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NEW SOLUTION AND ANALYTICAL TECHNIQUES OF THE IMPLICIT NUMERICAL METHOD FOR THE ANOMALOUS SUB-DIFFUSION EQUATION *

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Abstract. A physical-mathematical approach to anomalous diffusion is based on a generalized diffusion equation containing derivatives of fractional order. In this paper, an anomalous sub-diffusion equation (ASub-DE) is considered. A new implicit numerical method (INM) and two solution techniques for improving the order of convergence of the INM for solving the ASub-DE are proposed. The stability and convergence of the INM are investigated by the energy method. Some numerical examples are given. The numerical results demonstrate the effectiveness of theoretical analysis. These methods and supporting theoretical results can also be applied to other fractional integro-differential equations and higher-dimensional problems.

Key words. Anomalous sub-diffusion equation, implicit numerical method, stability, convergence, fractional integro-differential equation.

AMS subject classifications. 26A33, 45K05, 35K37, 65M12

1. Introduction. Fractional differential equations have attracted considerable interest because of their ability to model many phenomena, for example, in fractal media, mathematical biology, chemistry, statistical mechanics and biochemistry due to anomalous diffusion effects in constrained environments. A physical-mathematical approach to anomalous diffusion may be based on generalized partial differential equations containing derivatives of fractional order in space, or time, or space-time [1, 2]. These fractional diffusion equations can be derived asymptotically from basic random walk models or from generalized master equations. Anomalous diffusion, known since Richardson's treatise on turbulent diffusion in 1926, is ubiquitous in physical and biological systems where trapping and binding of particles can occur. In particular, the trapping of Brownian particles by static traps randomly distributed over either a Euclidean or a disordered substrate is a fundamental problem of non-equilibrium statistical mechanics and chemistry with a very wide range of applications [3]. Fractional kinetic equations have proved particularly useful in the context of anomalous subdiffusion [1]. The mean square displacement of the particles from the original starting site is no longer linear in time, but verifies a generalized Fick's second law. Subdiffusive motion is characterized by an asymptotic long-time behavior of the mean square displacement of the form

$$(1.1) \quad \langle x^2(t) \rangle \sim \frac{2K_\gamma}{\Gamma(1+\gamma)} t^\gamma, t \rightarrow \infty,$$

where γ (with $0 < \gamma < 1$) is the anomalous diffusion exponent and K_γ is the generalized diffusion coefficient. Ordinary (or Brownian) diffusion corresponds to $\gamma = 1$ with $K_1 = D$ (the ordinary diffusion coefficient).

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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. For anomalous subdiffusive random walkers, the continuum description via the ordinary diffusion equation is replaced by the fractional diffusion equation. It has been suggested that the probability density function (pdf) $u(x, t)$ that describes anomalous subdiffusion particles follows the anomalous sub-diffusion equation (ASub-DE) [1, 3, 4, 5]:

$$(1.2) \quad \frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left[K_\gamma \frac{\partial^2 u}{\partial x^2} \right], 0 \leq x \leq a, 0 < t \leq T,$$

where $u(x, t)$ is the probability density that the particle that started at 0 at time 0 is at x at time t , $\frac{\partial^{1-\gamma} u}{\partial t^{1-\gamma}}$ denotes the Riemann-Liouville fractional derivative of order $1 - \gamma$ defined by

$$(1.3) \quad \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} u(x, t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t \frac{u(x, \eta)}{(t - \eta)^{1-\gamma}} d\eta,$$

with $0 \leq \gamma \leq 1$. For $\gamma = 1$ one recovers the identity operator and for $\gamma = 0$ the ordinary first-order derivative. The integro-differential nature of the Riemann-Liouville fractional operator according to Eq. (1.3) ensures the non-Markovian nature of the subdiffusive process defined by Eq. (1.2). Eq. (1.2) can be rewritten as the following equivalent time fractional diffusion equation:

$$(1.4) \quad \frac{\partial^\gamma}{\partial t^\gamma} u(x, t) - \frac{t^{-\gamma}}{\Gamma(1-\gamma)} u_0(x) = K_\gamma \frac{\partial^2}{\partial x^2} u(x, t),$$

where $u_0(x)$ is the initial value.

Anomalous sub-diffusion equations have been widely studied. Schneider and Wyss [6] considered the following time fractional diffusion and wave equations:

$$(1.5) \quad \frac{\partial^\gamma u(\mathbf{x}, t)}{\partial t^\gamma} = \frac{\partial^2 u(\mathbf{x}, t)}{\partial \mathbf{x}^2}, \quad 0 < \gamma \leq 2.$$

They derived the corresponding Green functions in closed form for arbitrary space dimensions in terms of Fox functions. Huang and Liu [7] considered the time-fractional diffusion equation in n -dimensional whole-space and half-space. They investigated the explicit relationships between the problems in whole-space with the corresponding problems in half-space by the Fourier-Laplace transform. Mainardi [8] derived the fundamental solutions for the fractional diffusion-wave equation. Anh and Leonenko [9] presented spectral analysis of the fractional kinetic equation with random data; Gorenflo *et al.* [10] investigated mappings between solutions of fractional diffusion-wave equations; Kilbas *et al.* [11] presented solutions of Volterra integro-differential equations with kernels given in the form of generalized Mittag-Leffler functions.

Different numerical methods for solving the space, or time, or space-time fractional partial differential equations have been proposed. Liu *et al.* [12, 13] transformed the space fractional partial differential equation into a system of ordinary differential equations (method of lines) that was then solved using backward differentiation formulas. McLean *et al.* [14] considered time discretization via a Laplace transformation of an inhomogeneous integro-differential equation of parabolic type. The method is combined with a finite element discretization in the spatial variables to yield a fully discrete method. McLean [15] also proposed numerical methods for some fractional

differential equations and gave a convergence and stability analysis. Roop [16] investigated the numerical approximation of the variational solution to the fractional advection dispersion equation. Meerschaert *et al.* [17] examined finite difference approximations for fractional advection-dispersion flow equations. Shen *et al.* [18] proposed an explicit finite difference approximation for the space fractional diffusion equation and gave an error analysis. Liu *et al.* [19] discussed an approximation of the Lévy-Feller advection-dispersion process by a random walk and finite difference method. Zhang *et al.* [20] proposed a numerical approximation for the Lévy-Feller fractional diffusion equation. They used the finite difference method to discretize the integro-differential equation and gave an analysis of stability and convergence in the L_1 -norm. Liu *et al.* [21] derived an analysis of a discrete non-Markovian random walk approximation for the time fractional diffusion equation. Zhuang and Liu [22] analyzed an implicit difference approximation for the time fractional diffusion equation, and the stability and convergence of the method were also discussed. Liu *et al.* [23] also discussed the stability and convergence of the difference methods for the space-time fractional advection-diffusion equation. Lin and Liu [24] 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.

There have been some attempts on deriving numerical methods and analysis techniques for the ASub-DE (1.2). Cao *et al.* [25] presented a variable coefficient fractional derivative approximation scheme, and used embedding techniques to develop a variable stepsize implementation for solving time fractional differential equations. They gave a stability and order analysis for a fractional Euler method and a fractional trapezoidal method. Yuste and Acedo [4] proposed an explicit finite difference method and a new Von Neumann-type stability analysis for the ASub-DE (1.2). Langlands and Henry [5] also investigated this problem and proposed an implicit numerical scheme (L1 approximation). However, effective numerical methods and supporting error analyses for the ASub-DE (1.2) are still limited. The main purpose of this paper is to solve and analyze this problem by introducing an implicit numerical method and new solution techniques.

In Section 2, an implicit numerical method (INM) is proposed. In Sections 3 and 4, stability and convergence analyses are given for the INM. In Section 5, two solution techniques to improve the order of convergence are presented. Finally, some numerical results are given in Section 6 to evaluate the method.

