Chapter 1

Introduction

1.1 A Brief Overview of Fractional Calculus

The mathematical concept of Fractional Calculus (FC) is an old topic with more than 300 years of history, as it attracted the attention of many famous mathematicians such as G.W. Leibniz, L. Euler, Laplace, Liouville, Riemann, Fourier, Letnikov, M. Riesz and others [12, 13]. The study of FC deals with arbitrary real or complex exponents of the traditional definitions of the classical calculus operators (i.e. integer order derivatives and integrals) [14, 15]. The formula of fractional order derivative of a power function was developed by Lacroix in 1819. After that, the first practical application (tautochrone problem) of fractional calculus was discovered by the Abel in 1823 (see the related reference [16]). In recent years, a lot of attention has been paid to FC because it is an emerging area in mathematics with deep real world applications in all fields of science and engineering due to the nonlocality behavior of fractional operators (i.e. the current sate of fractional order system depends on the long memory). It has been demonstrated during the past few decades that the fractional operators seem to be potentially effective modeling tools and appealing in various fields such as physics [17, 18, 19], control [20, 21, 22, 23], signal and image processing [24, 25, 26], mechanics and dynamic systems [27, 28, 29], biology [30, 31], environmental science [32, 33, 34], and multidisciplinary in engineering fields [35, 36] etc.

1.2 Preliminaries

In the literature, there exist many definitions of fractional operators like, Riemann-Liouville, Grünwald-Letnikov, Hadamard, Weyl, Erdely-Kober and Caputo fractional derivative. In this thesis, we discuses some definitions of fractional operators used in subsequent chapters. We provide the definitions in left-side sense only (for right-side definitions can be found in [11, 14, 37]).

Definition 1.2.1. Let $Re(\alpha) > 0$ and function $f \in L^1[a, b]$, where $[a, b] \subset \mathbb{R}$. Then, the Riemann-Liouville integral ${}^{RL}\mathcal{I}^{\alpha}_{a,x} f(x)$ of order α is given as:

$$ {}^{RL}\mathcal{I}^{\alpha}_{a,x} f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-s)^{\alpha-1} f(s)ds, \quad x > a. \tag{1.1} $$

Definition 1.2.2. Let $n = [\alpha] + 1$, $Re(\alpha) \geq 0$ and function $f \in AC^n[a, b]$. Then, the Riemann-Liouville fractional derivative ${}^{RL}\mathcal{D}^{\alpha}_{a,x} f(x)$ of order α is given as:

$$ \begin{aligned} \left({}^{RL}\mathcal{D}^{\alpha}_{a,x} f\right)(x) &= \left(\frac{d}{dx}\right)^n \left({}^{RL}\mathcal{I}^{n-\alpha}_{a+} f\right)(x) \\ &= \frac{1}{\Gamma(n-\alpha)} \left(\frac{d}{dx}\right)^n \int_a^x (x-s)^{n-\alpha-1} f(s)ds, \quad x > a \qquad (1.2) \\ &= \sum_{k=0}^{n-1} \frac{(x-a)^{k-\alpha}}{\Gamma(1+k-\alpha)} f^{(k)}(a) + \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-s)^{n-\alpha-1} f^{(n)}(s)ds. \end{aligned} $$

Definition 1.2.3. Let $Re(\alpha) \geq 0$ and $f(x) \in AC^n[a,b]$. Then, the Caputo fractional derivative ${}^{C}\mathcal{D}^{\alpha}_{a,x}f(x)$ of order α is given as:

$$\begin{aligned}\left({}^{C}\mathcal{D}^{\alpha}_{a,x}f\right)(x) &= \left({}^{RL}\mathcal{I}^{n-\alpha}_{a}D^n f\right)(x)\\ &= \frac{1}{\Gamma(n-\alpha)}\int_a^x (x-s)^{n-\alpha-1}f^{(n)}(s)ds, \quad x>a. \end{aligned} \tag{1.3}$$

