\|\Delta_x\mathbf{Y}^{k+1}\|_2^2]\\ &+\tfrac{r_1}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})(|\eta_1^{k-j}|^2h+\|\Delta_x\mathbf{Y}^{k-j}\|_2^2)\\ &-\tfrac{\alpha r_2}{2}(1+b_k^{(\gamma)})\|\mathbf{Y}^{k+1}\|_2^2+\tfrac{\alpha r_2}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})\|\mathbf{Y}^{k-j}\|_2^2\\ &+\tfrac{\tau}{4}L\|\mathbf{Y}^k\|_2^2+\tfrac{3\tau}{4}L\|\mathbf{Y}^{k+1}\|_2^2\\ &+\tfrac{r_1h^2b_k^{(\gamma)}}{L_x^2}\|\mathbf{Y}^{k+1}\|_2^2+\tfrac{L_x^2}{4r_1h^2b_k^{(\gamma)}}\|\mathbf{R}_\gamma^{k+1}\|_2^2.\end{aligned}$$

Applying Lemma 2..5, we can obtain

$$\begin{aligned}\|\mathbf{Y}^{k+1}\|_2^2 \leqslant\ & \tfrac{1}{2}[\|\mathbf{Y}^{k+1}\|_2^2+\|\mathbf{Y}^k\|_2^2]-\tfrac{r_1}{2}[|\eta_1^{k+1}|^2h+\|\Delta_x\mathbf{Y}^{k+1}\|_2^2]\\ &+\tfrac{r_1}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})(|\eta_1^{k-j}|^2h+\|\Delta_x\mathbf{Y}^{k-j}\|_2^2)\\ &-\tfrac{\alpha r_2}{2}\|\mathbf{Y}^{k+1}\|_2^2+\tfrac{\alpha}{2}r_2\sum_{j=0}^{k-1}(b_j^{(\gamma)}-b_{j+1}^{(\gamma)})\|\mathbf{Y}^{k-j}\|_2^2\\ &+\tfrac{\tau}{4}L\|\mathbf{Y}^k\|_2^2+\tfrac{3\tau}{4}L\|\mathbf{Y}^{k+1}\|_2^2+\tfrac{L_x^2}{4r_1h^2b_k^{(\gamma)}}\|\mathbf{R}_\gamma^{k+1}\|_2^2.\end{aligned}$$

Also

$$\begin{aligned}&\|\mathbf{Y}^{k+1}\|_2^2+r_1\sum_{j=0}^{k}b_j^{(\gamma)}\left[|\eta_1^{k+1-j}|^2h+\|\Delta_x\mathbf{Y}^{k+1-j}\|_2^2\right]+\alpha r_2\sum_{j=0}^{k}b_j^{(\gamma)}\|\mathbf{Y}^{k+1-j}\|_2^2\\ &\leqslant \|\mathbf{Y}^k\|_2^2+r_1\sum_{j=0}^{k-1}b_j^{(\gamma)}\left[|\eta_1^{k-j}|^2h+\|\Delta_x\mathbf{Y}^{k-j}\|_2^2\right]+\alpha r_2\sum_{j=0}^{k-1}b_j^{(\gamma)}\|\mathbf{Y}^{k-j}\|_2^2\\ &+\tfrac{\tau}{2}L\|\mathbf{Y}^k\|_2^2+\tfrac{3\tau}{2}L\|\mathbf{Y}^{k+1}\|_2^2+\tfrac{L_x^2}{2r_1h^2b_k^{(\gamma)}}\|\mathbf{R}_\gamma^{k+1}\|_2^2.\end{aligned}$$

Let

$$\rho_k=\|\mathbf{Y}^k\|_2^2+r_1\sum_{j=0}^{k-1}b_j^{(\gamma)}\left[|\eta_1^{k-j}|^2h+\|\Delta_x\mathbf{Y}^{k-j}\|_2^2\right]+\alpha r_2\sum_{j=0}^{k-1}b_j^{(\gamma)}\|\mathbf{Y}^{k-j}\|_2^2.$$

Applying Lemma 2..6, we have

$$(1-\frac{3}{2}L\tau)\rho_{k+1}\leqslant(1+\frac{1}{2}L\tau)\rho_k+C_1b_k^{(\gamma)}\tau^\gamma(\tau+h^2)^2,$$

i.e.,

$$\rho_{k+1}\leqslant\frac{1+\frac{1}{2}L\tau}{1-\frac{3}{2}L\tau}\left[\rho_k+C_1b_k^{(\gamma)}\tau^\gamma(\tau+h^2)^2\right].$$