2. An implicit numerical method for the ASub-DE. In this section, we construct a new implicit numerical method for the ASub-DE

$$(2.1) \quad \frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left[K_\gamma \frac{\partial^2 u}{\partial x^2} + f(x, t) \right], \quad 0 \leq x \leq a, \quad 0 < t \leq T,$$

with initial and boundary conditions:

$$(2.2) \quad u(x, 0) = \phi(x), \quad 0 \leq x \leq a,$$

$$(2.3) \quad u(0, t) = \varphi_1(t), \quad u(a, t) = \varphi_2(t), \quad 0 \leq t \leq T,$$

where $0 < \gamma < 1$.

Yuste and Acedo [4] combined the forward time centered space (FTCS) method, which is well known for the numerical integration of ordinary diffusion equations, with the Grünwald-Letnikov discretization of the Riemann-Liouville derivative to obtain

an explicit FTCS scheme for the ASub-DE (1.2). However, they did not give the convergence analysis and pointed out that this is not such an easy task when implicit methods are considered. Langlands and Henry [5] proposed an implicit numerical scheme (L1 approximation) for the ASub-DE (1.2), and discussed the accuracy and stability of this scheme. However, the global accuracy of the implicit numerical scheme has not been derived and it seems that the unconditional stability for all γ in the range $0 < \gamma \leq 1$ has not been established.

Let $\Omega = [0, a] \times [0, T]$. We define the function space

$$G(\Omega) = \{w(x, t) \mid \frac{\partial^2 w}{\partial x^2} \in C^2(\Omega) \text{ and } \frac{\partial^5 w}{\partial x^4 \partial t} \in C(\Omega)\}.$$

In this paper, we suppose the continuous problem (2.1)-(2.3) has a smooth solution $u(x, t) \in G(\Omega)$.

Define $t_k = k\tau, k = 0, 1, 2, \dots, n, x_i = ih, i = 0, 1, 2, \dots, m$, where $\tau = \frac{T}{n}$ and $h = \frac{a}{m}$ are the space and time stepsizes, respectively. For convenience, we introduce the following notations:

$$Lu(x, t) = K_\gamma \frac{\partial^2 u(x, t)}{\partial x^2},$$

$$\delta_x^2 u(x, t) = u(x + h, t) - 2u(x, t) + u(x - h, t),$$

and

$$(2.4) \quad b_j = (j + 1)^\gamma - j^\gamma, j = 0, 1, 2, \dots, n.$$

Integrating both side of Eq. (2.1), we obtain

$$(2.5) \quad \begin{aligned} u(x_i, t_{k+1}) &= u(x_i, t_k) + \frac{1}{\Gamma(\gamma)} \int_0^{t_{k+1}} \frac{Lu(x_i, \eta) + f(x_i, \eta)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta \\ &\quad - \frac{1}{\Gamma(\gamma)} \int_0^{t_k} \frac{Lu(x_i, \eta) + f(x_i, \eta)}{(t_k - \eta)^{1-\gamma}} d\eta \\ &= u(x_i, t_k) + \frac{1}{\Gamma(\gamma)} \int_0^\tau \frac{Lu(x_i, \eta) + f(x_i, \eta)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta \\ &\quad + \frac{1}{\Gamma(\gamma)} \int_0^{t_k} \frac{Lv(x_i, \eta) + g(x_i, \eta)}{(t_k - \eta)^{1-\gamma}} d\eta, \end{aligned}$$

where $v(x, t) = u(x, t + \tau) - u(x, t)$ and $g(x, t) = f(x, t + \tau) - f(x, t)$. Letting

$$I_1 = \frac{1}{\Gamma(\gamma)} \int_0^\tau \frac{Lu(x_i, \eta) + f(x_i, \eta)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta,$$

and

$$I_2 = \frac{1}{\Gamma(\gamma)} \int_0^{t_k} \frac{Lv(x_i, \eta) + g(x_i, \eta)}{(t_k - \eta)^{1-\gamma}} d\eta,$$

Eq. (2.5) can be written as

$$u(x_i, t_{k+1}) = u(x_i, t_k) + I_1 + I_2.$$

For I_1 , we can use the following approximation:

$$\begin{aligned} I_1 &= \frac{1}{\Gamma(\gamma)} \int_0^\tau \frac{Lu(x_i, \tau) + f(x_i, \tau)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta + R_{11} \\ &= \frac{\tau^\gamma}{\Gamma(\gamma+1)} [(k+1)^\gamma - k^\gamma] [Lu(x_i, \tau) + f(x_i, \tau)] + R_{11} \\ &= \frac{\tau^\gamma}{\Gamma(\gamma+1)} b_k [K_\gamma \frac{1}{h^2} \delta_x^2 u(x_i, \tau) + R_{12} + f(x_i, \tau)] + R_{11} \\ &= \frac{\tau^\gamma}{\Gamma(\gamma+1)} b_k [K_\gamma \frac{1}{h^2} \delta_x^2 u(x_i, \tau) + f(x_i, \tau)] + R_1, \end{aligned}$$

where

$$R_{11} = \frac{1}{\Gamma(\gamma)} \int_0^\tau \frac{Lu(x_i, \eta) - Lu(x_i, \tau) + f(x_i, \eta) - f(x_i, \tau)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta,$$

$$R_{12} = K_\gamma \left[\frac{\partial^2 u(x_i, \tau)}{\partial x^2} - \frac{1}{h^2} \delta_x^2 u(x_i, \tau) \right]$$

and $R_1 = \frac{b_k \tau^\gamma}{\Gamma(\gamma+1)} R_{12} + R_{11}$. By noting that

$$\begin{aligned} Lu(x_i, \eta) + f(x_i, \eta) &= K_\gamma \frac{\partial^2 u(x_i, \eta)}{\partial x^2} + f(x_i, \eta) \\ &= K_\gamma \frac{\partial^2 u(x_i, \tau)}{\partial x^2} + f(x_i, \tau) + \left[K_\gamma \frac{\partial^3 u(x_i, \xi_1)}{\partial x^2 \partial t} + \frac{\partial f(x_i, \xi_1)}{\partial t} \right] (\eta - \tau), \end{aligned}$$

where $0 \leq \eta \leq \xi_1 \leq \tau$, we obtain

$$|R_{11}| \leq C_1 \tau \frac{1}{\Gamma(\gamma)} \int_0^\tau \frac{1}{(t_{k+1} - \eta)^{1-\gamma}} d\eta \leq \frac{C_1 \tau^{1+\gamma}}{\Gamma(\gamma+1)} b_k.$$

Again, it is apparent that

$$|R_{12}| \leq C_2 h^2.$$

Hence, we have $|R_1| \leq C b_k \tau^\gamma (\tau + h^2)$.

As for I_2 , we can obtain the following approximation:

$$\begin{aligned} I_2 &= \frac{1}{\Gamma(\gamma)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{Lv(x_i, \eta) + g(x_i, \eta)}{(t_k - \eta)^{1-\gamma}} d\eta \\ &= \frac{1}{\Gamma(\gamma)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{Lv(x_i, t_{j+1}) + g(x_i, t_{j+1})}{(t_k - \eta)^{1-\gamma}} d\eta + R_{21} \\ &= \frac{\tau^\gamma}{\Gamma(\gamma+1)} \sum_{j=0}^{k-1} b_{k-j-1} [Lv(x_i, t_{j+1}) + g(x_i, t_{j+1})] + R_{21} \\ &= \frac{\tau^\gamma}{\Gamma(\gamma+1)} \sum_{j=0}^{k-1} b_{k-j-1} [L_h v(x_i, t_{j+1}) + g(x_i, t_{j+1})] + R_{22} + R_{21}, \end{aligned}$$

where

$$R_{21} = \frac{1}{\Gamma(\gamma)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{Lv(x_i, \eta) - Lv(x_i, t_{j+1}) + g(x_i, \eta) - g(x_i, t_{j+1})}{(t_k - \eta)^{1-\gamma}} d\eta,$$

$$R_{22} = \frac{\tau^\gamma}{\Gamma(\gamma+1)} \sum_{j=0}^{k-1} b_{k-j-1} [Lv(x_i, t_{j+1}) - L_h v(x_i, t_{j+1})],$$

and $L_h u(x_i, t_j) = K_\gamma \frac{1}{h^2} \delta_x^2 u(x_i, t_j)$.