Definition 1.2.4. Let $Re(\alpha) > 0$ and function $f(x) \in L^1[a,b]$. Then, the weighted/scaled fractional integral $\mathcal{I}^{\alpha}_{[\zeta,\omega]}f(x)$ of order α with respect to weight $\omega(x)$ and scale $\zeta(x)$ functions is given as [11]:

$$\left(\mathcal{I}^{\alpha}_{[\zeta,\omega]}f\right)(x) = \frac{[\omega(x)]^{-1}}{\Gamma(\alpha)}\int_a^x [\zeta(x)-\zeta(s)]^{\alpha-1}\omega(s)f(s)\zeta'(s)ds, \quad x>a. \tag{1.4}$$

Definition 1.2.5. For $m \geq 1$, the weighted/scaled derivative of integer order $\mathcal{D}^{m}_{[\zeta,\omega]}f(x)$ with respect to the weight $\omega(x)$ and scale $\zeta(x)$ functions is given as [11]:

$$\left(\mathcal{D}^{m}_{[\zeta,\omega]}f\right)(x) = [\omega(x)]^{-1}\left[\left(\frac{1}{\zeta'(x)}\frac{d}{dx}\right)^m \left(\omega(x)f(x)\right)\right](x). \tag{1.5}$$

Definition 1.2.6. Let $Re(\alpha) > 0$ and $f \in L^1[a,b]$. Then, the generalized fractional integral (GFI) of order α with respect to weight $\omega(x)$ and scale $\zeta(x)$ functions is given as [11]:

$$\left(\mathcal{I}^{m-\alpha}_{a,x;[\zeta,\omega]}f\right)(x) = \frac{[\omega(x)]^{-1}}{\Gamma(m-\alpha)}\int_a^x [\zeta(x)-\zeta(s)]^{m-\alpha-1}\omega(s)f(s)\zeta'(s)ds. \tag{1.6}$$

Definition 1.2.7. Let $Re(\alpha) \geq 0$ and $f \in L^1[a,b]$, Then, the generalized fractional derivative of Riemann-Liouville type of order α with respect to weight $\omega(x)$ and scale $\zeta(x)$ functions is given as [11]:

$$\left(\mathcal{D}^{\alpha}_{a,x;[\zeta\omega]}\ f\right)(x) = \left(\mathcal{D}^{m}_{[\zeta,\omega]}\ \mathcal{I}^{m-\alpha}_{a,x;[\zeta,\omega]}f\right)(x). \tag{1.7}$$

Definition 1.2.8. Let $Re(\alpha) \geq 0$ and $f \in L^1[a,b]$, Then, the generalized fractional derivative of Caputo type of order α with respect to weight $\omega(x)$ and scale $\zeta(x)$ functions is given as [11]:

$$\big(\mathcal{D}^{\alpha}_{a,x;[\zeta\omega]}\, f\big)(x) = \big(\mathcal{I}^{m-\alpha}_{a,x;[\zeta,\omega]}\, \mathcal{D}^{\alpha}_{[\zeta,\omega]} f\big)(x). \tag{1.8}$$

1.3 Model Problems

In this section, we have provided a concise overview of the model problems explored in this thesis. Additionally, detailed explanations of these problems are provided at the beginning of the subsequent chapters. The following is a brief description of the models examined in this thesis:

1.3.1 Two-Dimensional Time Fractional Diffusion-Wave Equation

In **Chapter 2** we have considered the following two-dimensional time-fractional diffusion-wave (TFDW) equation:

$$^{C}\mathcal{D}^{\alpha}_{0,t}u(x,y,t) = u_{xx}(x,y,t) + u_{yy}(x,y,t) + f(x,y,t), \quad (x,y,t) \in \Omega \times (0,T], \tag{1.9}$$

$$u(x,y,t) = \Phi(x,y,t), \quad (x,y,t) \in \partial\Omega \times (0,T], \tag{1.10}$$

$$u(x,y,0) = \phi(x,y), \quad u_t(x,y,0) = \varphi(x,y), \quad (x,y) \in \Omega, \tag{1.11}$$

where $\Omega = (0,L_1) \times (0,L_2)$ and $\overline{\Omega} = \Omega \cup \partial\Omega$, the functions Φ, ϕ, φ and f are sufficiently smooth functions. The operator $^{C}\mathcal{D}^{\alpha}_{0,t}$ is the time-fractional Caputo derivative (TFCD) of order α ($1 < \alpha < 2$), which is defined in equation (1.2.3) of Chapter 1.