Therefore, we obtain

$$\rho_k\leqslant\left[\frac{1+\frac{1}{2}L\tau}{1-\frac{3}{2}L\tau}\right]^k\left[\rho_0+\sum_{j=0}^{k-1}C_1b_j^{(\gamma)}\tau^\gamma(\tau+h^2)^2\right].$$

Note that $\rho_0=0$, then there exists a positive constant C_2 such that

$$\|\mathbf{Y}^k\|_2^2\leqslant\rho_k\leqslant C_2k^\gamma\tau^\gamma(\tau+h^2)^2\leqslant C_2T^\gamma(\tau+h^2)^2.$$

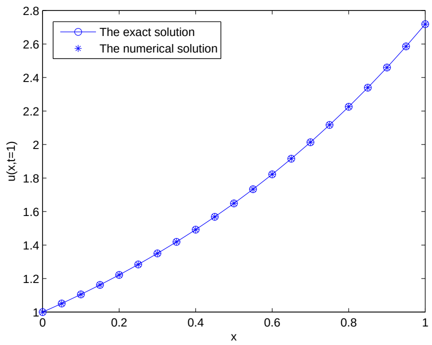

FIG. 1. Comparison of exact and numerical solutions at time $t = 1.0$ when $\gamma = 0.90$.

THEOREM 3..2 Suppose that the continuous problem (2..10)-(2..12) has a smooth solution $u(x,t) \in C^{4,2}_{x,t}(\Omega \times [0,T])$, then there exists a positive constant $C > 0$ such that

$$\|\mathbf{Y}^k\|_2 \leqslant C(\tau + h^2), k = 1, 2, \cdots, n. \tag{3..13}$$

Further, the FIDA defined by (3..1)- (3..3) is convergent.

4. Numerical results

In this section, three numerical examples are given to demonstrate our theoretical analysis.

EXAMPLE 4..1 Consider the following NFR-SubDE:

$$\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= {}_0D_t^{1-\gamma}\left[\frac{\partial^2 u(x,t)}{\partial x^2} - u + \frac{\Gamma(5+2\gamma)}{\Gamma(6+\gamma)} t^{5+\gamma} e^{2x}\right] \\
&\quad -u^2 + (2+\gamma) t^{1+\gamma} e^x, && (4..1)\\
u(x,0) &= 0, && (4..2)\\
u(0,t) &= t^{2+\gamma}, \quad u(1,t) = e t^{2+\gamma}, && (4..3)
\end{aligned}$$

where $0 \leqslant x \leqslant 1, \ \ t > 0$.

The exact solution of the NFR-SubDE (4..1)-(4..3) is

$$u(x,t) = t^{2+\gamma} e^x.$$

FIG.1 shows the exact solution and numerical solution of the FIDA, with $\tau = 1/400$ and $h = 1/20$, at time $t = 1.0$. From FIG.1, it can be seen that the numerical solution is in excellent agreement with the exact solution.

Table1 shows the maximum absolute numerical error of the exact solution and numerical solution of the FIDA at time $t = 1.0$ when $\gamma = 0.9$. From Table1, it can be seen that the FIDA yields convergence with rate $O(\tau + h^2)$.

TABLE 1 *Maximum error behavior versus gridsize reduction for Example 4..1 at time* $t = 1$.

h	τ	Maximum Error
$\frac{1}{10}$	$\frac{1}{100}$	1.6040E-3
$\frac{1}{15}$	$\frac{1}{225}$	7.4602E-4
$\frac{1}{20}$	$\frac{1}{400}$	4.2415E-4
$\frac{1}{25}$	$\frac{1}{625}$	2.7323E-4

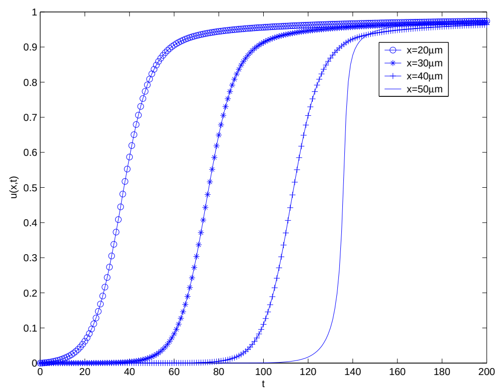

FIG. 2. Model simulation of a fertilization Ca^{2+} wave following (4..4) resulting in a travelling front for $\gamma = 0.50$ at four spatial positions.