LEMMA 2.1. *Let $u(x, t) \in G(\Omega)$ be the solution of (2.1)-(2.3). Then we have*

(1) $|R_{21}| \leq C\tau^2$; (2) $|R_{22}| \leq C\tau h^2$.

Proof. (1) When $t_j \leq \eta \leq t_{j+1}$, we have

$$\begin{aligned} Lv(x_i, \eta + \tau) + g(x_i, \eta + \tau) &= K_\gamma \frac{\partial^2 v(x_i, \eta + \tau)}{\partial x^2} + g(x_i, \eta + \tau) \\ &= K_\gamma \frac{\partial^2 v(x_i, t_{j+2})}{\partial x^2} + g(x_i, t_{j+2}) \\ &\quad + K_\gamma \frac{\partial^3 v(x_i, \tilde{\eta}_1)}{\partial x^2 \partial t} (\eta - t_{j+1}) + \frac{\partial g(x_i, \tilde{\eta}_1)}{\partial t} (\eta - t_{j+1}), \end{aligned}$$

where $\eta + \tau \leq \tilde{\eta}_1 \leq t_{j+2}$.

Again,

$$\begin{aligned} \frac{\partial^3 v(x_i, \tilde{\eta}_1)}{\partial x^2 \partial t} &= \frac{\partial^3 u(x_i, \tilde{\eta}_1 + \tau)}{\partial x^2 \partial t} - \frac{\partial^3 u(x_i, \tilde{\eta}_1)}{\partial x^2 \partial t} = \frac{\partial^4 u(x_i, \tilde{\eta}_2)}{\partial x^2 \partial t^2} \tau, \\ \frac{\partial g(x_i, \tilde{\eta}_1)}{\partial t} &= \frac{\partial f(x_i, \tilde{\eta}_1 + \tau)}{\partial t} - \frac{\partial f(x_i, \tilde{\eta}_1)}{\partial t} = \frac{\partial^2 f(x_i, \tilde{\eta}_3)}{\partial t^2} \tau, \end{aligned}$$

where $\tilde{\eta}_1 \leq \tilde{\eta}_2, \tilde{\eta}_3 \leq \tilde{\eta}_1 + \tau$. Consequently,

$$|Lu(x_i, \eta + \tau) - Lu(x_i, \eta) - [Lu(x_i, t_{j+2}) - Lu(x_i, t_{j+1})]| \leq C_3 \tau^2.$$

Thus, we have

$$|R_{21}| \leq C_3 \tau^2 \frac{1}{\Gamma(\gamma)} \int_0^{t_k} \frac{d\eta}{(t_k - \eta)^{1-\gamma}} \leq C\tau^2.$$

(2) Using Taylor's formula, we obtain

$$\begin{aligned} Lv(x_i, t_{j+1}) &= L_h v(x_i, t_{j+1}) + \frac{h^2}{12} \frac{\partial^4 v(\xi_2, t_{j+1})}{\partial x^4} \\ &= L_h v(x_i, t_{j+1}) + \frac{h^2}{12} \left[\frac{\partial^4 u(\xi_2, t_{j+2})}{\partial x^4} - \frac{\partial^4 u(\xi_2, t_{j+1})}{\partial x^4} \right] \\ &= L_h v(x_i, t_{j+1}) + \frac{h^2 \tau}{12} \frac{\partial^5 u(\xi_2, \tilde{\eta}_4)}{\partial x^4 \partial t}, \end{aligned}$$

$$|Lv(x_i, t_{j+1}) - L_h v(x_i, t_{j+1})| \leq C_3 \tau h^2 \tau.$$

Thus, we have

$$|R_{22}| \leq C_3 \tau h^2 \frac{\tau^\gamma}{\Gamma(\gamma + 1)} \sum_{j=0}^{k-1} b_{k-j+1} \leq C\tau h^2.$$

□

From the above results, we obtain

$$\begin{aligned} u(x_i, t_{k+1}) &= u(x_i, t_k) + r_1 b_k \delta_x^2 u(x_i, \tau) + r_2 b_k f(x_i, \tau) \\ &\quad + r_1 \sum_{j=0}^{k-1} b_{k-j-1} [\delta_x^2 u(x_i, t_{j+2}) - \delta_x^2 u(x_i, t_{j+1})] \\ &\quad + r_2 \sum_{j=0}^{k-1} b_{k-j-1} [f(x_i, t_{j+2}) - f(x_i, t_{j+1})] + R_i^{k+1}, \end{aligned}$$

where $r_1 = K_\gamma \frac{\tau^\gamma}{\Gamma(\gamma+1)h^2}$, $r_2 = \frac{\tau^\gamma}{\Gamma(\gamma+1)}$, and

$$(2.6) \quad |R_i^{k+1}| \leq C(b_k \tau^\gamma + \tau)(\tau + h^2).$$

LEMMA 2.2. *The coefficients $b_k (k = 0, 1, 2, \dots)$ defined by (2.4) satisfy:*

- (1) $b_0 = 1, b_k > 0, k = 0, 1, 2, \dots$;
- (2) $b_k > b_{k+1}, k = 0, 1, 2, \dots$;
- (3) *there exists a positive constant $C > 0$, such that*

$$\tau \leq C b_k \tau^\gamma, k = 1, 2, \dots.$$

Proof. Let $\psi_1(x) = x^\gamma$ and $\psi_2(x) = (x+1)^\gamma - x^\gamma$. For $x > 0$, it can be seen that $\psi_1(x)$ is monotone increasing and $\psi_2(x)$ is monotone decreasing. Thus, (1) and (2) in Lemma 2.2 hold.

For (3) in Lemma 2.2, using

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

we have

$$\frac{n^{\gamma-1}}{b_n} \leq C_1,$$

or

$$n^{-1} \leq C_1 b_n n^{-\gamma} \leq C_1 b_k n^{-\gamma}.$$

Thus, from $\tau = \frac{T}{n}$, the inequality (3) can be obtained. \square

Let $\mathbf{R}^k = (R_1^k, R_2^k, \dots, R_{m-1}^k)^T$. Applying Lemma 2.2 with (2.6), we obtain the following lemma.

LEMMA 2.3. *Suppose that $\|\mathbf{R}^k\|_2 = \sqrt{\sum_{i=1}^{m-1} |R_i^k|^2}$. If $u(x, t) \in G(\Omega)$ is the solution of (2.1)-(2.3), then we have*

$$\|\mathbf{R}^{k+1}\|_2 \leq C b_k \tau^\gamma (\tau + h^2).$$

Let u_i^k be the numerical approximation to $u(x_i, t_k)$, $f_i^k = f(x_i, t_k)$ and introduce the following notations:

$$(2.7) \quad \delta_x^2 u_i^k = u_{i+1}^k - 2u_i^k + u_{i-1}^k, \quad \Delta_x u_i^k = u_{i+1}^k - u_i^k.$$

We obtain the following implicit difference scheme:

$$\begin{aligned} u_i^{k+1} &= u_i^k + r_1 b_k \delta_x^2 u_i^1 + r_2 b_k f_i^1 \\ &+ r_1 \sum_{j=0}^{k-1} b_{k-j-1} \left[\delta_x^2 u_i^{j+2} - \delta_x^2 u_i^{j+1} \right] + r_2 \sum_{j=0}^{k-1} b_{k-j-1} \left[f_i^{j+2} - f_i^{j+1} \right]. \end{aligned}$$

The implicit numerical method (INM) can be rewritten in the following form:

$$(2.8) \quad \begin{aligned} u_i^{k+1} &= u_i^k + r_1 \delta_x^2 u_i^{k+1} + r_1 \sum_{j=0}^{k-1} (b_{j+1} - b_j) \delta_x^2 u_i^{k-j} \\ &+ r_2 f_i^{k+1} + r_2 \sum_{j=0}^{k-1} (b_{j+1} - b_j) f_i^{k-j}, \end{aligned}$$

for $i = 1, 2, \dots, m-1, k = 0, 1, 2, \dots, n-1$.