1.3.2 Two-Dimensional Nonlinear Time-Fractional Mixed Diffusion and Diffusion-Wave Equation:

We have discussed and analyzed following two-dimensional nonlinear time-fractional mixed diffusion and diffusion-wave (TFMDW) equation in **Chapter 3**:

$$ {}^{C}\mathcal{D}^{\alpha}_{0,t}u + {}^{C}\mathcal{D}^{\beta}_{0,t}u + F(u) = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + f(x,y,t), \quad (x,y,t) \in \Omega \times (0,T], \tag{1.12} $$

$$ u(x,y,0) = \phi(x,y), \qquad \frac{\partial u(x,y,0)}{\partial t} = \varphi(x,y), \quad (x,y) \in \Omega, \tag{1.13} $$

$$ u(x,y,t) = \Phi(x,y,t), \qquad (x,y,t) \in \partial\Omega \times (0,T], \tag{1.14} $$

where, $\overline{\Omega} \times [0,T] := [0,L_1] \times [0,L_2] \times [0,T]$, $\overline{\Omega} = \Omega \cup \partial\Omega$, $\phi \in C(\overline{\Omega})$, $\varphi \in C(\overline{\Omega})$, $\Phi \in C(\overline{\Omega} \times [0,T])$, and $f \in C(\overline{\Omega} \times [0,T])$. Furthermore, the operators ${}^{C}\mathcal{D}^{\alpha}_{0,t}$, ${}^{C}\mathcal{D}^{\beta}_{0,t}$ denotes the time-fractional Caputo derivatives (TFCDs) of order β ($0 < \beta < 1$) and α ($1 < \alpha < 2$), respectively. The TFCDs of a function u are defined in equation (1.2.3) of Chapter 1.

1.3.3 Nonlinear Time-Fractional Diffusion-Wave Equation with Variable Coefficients

In **Chapter 4**, we analyze and present the numerical simulation for the following model problem:

$$ {}^{C}\mathcal{D}_{0,t}^{\alpha}u(x,t) + q(x)F(u) = \frac{\partial}{\partial x}\left(p(x)\,\frac{\partial u(x,t)}{\partial x}\right) + f(x,t),\ x \in \Omega,\ t \in (0,T], \tag{1.15} $$

$$ u(x,0) = \phi(x), \quad u_t(x,0) = \varphi(x), \quad x \in \overline{\Omega}(\equiv \Omega \cup \partial\Omega), \tag{1.16} $$

$$ u(x,t) = \Phi(x,t), \qquad x \in \partial\Omega,\ t \in (0,T], \tag{1.17} $$

where $\Omega = (0,L)$, $p \in C^1(\overline{\Omega})$, $q \in C(\overline{\Omega})$, $0 < c_1 \leq p(x) \leq c_2$, $q(x) \geq 0$, $\forall x \in \overline{\Omega}$, $\phi \in C(\overline{\Omega})$, $\varphi \in C(\overline{\Omega})$, $\Phi \in C(\overline{\Omega} \times [0,T])$, $f \in C(\overline{\Omega} \times [0,T])$, where the function $F(u)$ satisfies the Lipschitz condition with Lipschitz constant $\mathcal{L}$ i.e.

$$ |F(u) - F(\widehat{u})| \leq \mathcal{L}|u - \widehat{u}|, \quad \forall\ u,\ \widehat{u}, \tag{1.18} $$

and the operator ${}^{C}\mathcal{D}_{0,t}^{\alpha}$ denotes the Caputo fractional derivative of order $\alpha \in (1,2)$.

1.3.4 Generalized Time-Fractional Advection-Diffusion Equation

Chapter 5 includes the numerical solution of following generalized fractional advection-diffusion equation:

$$ {}^{C}\mathcal{D}^{\alpha}_{0,t;[\zeta(t),\omega(t)]}U(x,t) = D\frac{\partial^2 U(x,t)}{\partial x^2} - A\frac{\partial U(x,t)}{\partial x} + g(x,t), \;\; x \in \Omega, \;\; t \in (0,T], \quad (1.19) $$

$$ U(x,0) = U_0(x), \qquad x \in \overline{\Omega} = \Omega \cup \partial\Omega, \quad (1.20) $$

$$ U(0,t) = \rho_1(t), \;\; U(a,t) = \rho_2(t), \qquad t \in (0,T], \quad (1.21) $$

where $\Omega = (0,a)$ is a bounded domain with boundary $\partial\Omega$, and the notation ${}^{C}\mathcal{D}^{\alpha}_{0,t,[\zeta(t),\omega(t)]}$ denotes the generalized Caputo fractional derivative (see [11], and related references therein) with respect to weight $\omega(t)$ and scale function $\zeta(t)$ of order α.