EXAMPLE 4..2 Consider a travelling wave of a concentration of a molecular species in a crowded environment. The following nonlinear reaction diffusion equation is used(See Cao *et al.* (2006)):

$$\frac{\partial u}{\partial t} = {}_0D_t^{1-\gamma}\left[K_\gamma \frac{\partial^2 u(x,t)}{\partial x^2} + f(u)\right], 0 \leqslant x \leqslant L_x, 0 < t \leqslant T, \quad (4..4)$$

with the boundary conditions $\frac{\partial u}{\partial x}|_{x=0,L_x} = 0$ and the initial condition

$$u(x,0) = \begin{cases} 1, & 0 \leqslant x \leqslant l, \\ 0, & l < x \leqslant L_x, \end{cases}$$

where $f(u)$ is the cubic polynomial $f(u) = K_\gamma u(1-u)(u-\theta)$ with $0 < \theta < 0.5$. The reaction term has realistic chemical reaction features. This equation has been used to describe features of action potential propagation in nerve axons, and calcium fertilization waves in frog eggs in a crowded spatial environment(See Fall *et al.* (2002)). In this example, we take $K_\gamma = 2.25$, $\theta = 0.2$, $T = 200$, $L_x = 500\mu m$, $l = 10\mu m$, and $\tau = 0.01$, $h = 0.1$.

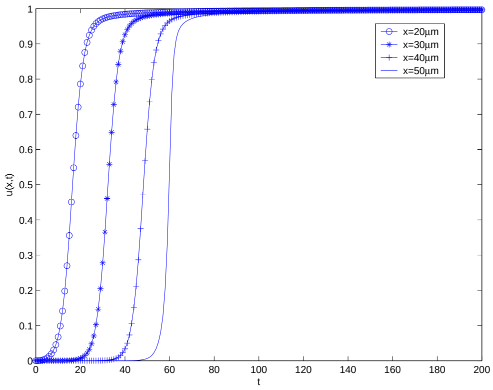

FIG. 3. Model simulation of a fertilization Ca^{2+} wave following (4..4) resulting in a travelling front for $\gamma = 0.75$ at four spatial positions.

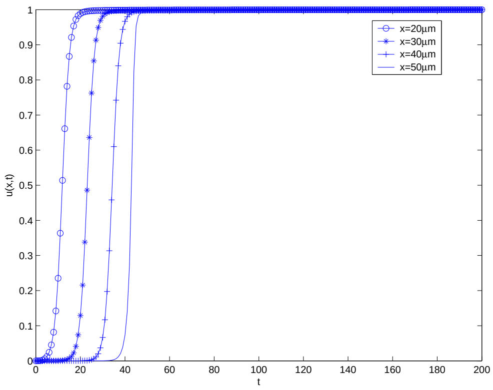

FIG. 4. Model simulation of a fertilization Ca^{2+} wave following (4..4) resulting in a travelling front for $\gamma = 0.95$ at four spatial positions.

FIG.2, FIG.3 and FIG.4 show model simulation of a fertilization Ca^{2+} following (4..4) in a travelling front for $\gamma = 0.5$, $\gamma = 0.75$ and $\gamma = 0.95$ at different x , respectively. FIG.5, FIG.6 and FIG.7 show the numerical simulation of the equation (4..4) when $\gamma = 0.5$, $\gamma = 0.75$ and $\gamma = 0.95$, respectively. From these figures, we find that the wave travels more slowly as γ decreases as to be expected.

EXAMPLE 4..3 Consider the following Michaelis-Menten reaction-diffusion equations (See Cao *et al.* (2006)):

$$\begin{aligned} \frac{\partial A}{\partial t} &= {}_0D^{1-\gamma}(K_\gamma \frac{\partial^2 A}{\partial x^2} - k_1 AB) + (k_2 + k_3)C, \\ \frac{\partial B}{\partial t} &= {}_0D^{1-\gamma}(K_\gamma \frac{\partial^2 B}{\partial x^2} - k_1 AB) + k_2 C, \\ \frac{\partial C}{\partial t} &= {}_0D^{1-\gamma}(K_\gamma \frac{\partial^2 C}{\partial x^2} + k_1 AB) - (k_2 + k_3)C, \end{aligned} \tag{4..5}$$

where A, B, C denote concentrations, K_γ is the generalized diffusion coefficient, and k_1, k_2, k_3 are the rate

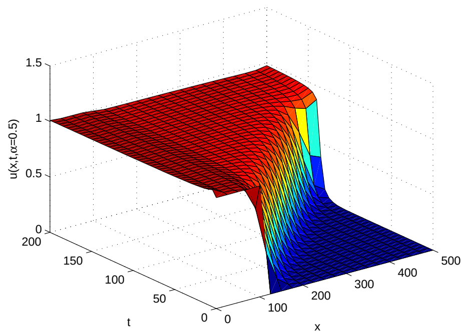

FIG. 5. The solution $u(x,t)$ of (4..4) when $\gamma = 0.50$.