The initial and boundary conditions are

$$(2.9) \quad \begin{aligned} u_i^0 &= \phi(ih), \quad i = 0, 1, 2, \dots, m, \\ u_0^k &= \varphi_1(k\tau), \quad u_m^k = \varphi_2(k\tau), \quad k = 1, 2, \dots, n. \end{aligned}$$

Eqs. 2.8 and 2.9 can be rewritten as the following matrix form

$$(2.10) \quad \begin{cases} A\mathbf{u}^1 = \mathbf{u}^0 + r_1\mathbf{v}^1 + r_2\mathbf{f}^1 \\ A\mathbf{u}^{k+1} = \mathbf{u}^k + r_1\mathbf{v}^{k+1} + r_1\mathbf{w}^{k+1} + r_2\mathbf{g}^{k+1}, \quad k > 0 \\ \mathbf{u}^0 = \Phi \end{cases}$$

where

$$(2.11) \quad A = \begin{bmatrix} 1 + 2r_1 & -r_1 & 0 & \cdots & 0 & 0 \\ -r_1 & 1 + 2r_1 & -r_1 & \cdots & 0 & 0 \\ 0 & -r_1 & 1 + 2r_1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 + 2r_1 & -r_1 \\ 0 & 0 & 0 & \cdots & -r_1 & 1 + 2r_1, \end{bmatrix}$$

$$(2.12) \quad \mathbf{u}^k = \begin{bmatrix} u_1^k \\ u_2^k \\ \vdots \\ u_{m-2}^k \\ u_{m-1}^k \end{bmatrix}, \quad \mathbf{f}^k = \begin{bmatrix} f_1^k \\ f_2^k \\ \vdots \\ f_{m-2}^k \\ f_{m-1}^k \end{bmatrix}, \quad \mathbf{v}^{k+1} = \begin{bmatrix} u_0^{k+1} \\ 0 \\ \vdots \\ 0 \\ u_m^{k+1} \end{bmatrix}, \quad \Phi = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{m-2} \\ \phi_{m-1} \end{bmatrix},$$

$$\text{and } \mathbf{w}^{k+1} = \sum_{j=0}^{k-1} (b_{j+1} - b_j)\delta_x^2 \mathbf{u}^{k-j}, \quad \mathbf{g}^{k+1} = \mathbf{f}^{k+1} + \sum_{j=0}^{k-1} (b_{j+1} - b_j)\mathbf{f}^{k-j}, \quad \phi_i = \phi(ih).$$

In (2.11) we see that the matrix A is strictly diagonally dominant with positive diagonal terms and nonpositive offdiagonal terms. Hence, the following theorem can be obtained.

THEOREM 2.4. *The discretization matrix A is invertible. Further, the equations (2.8) and (2.9) has a unique solution.*

3. Stability of the INM. For $\mathbf{u} = (u_1, u_2, \dots, u_{m-1})^T$, $\mathbf{v} = (v_1, v_2, \dots, v_{m-1})^T$, we define

$$(3.1) \quad (\mathbf{u}, \mathbf{v}) = \sum_{j=1}^{m-1} u_j v_j h, \quad \|\mathbf{u}\|_2 = \sqrt{(\mathbf{u}, \mathbf{u})} = \left(\sum_{j=1}^{m-1} u_j^2 h \right)^{\frac{1}{2}}.$$

We suppose that \tilde{u}_i^k , $i = 0, 1, 2, \dots, m$; $j = 0, 1, 2, \dots, n$ is the approximate solution of (2.8) and (2.9). The rounding error $\varepsilon_i^k = \tilde{u}_i^k - u_i^k$ satisfies

$$(3.2) \quad \varepsilon_i^{k+1} = \varepsilon_i^k + r_1 \delta_x^2 \varepsilon_i^{k+1} + r_1 \sum_{j=0}^{k-1} (b_{j+1} - b_j) \delta_x^2 \varepsilon_i^{k-j}$$

and

$$(3.3) \quad \varepsilon_0^k = 0, \quad \varepsilon_m^k = 0, \quad k = 1, 2, \dots, n.$$

Let $\mathbf{E}^k = (\varepsilon_1^k, \varepsilon_2^k, \dots, \varepsilon_{m-1}^k)^T$. Multiplying (3.2) by $h\varepsilon_i^{k+1}$ and summing i from 1 to $m-1$, we obtain

$$\begin{aligned}
\|\mathbf{E}^{k+1}\|_2^2 &= (\mathbf{E}^{k+1}, \mathbf{E}^k) + r_1(\delta_x^2 \mathbf{E}^{k+1}, \mathbf{E}^{k+1}) + r_1 \sum_{j=0}^{k-1} (b_{j+1} - b_j)(\delta_x^2 \mathbf{E}^{k-j}, \mathbf{E}^{k+1}) \\
&= (\mathbf{E}^{k+1}, \mathbf{E}^k) - r_1[(\varepsilon_1^{k+1})^2 h + \|\Delta_x \mathbf{E}^{k+1}\|_2^2] \\
&\quad + r_1 \sum_{j=0}^{k-1} (b_{j+1} - b_j)[- \varepsilon_1^{k-j} \varepsilon_1^{k+1} h - (\Delta_x \mathbf{E}^{k-j}, \Delta_x \mathbf{E}^{k+1})] \\
&\leq \frac{1}{2}[\|\mathbf{E}^{k+1}\|_2^2 + \|\mathbf{E}^k\|_2^2] - r_1|\varepsilon_1^{k+1}|^2 h - r_1\|\Delta_x \mathbf{E}^{k+1}\|_2^2 \\
&\quad + \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j - b_{j+1})[|\varepsilon_1^{k+1}|^2 h + |\varepsilon_1^{k-j}|^2 h] \\
&\quad + \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j - b_{j+1})[\|\Delta_x \mathbf{E}^{k-j}\|_2^2 + \|\Delta_x \mathbf{E}^{k+1}\|_2^2].
\end{aligned}$$

Noting that $\sum_{j=0}^{k-1} (b_j - b_{j+1}) = b_0 - b_k = 1 - b_k$ and $b_k > 0$, we have

$$\begin{aligned}
\|\mathbf{E}^{k+1}\|_2^2 &\leq \frac{1}{2}[\|\mathbf{E}^{k+1}\|_2^2 + \|\mathbf{E}^k\|_2^2] - \frac{r_1}{2}(1 + b_k)[|\varepsilon_1^{k+1}|^2 h + \|\Delta_x \mathbf{E}^{k+1}\|_2^2] \\
&\quad + \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j - b_{j+1})(|\varepsilon_1^{k-j}|^2 h + \|\Delta_x \mathbf{E}^{k-j}\|_2^2) \\
&\leq \frac{1}{2}[\|\mathbf{E}^{k+1}\|_2^2 + \|\mathbf{E}^k\|_2^2] - \frac{r_1}{2}[|\varepsilon_1^{k+1}|^2 h + \|\Delta_x \mathbf{E}^{k+1}\|_2^2] \\
&\quad + \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j - b_{j+1})(|\varepsilon_1^{k-j}|^2 h + \|\Delta_x \mathbf{E}^{k-j}\|_2^2),
\end{aligned}$$

i.e.,

$$\begin{aligned}
(3.4) \quad \|\mathbf{E}^{k+1}\|_2^2 &+ r_1 \sum_{j=0}^k b_j \{|\varepsilon_1^{k+1-j}|^2 h + \|\Delta_x \mathbf{E}^{k+1-j}\|_2^2\} \\
&\leq \|\mathbf{E}^k\|_2^2 + r_1 \sum_{j=0}^{k-1} b_j \{|\varepsilon_1^{k-j}|^2 h + \|\Delta_x \mathbf{E}^{k-j}\|_2^2\}.
\end{aligned}$$

Defining the energy norm $\|\mathbf{E}^k\|_E^2 = \|\mathbf{E}^k\|_2^2 + r_1 \sum_{j=0}^{k-1} b_j \{|\varepsilon_1^{k-j}|^2 h + \|\Delta_x \mathbf{E}^{k-j}\|_2^2\}$, we have

$$\|\mathbf{E}^{k+1}\|_2^2 \leq \|\mathbf{E}^{k+1}\|_E^2 \leq \|\mathbf{E}^k\|_E^2 \leq \dots \leq \|\mathbf{E}^1\|_E^2.$$