1.4 Literature Review

Over the past few decades, several research papers appeared in the literature handling numerical solutions of time-fractional PDEs [38, 39, 40, 41, 42, 43, 44, 45, 46]. Among them, we are interested in numerical solutions of time-fractional diffusion (i.e., sub-diffusion) [47, 48, 49] and time-fractional wave equations (i.e., super-diffusion) [50, 51, 52, 53, 53]. It is difficult task to find the analytical solutions of such type problems. The discretization is a productive way to handle time fractional PDEs via developing an efficient numerical scheme with good accuracy and minimum computational time.

1.4.1 Literature Review on Time-Fractional Diffusion-Wave Equation

Firstly, there are several numerical methods have been introduced in the literature to approximate the TFCDs of order β $(0 < \beta < 1)$ like $L1$ method [3, 54], $L1-2$ method [3], $L2{-}1_\sigma$ method [55], $L1{-}2{-}3$ method [4, 56], and for order α $(1 < \alpha < 2)$ such as $L2$ and $L2$C methods [57, 58], H2N2 method [59, 60], Crank-Nicolson $L1$ method [61, 62], Crank-Nicolson $L1-2$ method [63], and $L2-1_\sigma$ method [64] etc. Here, we discuss some of them in brief. Suppose uniform partition $0 = t_0 < t_1 < ... < t_N = T$ of the interval $[0, T]$ with τ temporal step size. Define some notations $t_n = n\tau$, $\delta_t u(t_{k-\frac{1}{2}}) = \frac{u(t_k)-u(t_{k-1})}{\tau}$, $\delta_t^2 u(t_k) = \frac{\delta_t u(t_{k+\frac{1}{2}})-\delta_t u(t_{k-\frac{1}{2}})}{\tau}$, and the TFCD defined in (1.2.3) at $t = t_n$,

$$ {}_0^C D_t^\alpha u(t_n) = \sum_{k=1}^{n} \int_{t_{k-1}}^{t_k} \omega_{2-\alpha}(t_n - s) u''(s) ds, \quad 1 \le n \le N. \tag{1.22} $$

- In $L2$ method [58], approximating the $u''(s)$ by the operator $\frac{u(t_{k+1})-2u(t_k)+u(t_{k-1})}{\tau^2}$ $(\equiv \delta_t^2 u(t_k))$ on the interval $[t_{k-1}, t_k]$, we obtain

$$ {}_0^C D_t^\alpha u(t_n) \approx \frac{1}{\nu} \sum_{k=0}^{n-1} \lambda_{n-k} \delta_t^2 u(t_k), \quad 1 \le n \le N, \tag{1.23} $$

  where, $\lambda_k = (k+1)^{2-\alpha} - k^{2-\alpha}$ and $\nu = \tau^\alpha \Gamma(3-\alpha)$, $1 < \alpha < 2$.

- For the $L2C$ method [58], we approximate $u''(s)$ by the four point discretization $\frac{u(t_{k+1})-u(t_k)-u(t_{k-1})+u(t_{k-2})}{2\tau^2}$ on the interval $[t_{k-1}, t_k]$, we obtain $(1 \le n \le N)$

$$ {}^C D_{0,t}^\alpha u(t_n) \approx \frac{1}{2\nu} \sum_{k=0}^{n-1} \lambda_{n-k} [u(t_{k+1}) - u(t_k) - u(t_{k-1}) + u(t_{k-2})], \tag{1.24} $$

  with $u(t_{-1}) = u(t_0)$.