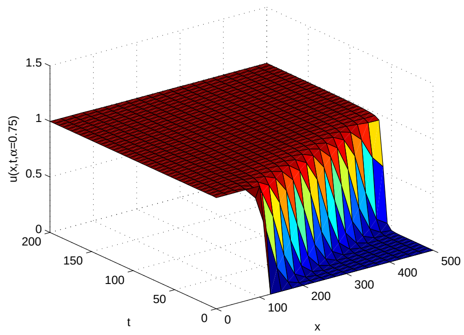

FIG. 6. The solution $u(x,t)$ of (4..4) when $\gamma = 0.75$.

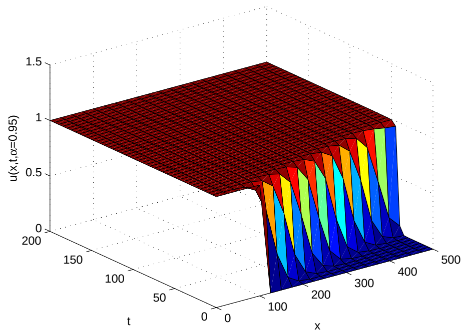

FIG. 7. The solution $u(x,t)$ of (4..4) when $\gamma = 0.95$.

coefficients. Here,

$$K_\gamma = 10^{-5}, k_1 = 0.01, k_2 = 0.02, k_3 = 0.03, L_x = 1, T = 600.$$

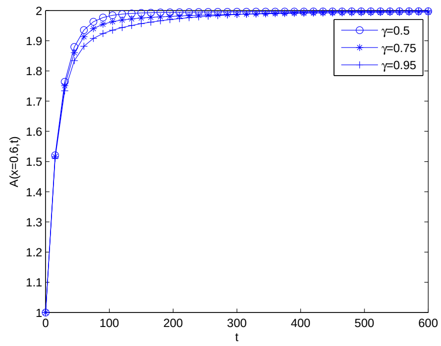

FIG. 8. Concentration A as a function of t at $x = 0.6$ for various γ.

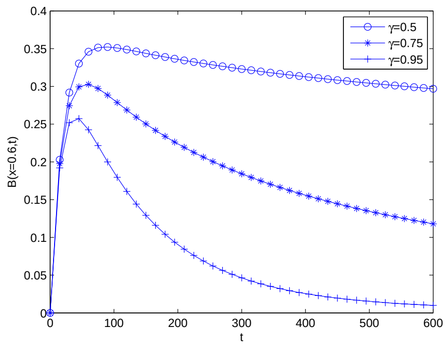

FIG. 9. Concentration B as a function of t at $x = 0.6$ for various γ.

We suppose the periodic boundary condition, i.e.,

$$A(0,t) = A(L_x,t), B(0,t) = B(L_x,t), C(0,t) = C(L_x,t),$$

and initial conditions: $A(x,0) = 1$, $B(x,0) = 0$, $C(x,0) = 1$. In this simulation, we choose $h = 0.1, \tau = 0.01$. The results of the simulation are shown in FIG.8, FIG.9 and FIG.10.

These figures compare the response of the diffusion system with different real numbers γ for $A(x,t)$, $B(x,t)$ and $C(x,t)$ concentrations, respectively.

5. Conclusions

In this paper, we have proposed an implicit numerical method to model the nonlinear fractional reaction-subdiffusion process. We have proved the stability and convergence of the method. Some numerical

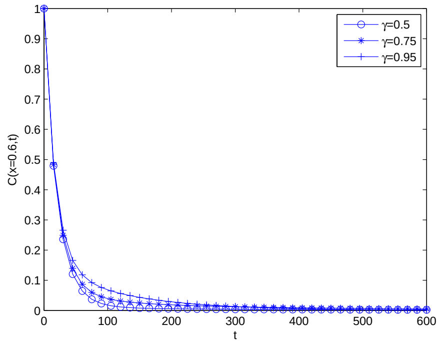

FIG. 10. Concentration C as a function of t at $x = 0.6$ for various γ.

examples are presented to show the application of the present technique. This method and supporting theoretical results can also be applied to fractional integro-differential equations.

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