Because $\varepsilon_i^1 = \varepsilon_i^0 + r_1 \delta_x^2 \varepsilon_i^1$, we obtain

$$\begin{aligned}
\|\mathbf{E}^1\|_2^2 &= (\mathbf{E}^1, \mathbf{E}^0) + r_1(\delta_x^2 \mathbf{E}^1, \mathbf{E}^1) \\
&= (\mathbf{E}^1, \mathbf{E}^0) - r_1[(\varepsilon_1^1)^2 h + \|\Delta_x \mathbf{E}^1\|_2^2] \\
&\leq \frac{1}{2}[\|\mathbf{E}^1\|_2^2 + \|\mathbf{E}^0\|_2^2] - r_1|\varepsilon_1^1|^2 h - r_1\|\Delta_x \mathbf{E}^1\|_2^2,
\end{aligned}$$

i.e.,

$$(3.5) \quad \|\mathbf{E}^1\|_E^2 = \|\mathbf{E}^1\|_2^2 + r_1 \sum_{j=0}^k b_j \{|\varepsilon_1^{1-j}|^2 h + \|\Delta_x \mathbf{E}^{1-j}\|_2^2\} \leq \|\mathbf{E}^0\|_2^2,$$

so that $\|\mathbf{E}^{k+1}\|_2^2 \leq \|\mathbf{E}^0\|_2^2$.

Hence, the following theorem of stability is obtained.

THEOREM 3.1. *The fractional implicit numerical method defined by (2.8) is unconditionally stable.*

4. Convergence of the INM. In this section, we discuss the convergence of the INM. Let $u(x_i, t_k), i = 0, 1, 2, \dots, m; k = 0, 1, 2, \dots, n$ be the exact solution of the ASub-DE (2.1) - (2.3) at mesh point (x_i, t_k) . Suppose that $u(x, t)$ is the solution of (2.1)-(2.3) and $u(x, t) \in G(\Omega)$.

Define

$$\eta_i^k = u(x_i, t_k) - u_i^k, \quad i = 0, 1, 2, \dots, m; \quad k = 0, 1, 2, \dots, n$$

and $\mathbf{Y}^k = (\eta_1^k, \eta_2^k, \dots, \eta_{m-1}^k)^T$. Using $u_i^k = u(x_i, t_k) - \eta_i^k$, substitution into (2.8) leads to

$$(4.1) \quad \eta_i^{k+1} = \eta_i^k + r_1 \delta_x^2 \eta_i^{k+1} + r_1 \sum_{j=0}^{k-1} (b_{j+1} - b_j) \delta_x^2 \eta_i^{k-j} + R_i^k,$$

where $i = 1, 2, \dots, m-1; k = 0, 1, 2, \dots, n-1$, and

$$\begin{aligned} \eta_i^0 &= 0, \quad i = 0, 1, \dots, m, \\ \eta_0^k &= \eta_m^k = 0, \quad k = 0, 1, \dots, n. \end{aligned}$$

Multiplying (4.1) by $h\eta_i^{k+1}$ and summing i from 1 to $m-1$, we obtain

$$(4.2) \quad \begin{aligned} \|\mathbf{Y}^{k+1}\|_2^2 &= (\mathbf{Y}^{k+1}, \mathbf{Y}^k) + r_1 (\delta_x^2 \mathbf{Y}^{k+1}, \mathbf{Y}^{k+1}) \\ &\quad + r_1 \sum_{j=0}^{k-1} (b_{j+1} - b_j) (\delta_x^2 \mathbf{Y}^{k-j}, \mathbf{Y}^{k+1}) + (\mathbf{R}^k, \mathbf{Y}^{k+1}). \end{aligned}$$

For $j = 0, 1, \dots, k+1$, we have

$$(\delta_x^2 \mathbf{Y}^j, \mathbf{Y}^{k+1}) = -\eta_1^j \eta_1^{k+1} - (\Delta_x \mathbf{Y}^j, \Delta_x \mathbf{Y}^{k+1}).$$

Using $|v \cdot w| \leq \sigma v^2 + \frac{1}{4\sigma} w^2$, $\sigma > 0$, we obtain

$$(4.3) \quad (\mathbf{Y}^{k+1}, \mathbf{Y}^j) \leq \frac{1}{2} [\|\mathbf{Y}^{k+1}\|_2^2 + \|\mathbf{Y}^j\|_2^2],$$

$$(4.4) \quad \eta_1^{k+1} \eta_1^j \leq \frac{1}{2} [|\eta_1^{k+1}|^2 + |\eta_1^j|^2]$$

and

$$(4.5) \quad |(\mathbf{R}^{k+1}, \mathbf{Y}^{k+1})| \leq \frac{r_1 h^2 b_k}{a^2} \|\mathbf{Y}^{k+1}\|_2^2 + \frac{a^2}{4r_1 h^2 b_k} \|\mathbf{R}^{k+1}\|_2^2.$$

Noting that $\sum_{j=0}^{k-1} (b_j - b_{j+1}) = b_0 - b_k = 1 - b_k$ and $b_k > 0$, similarly to the proof of the stability, we have

$$(4.6) \quad \begin{aligned} \|\mathbf{Y}^{k+1}\|_2^2 &\leq \frac{1}{2} [\|\mathbf{Y}^{k+1}\|_2^2 + \|\mathbf{Y}^k\|_2^2] - \frac{r_1}{2} (1 + b_k) [|\eta_1^{k+1}|^2 h + \|\Delta_x \mathbf{Y}^{k+1}\|_2^2] \\ &\quad + \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j - b_{j+1}) (|\eta_1^{k-j}|^2 h + \|\Delta_x \mathbf{Y}^{k-j}\|_2^2) \\ &\quad + \frac{r_1 h^2 b_k}{a^2} \|\mathbf{Y}^{k+1}\|_2^2 + \frac{a^2}{4r_1 h^2 b_k} \|\mathbf{R}^{k+1}\|_2^2. \end{aligned}$$

LEMMA 4.1. Given $\|\mathbf{Y}^k\|_\infty = \max_{1 \leq i \leq m-1} |\eta_i^k|$, then

$$\|\mathbf{Y}^k\|_2^2 \leq a \|\mathbf{Y}^k\|_\infty^2 \leq \frac{a^2}{2h^2} [h|\eta_1^k|^2 + \|\Delta_x \mathbf{Y}^k\|_2^2].$$

Proof. The first inequality is apparent.

For the second inequality, let $|\eta_{i_0}^k| = \max_{1 \leq i \leq m-1} |\eta_i^k|$, then

$$\eta_{i_0}^k = \eta_1^k + \sum_{j=1}^{i_0-1} \Delta_x \eta_j^k, \quad \eta_{i_0}^k = - \sum_{j=i_0}^{m-1} \Delta_x \eta_j^k.$$

Thus

$$2|\eta_{i_0}^k| \leq |\eta_1^k| + \sum_{j=1}^{m-1} |\Delta_x \eta_j^k|.$$

Using the Cauchy-Schwarz inequality, we have

$$\begin{aligned} 4|\eta_{i_0}^k|^2 &\leq 2m \left[|\eta_1^k| + \sum_{j=1}^{m-1} |\Delta_x \eta_j^k| \right]^2 \\ &\leq \frac{2a}{h^2} [h|\eta_1^k|^2 + \|\Delta_x \mathbf{Y}^k\|_2^2]. \end{aligned}$$

Therefore,

$$\|\mathbf{Y}^k\|_\infty^2 \leq \frac{a}{2h^2} [h|\eta_1^k|^2 + \|\Delta_x \mathbf{Y}^k\|_2^2].$$