- For the Crank-Nicolson $L1$ method or modified $L1$ method [62], the linear interpolation polynomials are constructed using $(u'(t_{k-1}), t_{k-1})$ and $(u'(t_k), t_k)$ to approximate $u''(s)$. Further, once obtains the approximations

$$ {}^C D_{0,t}^{\alpha} u(t_{n-\frac{1}{2}}) \approx \frac{\tau}{\nu}\Big[\lambda_0 \delta_t u(t_{n-\frac{1}{2}}) + \sum_{k=1}^{n-1} (\lambda_{n-k} - \lambda_{n-k-1})\delta_t u(t_{k-\frac{1}{2}}) - \lambda_{n-1} u'(t_0)\Big]. \tag{1.25} $$

- For $H2N2$ method [59], we use Hermite quadratic interpolation polynomial to approximate the function u on the interval $[t_0, t_{\frac{1}{2}}]$ using $(t_0, u(t_0))$, $(t_1, u(t_1))$, $(t_0, u'(t_0))$ and quadratic interpolation polynomial on the other subintervals $[t_{k-\frac{1}{2}}, t_{k+\frac{1}{2}}]$ using $(t_{k-1}, u(t_{k-1}))$, $(t_k, u(t_k))$, $(t_{k+1}, u(t_{k+1}))$. Then the $H2N2$ method approximation of TFCD at $t_{n-\frac{1}{2}}$ takes the following forms

$$ {}_0^C D_t^{\alpha} u(t_{n-\frac{1}{2}}) \approx \frac{\tau}{\nu}\Big[b_{n-1}(\delta_t u(t_{\frac{1}{2}}) - u'(t_0)) + \sum_{k=1}^{n-1} b_{n-k-1}(\delta_t u(t_{k+\frac{1}{2}}) - \delta_t u(t_{k-\frac{1}{2}}))\Big], \tag{1.26} $$

where, $b_{n-1} = 2[(n-\frac{1}{2})^{2-\alpha} - (n-1)^{2-\alpha}]$, and $b_{n-k-1} = (n-k)^{2-\alpha} - (n-k-1)^{2-\alpha}$, $1 \le k \le n-1$.

In novel TFCD discretization, the time domain $[0, T]$ is discretized on the intervals $[t_0, t_{\frac{1}{2}}]$ and $[t_{k-\frac{1}{2}}, t_{k+\frac{1}{2}}]$ ([1]) instead of the interval $[t_{k-1}, t_{k+1}]$ $(k \ge 1)$. We extend it on nonuniform temporal mesh to handle the singular behavior of kernel at initial mesh point $t = 0$. This discretization has an advantage in calculation, it reduces the two-step approximation at grid point $t_{n-\frac{1}{2}}$ into single-step at t_n with good accuracy.

$$
\begin{aligned}
{}^{C}\mathcal{D}_{0,t}^{\alpha} u(t_n) = & \int_{t_{n-\frac{1}{2}}}^{t_n} \omega_{2-\alpha}(t_{n-\frac{1}{2}} - s) u''(s) ds \\
& + \sum_{k=1}^{n-1} \int_{t_{k-\frac{1}{2}}}^{t_{k+\frac{1}{2}}} \omega_{2-\alpha}(t_{n-\frac{1}{2}} - s) u''(s) ds. \qquad (1.27)
\end{aligned}
$$

- In novel $L1$ method [1], we approximate the u'' by the linear interpolation polynomials using $v(t_{n-\frac{3}{2}})$, $v(t_{n-\frac{1}{2}})$ and $v(t_{k-\frac{1}{2}})$, $v(t_{k+\frac{1}{2}})$, $(1 \leq k \leq n-1)$ on the first and second integration of the above equation (1.27), respectively. Then the $L1$ method with novel discretization is define as follows:

$$
\begin{aligned}
{}_{0}^{C}D_{t}^{\alpha} u(t_n) \approx \frac{\tau}{\nu} \Bigg[& \Lambda_1 \delta_t u(t_{n-\frac{1}{2}}) + \sum_{k=1}^{n-1} (\Lambda_{n-k+1} - \Lambda_{n-k}) \delta_t u(t_{k-\frac{1}{2}}) \\
& - \Lambda_n \delta_t u(t_{-\frac{1}{2}}) + \frac{1}{2^{2-\alpha}} [\delta_t u(t_{n-\frac{1}{2}}) - \delta_t u(t_{n-\frac{3}{2}})] \Bigg], \qquad (1.28)
\end{aligned}
$$

where, $\delta_t u(t_{-\frac{1}{2}}) = v(t_{-\frac{1}{2}})$ defined in [1], and $\Lambda_k = (k+\frac{1}{2})^{2-\alpha} - (k-\frac{1}{2})^{2-\alpha}$.