□

Applying Lemma 4.1, we have

$$(4.7) \quad \frac{r_1 h^2 b_k}{a^2} \|\mathbf{Y}^{k+1}\|_2^2 \leq \frac{r_1 h^2 b_k}{a^2} \cdot a \|\mathbf{Y}^{k+1}\|_\infty^2 \leq \frac{b_k}{2} r_1 [|\eta_1^{k+1}|^2 h + \|\Delta_x \mathbf{Y}^{k+1}\|_2^2].$$

Hence, from (4.6) and (4.7), we have

$$\begin{aligned} \|\mathbf{Y}^{k+1}\|_2^2 &\leq \frac{1}{2} [\|\mathbf{Y}^{k+1}\|_2^2 + \|\mathbf{Y}^k\|_2^2] - \frac{r_1}{2} [|\eta_1^{k+1}|^2 h + \|\Delta_x \mathbf{Y}^{k+1}\|_2^2] \\ &\quad + \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j - b_{j+1}) (|\eta_1^{k-j}|^2 h + \|\Delta_x \mathbf{Y}^{k-j}\|_2^2) + \frac{a^2}{4r_1 h^2 b_k} \|\mathbf{R}^{k+1}\|_2^2. \end{aligned}$$

Let $\rho_k = \|\mathbf{Y}^k\|_2^2 + r_1 \sum_{j=0}^{k-1} b_j \{|\eta_1^{k-j}|^2 h + \|\Delta_x \mathbf{Y}^{k-j}\|_2^2\}$, then

$$(4.8) \quad \rho_{k+1} \leq \rho_k + \frac{a^2}{4r_1 h^2 b_k} \|\mathbf{R}^{k+1}\|_2^2,$$

$$(4.9) \quad \rho_0 = 0.$$

According to Lemma 2.3, and $r_1 = K_r \frac{\tau^\gamma}{\Gamma(\gamma+1)h^2}$, we have

$$(4.10) \quad \rho_{k+1} \leq \rho_k + C b_k \tau^\gamma (\tau + h^2)^2.$$

Hence, we obtain

$$(4.11) \quad \rho_{k+1} \leq C \sum_{j=0}^k b_j \tau^\gamma (\tau + h^2)^2.$$

Noting that $\sum_{j=0}^k b_j \tau^\gamma = (k+1)^\gamma \tau^\gamma \leq T^\gamma$ and $\|\mathbf{Y}^{k+1}\|_2^2 \leq \rho_{k+1}$, we have

$$\|\mathbf{Y}^{k+1}\|_2^2 \leq CT^\gamma (\tau + h^2)^2.$$

Consequently, the following theorem of convergence is obtained.

THEOREM 4.2. *Let $u(x, t) \in G(\Omega)$ be the solution of (2.1)-(2.3). Then the fractional implicit difference scheme defined by (2.8) is convergent, and there exists a positive constant $C > 0$ such that*

$$(4.12) \quad \|\mathbf{Y}^{k+1}\|_2 \leq C(\tau + h^2), k = 0, 1, 2, \dots, n-1.$$

5. Improving the order of convergence of the INM. In this section, we propose two techniques to improve the rate of convergence of the INM.

5.1. The extrapolation method (EM). According to Theorem 4.2, we know that the INM converges at the rate $O(\tau + h^2)$. In order to improve the order of convergence, we apply the INM on a (coarse) grid $\Delta t = \tau$, and then on a finer grid of size $\tau/2$ with the same Δx . The extrapolated solution is then computed from $u(x_i, t) \approx 2u_i^{2k}(\tau/2) - u_i^k(\tau)$, $i = 1, 2, \dots, m-1$, where $t = t_k$ on the coarse grid, while $t = t_{2k}$ on the fine grid. Here, $u_i^k(\tau)$ and $u_i^{2k}(\tau/2)$ are numerical solutions on the coarse grid and the fine grid, respectively. Thus, the extrapolation method can be used to obtain a solution with convergence order $O(\tau^2 + h^2)$.

5.2. Improved difference scheme (IDS). We use a technique of increasing the order of local truncation error to obtain an improved difference scheme (IDS). Integrating both sides of Eq. (2.1) for t , we obtain

$$u(x_i, t_{k+1}) = u(x_i, 0) + \frac{1}{\Gamma(\gamma)} \int_0^{t_{k+1}} \frac{K_\gamma \frac{\partial^2 u(x_i, \eta)}{\partial x^2} + f(x_i, \eta)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta,$$

or

$$u(x_i, t_{k+1}) = u(x_i, 0) + \frac{1}{\Gamma(\gamma)} \sum_{j=0}^k \int_{t_j}^{t_{j+1}} \frac{K_\gamma \frac{\partial^2 u(x_i, \eta)}{\partial x^2} + f(x_i, \eta)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta.$$

LEMMA 5.1. *If the function $v(x, t)$ is sufficiently smooth, then*

$$(5.1) \quad v(x_i, \eta) = \frac{(t_{j+1} - \eta)v(x_i, t_j) + (\eta - t_j)v(x_i, t_{j+1})}{\tau} + O(\tau^2).$$

Proof. The estimate (5.1) can be obtained from the following formulae:

$$\begin{aligned} v(x_i, t_j) &= v(x_i, \eta) + \frac{\partial v(x_i, \eta)}{\partial t} (t_j - \eta) + \frac{1}{2} \frac{\partial^2 v(x_i, \xi_1)}{\partial t^2} (t_j - \eta)^2, \\ v(x_i, t_{j+1}) &= v(x_i, \eta) + \frac{\partial v(x_i, \eta)}{\partial t} (t_{j+1} - \eta) + \frac{1}{2} \frac{\partial^2 v(x_i, \xi_2)}{\partial t^2} (t_{j+1} - \eta)^2, \end{aligned}$$

where $t_j \leq \xi_1 \leq \eta \leq \xi_2 \leq t_{j+1}$. \square

Applying Lemma 5.1, we have

$$(5.2) \quad \begin{aligned} u(x_i, t_{k+1}) &= u(x_i, 0) + r_1 \sum_{j=0}^k \left[c_j^{(1)} \delta_x^2 u(x_i, t_{k-j+1}) + c_j^{(2)} \delta_x^2 u(x_i, t_{k-j}) \right] \\ &\quad + r_2 \sum_{j=0}^k \left[c_j^{(1)} f(x_i, t_{k-j+1}) + c_j^{(2)} f(x_i, t_{k-j}) \right] + R_i^{k+1}, \end{aligned}$$

where $r_1 = \frac{K\gamma\tau^\gamma}{\Gamma(\gamma+1)h^2}$, $r_2 = \frac{\tau^\gamma}{\Gamma(\gamma+1)}$, and

$$(5.3) \quad c_j^{(1)} = (j+1)^\gamma - \frac{1}{\gamma+1} [(j+1)^{\gamma+1} - j^{\gamma+1}],$$

$$(5.4) \quad c_j^{(2)} = \frac{1}{\gamma+1} [(j+1)^{\gamma+1} - j^{\gamma+1}] - j^\gamma,$$

$$(5.5) \quad |R_i^{k+1}| \leq Ct_{k+1}^{\gamma+1}(\tau^2 + h^2).$$

Thus, we obtain the following improved difference scheme:

$$u_i^{k+1} = u_i^0 + r_1 \sum_{j=0}^k \left[c_j^{(1)} \delta_x^2 u_i^{k-j+1} + c_j^{(2)} \delta_x^2 u_i^{k-j} \right] + r_2 \sum_{j=0}^k \left[c_j^{(1)} f_i^{k-j+1} + c_j^{(2)} f_i^{k-j} \right].$$

6. Numerical results. In order to demonstrate the effectiveness of our theoretical analysis, two examples are now presented. To simplify the computation, Eq. (2.8) is rewritten as

$$(6.1) \quad \begin{aligned} u_i^{l+1} - u_i^l &= r_1 \delta_x^2 u_i^{l+1} + r_1 \sum_{j=0}^{l-1} (b_{j+1} - b_j) \delta_x^2 u_i^{l-j} \\ &\quad + r_2 f_i^{l+1} + r_2 \sum_{j=0}^{l-1} (b_{j+1} - b_j) f_i^{l-j}. \end{aligned}$$

Summing l from 0 to $k-1$, we obtain

$$u_i^k = u_i^0 + r_1 \sum_{j=0}^{k-1} b_j \delta_x^2 u_i^{k-j} + r_2 \sum_{j=0}^{k-1} b_j f_i^{k-j},$$

where $i = 1, 2, \dots, m-1$; $k = 1, 2, \dots, n$.

Example 1. Consider the following ASub-DE:

$$(6.2) \quad \frac{\partial u(x, t)}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left[0.5\Gamma(\gamma+3) \frac{\partial^2 u(x, t)}{\partial x^2} + 0.5\Gamma(\gamma+3)(t^2 - t^{2+\gamma})e^x \right],$$

with the boundary and initial conditions

$$(6.3) \quad u(0, t) = t^{2+\gamma}, \quad u(1, t) = et^{2+\gamma}, \quad u(x, 0) = 0.$$

The exact solution of the equations (6.2) and (6.3) is $u(x, t) = t^{2+\gamma}e^x$, which can be obtained by evaluating the fractional derivative formula [26, 27].

TABLE 6.1

The error $\|\mathbf{Y}^n\|_2$ for INM, EM and IDS and the effect of the grid size reduction at time $t=1.0$ ($\gamma = 0.9$)

Δx	Δt	INM	EM	IDS
$\frac{1}{10}$	$\frac{1}{10}$	1.4252E-2	3.5158E-4	3.5663E-5
$\frac{1}{15}$	$\frac{1}{15}$	9.6200E-3	1.6191E-4	8.4894E-6
$\frac{1}{20}$	$\frac{1}{20}$	7.2613E-3	1.2173E-4	8.1641E-6
$\frac{1}{25}$	$\frac{1}{25}$	5.8285E-3	1.1443E-4	6.4540E-6

Table 6.1 shows the numerical errors at $t = 1$ between the exact solution and the numerical solution obtained by the INM, the EM and the IDS. From Table 1, all the three methods are in excellent agreement with the exact solution and the convergence order of EM and IDS is improved significantly.

A comparison of the exact solution and the numerical solution using INM with various time and space steps for ASUB-DE at $t = 1.0$ and $\gamma = 0.9$ is shown in Figure 6.1. It is apparent that the numerical solution (INM) is in excellent agreement with the exact solution.

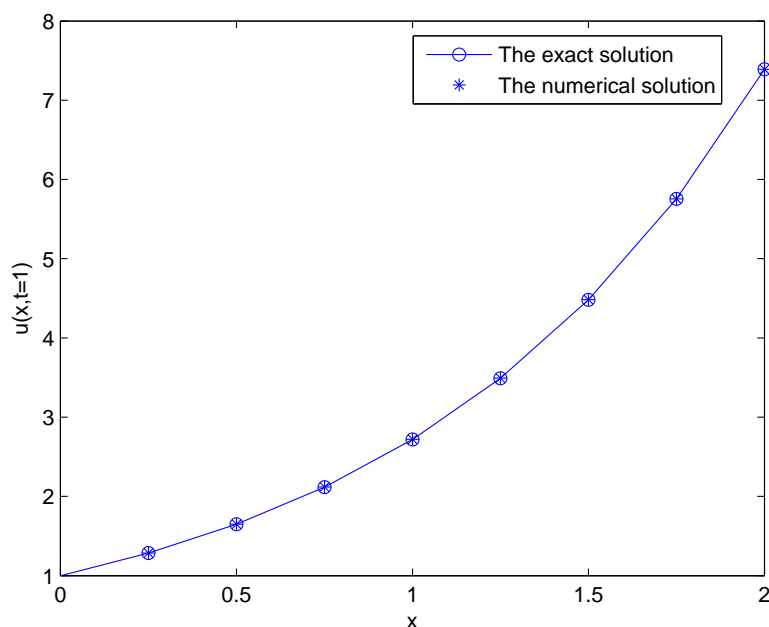


FIG. 6.1. The compare of the exact solution and the numerical solution (INM) when $\gamma = 0.9$ and $t = 1$.

Example 2 Consider the following ASUB-DE:

$$(6.4) \quad \frac{\partial u(x, t)}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left[\frac{\partial^2 u(x, t)}{\partial x^2} \right],$$

with initial and boundary conditions

$$u(x, 0) = \begin{cases} 2x, & 0 \leq x \leq 0.5, \\ \frac{4-2x}{3}, & 0.5 \leq x \leq 2, \end{cases}$$

$$u(0, t) = u(2, t) = 0, \quad 0 \leq t \leq 0.4.$$

The evolution results for the INM when $\gamma = 0.8$, $0 \leq t \leq 0.4$, $0 \leq x \leq 2$, and $0.1 \leq \gamma \leq 1$, $0 \leq t \leq 0.4$, $x = 0.6$, and $0.1 \leq \gamma \leq 1$, $t = 0.4$, $0 \leq x \leq 2$ are shown in Figures 6.2, 6.3 and 6.4 respectively. Figures 6.2-6.4 show that the system exhibits sub-diffusion behaviors. From Figure 6.4, it can be seen that the solution continuously depends on time fractional derivative.

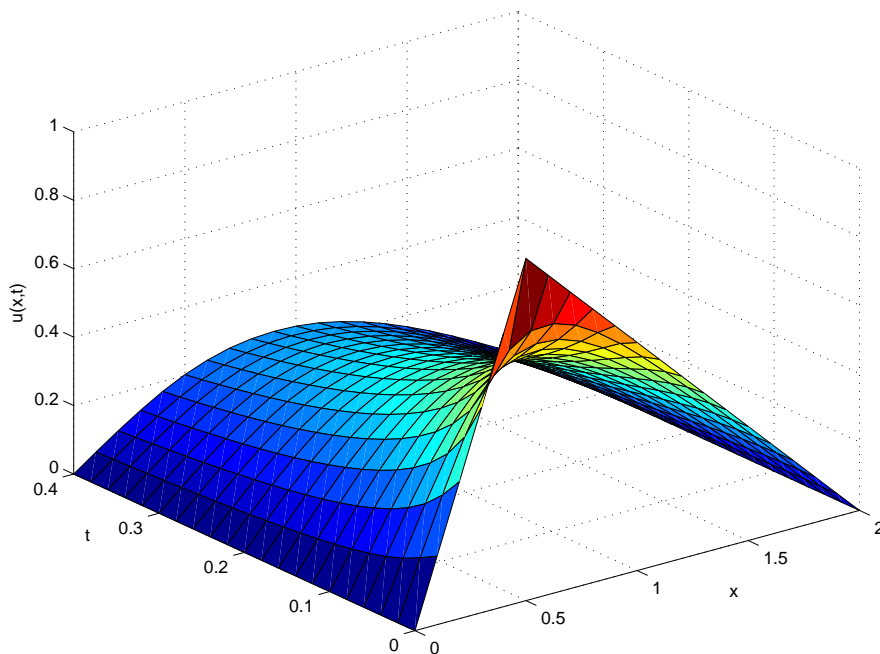


FIG. 6.2. The numerical approximation when $\gamma = 0.8$.

7. Conclusions. In this paper, an INM for the fractional sub-diffusion equation in a bounded domain has been described and demonstrated. We prove that the INM is unconditionally stable and convergent. Two techniques to improve the convergence rate are presented. Both the EM and IDS techniques provide computationally effective tools for simulating the behavior of the solution of the ASub-DE. These methods and analytical techniques can also be extended to any fractional integro-differential equations and higher-dimensional problems.

REFERENCES

- [1] R. Metzler and J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Phys. Rep. 339 (2000) 1-77.