- In Crank-Nicolson $L1-2$ method [63], authors use the linear interpolation polynomial to approximate the function u on the interval $[t_0, t_1]$ and the quadratic interpolation polynomials for the other subintervals $[t_{k-2}, t_k]$, $k \geq 2$. Then the Crank-Nicolson $L1-2$ method for the TFCD discretization at the point $t = t_{n-\frac{1}{2}}$ becomes

$$
\begin{aligned}
{}^{C}\mathcal{D}_{0,t}^{\alpha} u(t_{n-\frac{1}{2}}) \approx \frac{\tau^{1-\alpha}}{\Gamma(3-\alpha)} \Bigg[& w_0 v(t_{n-\frac{1}{2}}) + \sum_{k=2}^{n} (w_{n-k} \\
& - w_{n-k-1}) v(t_{k-\frac{1}{2}}) - w_{n-1} u'(t_0) \Bigg], \qquad (1.29)
\end{aligned}
$$

where, $v = u'$ and $\tilde{\lambda}_k = \frac{1}{(3-\alpha)}[(k+1)^{3-\alpha} - k^{3-\alpha}] - \frac{1}{2}[(k+1)^{2-\alpha} + k^{2+\alpha}]$, $(k \geq 0)$. For $n \geq 2$,

$$w_k = \begin{cases} \lambda_0 + \tilde{\lambda}_0; \quad k = 0 \\ \lambda_k + \tilde{\lambda}_k - \tilde{\lambda}_{k-1}; \quad 1 \leq k \leq n-2, \\ \lambda_k - \tilde{\lambda}_{k-1}; \quad k = n-1. \end{cases} \tag{1.30}$$

- For $L2 - 1_\sigma$ Crank-Nicolson method [64], by using the linear interpolation polynomial and quadratic interpolation polynomial as discussed in [64], the expression of the Caputo derivative approximation at the point $t = t_{n-\frac{1}{2}-\sigma}$ is as follows:

$$\begin{cases} {}^C\mathcal{D}^\alpha_{0,t} u(t_{\frac{1}{2}-\frac{\sigma}{2}}) \approx \overline{\lambda}_1 [v(t_{\frac{1}{2}}) - u'(t_0)], \quad n = 1 \\ {}^C\mathcal{D}^\alpha_{0,t} u(t_{n-\frac{1}{2}-\sigma}) \approx \overline{\lambda}_n [v(t_{\frac{1}{2}}) - u'(t_0)] + \sum_{k=1}^{n-1} \overline{\lambda}_{n-k} [v(t_{k+\frac{1}{2}}) - v(t_{k-\frac{1}{2}})], \quad n \geq 2 \\ v(t_{n-\frac{1}{2}}) \approx \delta_t u(t_{n-\frac{1}{2}}), \quad n \geq 1, \end{cases} \tag{1.31}$$

where

$$\begin{aligned}
\mathfrak{a}_1 &= \int_0^{t_{\frac{1}{2}-\frac{\sigma}{2}}} \omega_{2-\alpha}(t_{\frac{1}{2}-\frac{\sigma}{2}} - s)ds \qquad (n = 1),\\
\mathfrak{a}_1 &= \int_{t_{n-\frac{3}{2}}}^{t_{n-\frac{1}{2}-\sigma}} \omega_{2-\alpha}(t_{n-\frac{1}{2}-\sigma} - s)ds \qquad (n \geq 2),\\
\mathfrak{a}_n &= \int_0^{t_{\frac{1}{2}}} \omega_{2-\alpha}(t_{n-\frac{1}{2}-\sigma} - s)ds \qquad (n \geq 2),\\
\mathfrak{b}_n &= \frac{4}{3\tau}\int_0^{t_{\frac{1}{2}}} \omega_{2-\alpha}(t_{n-\frac{1}{2}-\sigma} - s)(s - t_{\frac{1}{4}})ds \qquad (n \geq 2),\\
\mathfrak{a}_{n-k} &= \int_{t_{k-\frac{1}{2}}}^{t_{k+\frac{1}{2}}} \omega_{2-\alpha}(t_{n-\frac{1}{2}-\sigma} - s)ds, \qquad (n \geq 3)\\
\mathfrak{b}_{n-k} &= \frac{1}{\tau}\int_{t_{k-\frac{1}{2}}}^{t_{k+\frac{1}{2}}} \omega_{2-\alpha}(t_{n-\frac{1}{2}-\sigma} - s)(s - t_k)ds \qquad (n \geq 3),
\end{aligned} \tag{1.32}$$