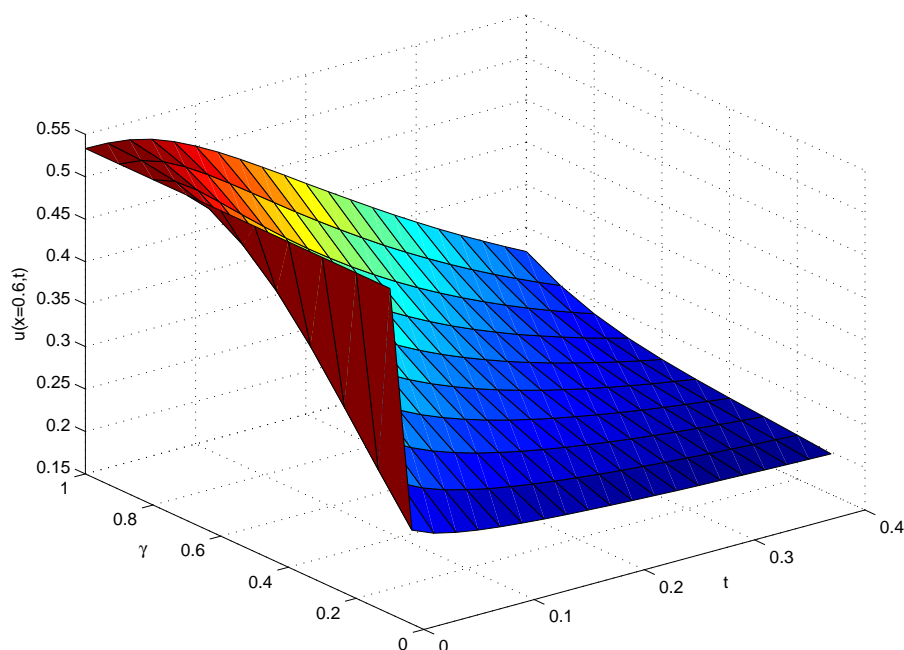


FIG. 6.3. The numerical approximation $u(x, t)$ for various γ when $x = 0.6$.

- [2] R. Kutner, A. Pekalski, K. Sznajd-Weron, Anomalous Diffusion, Basics to Application, Springer, Berlin, 1999.
- [3] S.B. Yuste and L. Acedo, Some exact results for the trapping of subdiffusive particles in one dimension, *Physica A*, 336(2004) 334-346.
- [4] S.B. Yuste and L. Acedo, An explicit finite difference method and a new Von Neumann-type stability analysis for fractional diffusion equations, *SIAM J. Numer. Anal.*, 42(5) (2005) 1862-1874.
- [5] T.A.M. Langlands and B.I. Henry, The accuracy and stability of an implicit solution method for the fractional diffusion equation, *J. Comp. Phys.*, 205 (2005) 719-736.
- [6] W.R. Schneider and W. Wyss, Fractional diffusion and wave equations, *J. Math. Phys.*, 30 (1989) 134-144.
- [7] F. Huang and F. Liu, The time fractional diffusion and advection-dispersion equation, *ANZIAM J.*, 46 (2005) 317-330.
- [8] Mainardi, F., The fundamental solutions for the fractional diffusion-wave equation, *Appl. Math. Letters*, 9(6) (1996) 23-28
- [9] V.V.Anh, N.N. Leonenko, Spectral analysis of fractional kinetic equations with random data, *J.Stat.Phys.*, 104 (2001) 1349-1387.
- [10] R.Gorenflo, A.Iskenderov and Yu. Luchko, Mapping between solutions of fractional diffusion-wave equations, *Fract. Calculus and Appl. Math.*, 3(1) (2000) 75-86.
- [11] A.A.Kilbas, M.Saigo and R.K.Saxena, Solutions of Volterra integro-differential equations with generalised Mittag-Leffler function in the kernels, *Journal of Integral Equations*, 14(4) (2002) 377-396.
- [12] F. Liu, V. Anh, I. Turner, Numerical Solution of the Space Fractional Fokker-Planck Equation, *J. Comp. Appl. Math.*, 166 (2004) 209-219.
- [13] F. Liu, V. Anh, I. Turner, P. Zhuang, Numerical simulation for solute transport in fractal porous media, *ANZIAM J.* 45 (2004) 461-473.
- [14] W. McLean, I. H. Sloan and V. Thomée, Time discretization via Laplace transformation of an integro-differential equation of parabolic type, *Numerische Mathematik*, 102(3) (2006) 497-522.
- [15] W. McLean, K. Mustapha and V. Thomee, Numerical methods for Numerical methods for some fractional-order partial differential equations, *International Symposium on Fractional Calculus*, Dunedin, 9-13 January, 2006.

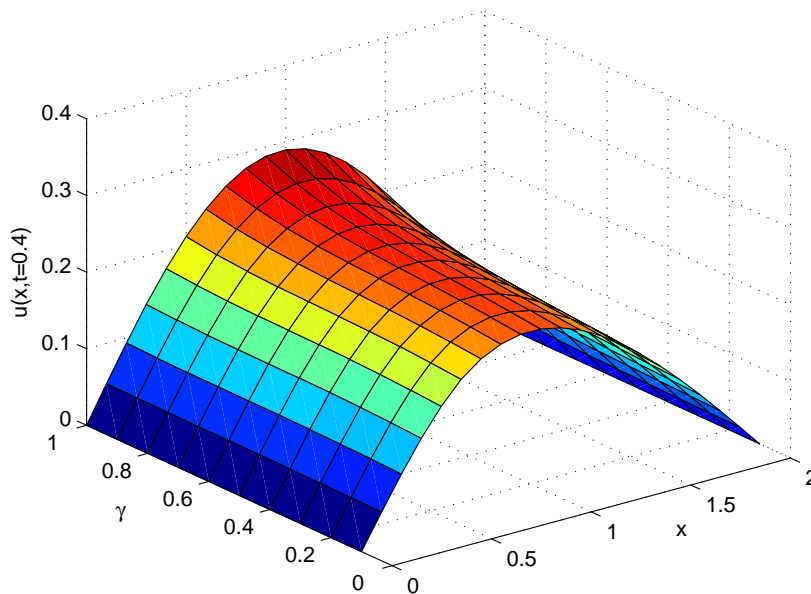


FIG. 6.4. The numerical approximation $u(x, t)$ for various γ when $t = 0.4$.

- [16] J.P. Roop, Computational aspects of FEM approximation of fractional advection dispersion equation on bounded domains in \mathbb{R}^2 , *J. Comp. Appl. Math.*, 193(1) (2006) 243–268.
- [17] M. Meerschaert and C. Tadjeran, Finite difference approximations for fractional advection-dispersion flow equations, *J. Comp. and Appl. Math.*, 172 (2004) 65-77.
- [18] S. Shen S and F. Liu, Error analysis of an explicit finite difference approximation for the space fractional diffusion, *ANZIAM J.*, 46 (2005) 871-887.
- [19] Q. Liu, F. Liu, I. Turner and V. Anh, Approximation of the Levy-Feller advection-dispersion process by random walk and finite difference method, *J. Phys. Comp.*, 222 (2007) 57-70.
- [20] H. Zhang, F. Liu and V. Anh, Numerical approximation of Levy-Feller diffusion equation and its probability interpretation, *Journal of Computational and Applied Mathematics*, 206 (2007) 1098-1115.
- [21] F. Liu, S. Shen, V. Anh and I. Turner, Analysis of a discrete non-Markovian random walk approximation for the time fractional diffusion equation, *ANZIAM J.*, 46 (2005) 488-504.
- [22] P. Zhuang and F. Liu, Implicit difference approximation for the time fractional diffusion equation, *J. Appl. Math. Computing*, 22 (2006) 87-99.
- [23] F. Liu, P. Zhuang, V. Anh, I. Turner and K. Burrage , Stability and convergence of the difference methods for the space-time fractional advection-diffusion equation, *Appl. Math. Comp.*, (2007), in press.
- [24] R. Lin and F. Liu, Fractional high order methods for the nonlinear fractional ordinary differential equation. *Nonlinear Analysis*, 66 (2007) 856-869.
- [25] X. Cao, K. Burrage and F. Abdullah, A variable stepsize implementation for fractional differential equations, Submitted to BIT, 2006.
- [26] K.B. Oldham, J. Spanier, *The Fractional Calculus*, New York and London: Academic Press, 1974.
- [27] I. Sokolov, J.klafter and A. Blumen, Fractional Kinetics, *Physics Today*, November, (2002) 48-54. (<http://www.physicstoday.org>).