and

$$\bar{\lambda}_1 = \frac{2}{\tau}\mathfrak{a}_1, \quad \bar{\lambda}_{n-k} = \frac{1}{\tau}\begin{cases} 2(\mathfrak{a}_n - \mathfrak{b}_n); \quad k = 0, \quad n \geq 2,\\ \mathfrak{a}_{n-k} + \mathfrak{b}_{n-k+1} - \mathfrak{b}_{n-k}; \quad 1 \leq k \leq n-2, \ n \geq 3,\\ \mathfrak{a}_1 + \mathfrak{b}_2; \quad k = n-1, n \geq 2. \end{cases} \tag{1.33}$$

Over the last decade, several numerical methods were investigated to find the numerical solution of one-dimensional (1D) TFDW equation. For example, Agrawal [52, 65, 66] considered the sine transform technique to convert the FDE from space domain to wave number domain and then resulting equation is reduced into ordinary algebraic equation using the Laplace transform. To obtain final solution they used inverse sine transform and inverse Laplace transform. In [67, 68], authors simulated approximate solution for the time-fractional diffusion-wave equations using the meshless Galerkin method utilizing radial basis functions. The authors used finite difference method for discretization of time derivative and finite element and interpolating element free Galerkin methods for the spatial derivatives. In [2, 69, 70] authors developed meshless method based on radial basis function to solve the 1D and multi-dimensional mixed diffusion and diffusion-wave equations. In [58, 59, 61, 62, 63, 64] authors used finite difference methods to approximate the TFCD and the central difference approximation for spatial derivatives to solve the 1D TFDW equation. In [71, 72] authors investigated finite element method in space and $L1$ method in time to solve TFDW equation of Krichhoff type. Zhang et al. [73] considered $L1$ method for time fractional derivative discretization and compact difference operator for approximation of spatial derivatives. They solved the 2D TFDW equation by using ADI approach. Li et al. [74] presented numerical scheme to solve 2D TFDW equation by using Crank–Nicolson method for TFCD approximation and Galerkin finite element is applied for space derivatives discretization. Moreover, there are some recent research articles on numerically solving the time-fractional PDEs with $\alpha \in (1, 2)$ order time-fractional derivative. Lyu et al. [75] considered the fractional Benjamin-Bona-Mahony-type equation. They used a nonuniform $L2$ approximation method to discretize the TFCD of order $\alpha \in (1, 2)$ and presented a linearized difference scheme for the considered model. Du and Sun [76] considered the $L2 - 1_\sigma$ approximation approach for the time-fractional derivatives and central difference formulas for spatial derivative approximation. They presented a numerical scheme for solving multi-term time fractional mixed diffusion-wave equations. Lyu et al. [77] used the $L2 - 1_\sigma$ method for the approximation of multi-term Caputo derivative and proposed a fast linearized finite difference scheme. In this study, authors solved nonlinear distributed order time-fractional wave equation numerically. Zhang and Wang [78] considered the $L1$ method on uniform time discretization and compact difference operator for space derivative approximation in solving TFDWE with time delay. Sun et al. [79] presented a numerical method in solving one and two-dimensional time-fractional diffusion-wave equations. Authors used $L2-1_\sigma$ formula for time fractional derivative discretization and central difference approximation in space. In [80, 81] authors considered the alternating direction implicit approach to construct finite difference scheme in addressing the numerical solution of the time-fractional mixed diffusion and diffusion-wave equation in two-dimension.

1.4.2 Literature Review on Time-Fractional Mixed Diffusion and Diffusion-Wave Equation

The mixed diffusion and diffusion-wave equation can be employed to investigate the intermediate processes between diffusion and diffusion-wave equations. The considered problem (1.12) is generalization of the time-fractional telegraph equation. The problem (1.12) contains both time-fractional diffusion (or sub-diffusion) and the time-fractional wave equation (or super-diffusion) terms together, due to which it becomes more challenging to develop computational algorithm for solving higher dimension problems. Also it is difficult task to find the analytical solutions of such type problems. The discretization is a productive way to handle many time-fractional PDEs via developing an efficient numerical scheme with good accuracy and minimum computational time. Sun et al. [82] considered the Crank-Nicolson $L1$ method on uniform mesh to approximate the TFCDs of order $\beta \in (0, 1)$ and $\alpha \in (1, 2)$. They used central difference operator for approximation of space derivatives and then solve the time fractional mixed diffusion-wave equation. Bhardwaj et al. [2, 70] used finite difference method to discretize the time fractional derivatives on uniform mesh and applied meshless method based on radial basis function for spatial discretization to find numerical solution of time-fractional mixed diffusion-wave equation. Du et al. [76] presented numerical solution of the multi-term time fractional mixed diffusion-wave equation by using $L2-1_\sigma$ method. Liu et al. [83] discussed the Crank-Nicolson $L1$ scheme for the approximation of TFCDs of order $\beta \in (0,1)$ and $\alpha \in (1,2)$ and Legendre spectral approximation for space derivative approximation to solve multi-term TFMDW equation numerically. Liu et al. [84] considered Legendre spectral method for space derivatives and finite difference approximation for the time discretization in solving 2D time-fractional linear mixed diffusion and diffusion-wave equations by using ADI approach. Mingrong Cui [81] used compact difference operator for the space side approximation and finite difference algorithm for the time fractional derivatives to solve the time-fractional linear mixed diffusion and diffusion-wave equation. Nikan et al. [85] considered local radial basis finite difference method in solving the nonlinear time-fractional telegraph equation. The authors used same process as discussed in [86] to approximate the Caputo derivative on uniform meshes and they obtained the convergence order $(3-\alpha)$, $1<\alpha<2$. Although, the semi-linear time-fractional mixed diffusion and diffusion-wave equations have initial layer in the solution u at $t=0$, these studies are still remaining in the literature to examine in details. Our interest in this thesis to provide a numerical scheme to handle such behavior of solutions, and describe the theoretical and numerical analysis for the considered problems.

1.4.3 Literature Review on Generalized Time-Fractional Advection-Diffusion Equation

The advection-diffusion equation is basically a transport problem that transport a passive scalar quantity in a fluid flow. Due to diffusion and advection, this model represents physical phenomenon of species concentration for mass transfer and temperature in heat transfer; for more details, we refer to [87, 88, 89, 90, 91], and

[92, 93, 94, 95, 96] for further history and significance of advection-diffusion equation in physics, chemistry and biology.

Mostly used fractional derivatives in the problem formulation are the Riemann-Liouville and the Caputo derivatives [14]. In the year 2012, the generalizations of fractional integrals and derivatives were discussed by Agrawal [11]. Two functions, scale $\zeta(t)$ and weight $\omega(t)$ in one parameter, appear in the definition of the generalized fractional derivative (1.2.8) of $u(t)$. If $\omega(t) = 1$ and $\zeta(t) = t$ then generalized fractional derivative reduces to the Riemann-Liouville (R-L) and the Caputo derivative, whereas if $\omega(t) = 1$, $\zeta(t) = ln(t)$, and $\omega(t) = t^{\sigma\eta}$, $\zeta(t) = t^{\sigma}$ then it will convert to Hadamard [97], and modified Erdélyi-Kober fractional derivatives, respectively. In [98] studied the generalized form of R-L and the Hadamard fractional integrals, which is a special case of the Erdélyi-Kober generalized fractional derivative, and some properties of this operator. In generalized derivative, scale function $\zeta(t)$ manages the considered time domain, it can stretch or contract accordingly to capture the phenomena accurately over desired time range. The weight function $\omega(t)$ allows the events to be estimated differently at different time.

Over the last decade, many numerical methods were investigated to approximate the Generalized Caputo and Caputo fractional derivatives. For example, Mustapha et al. [99] presented $L1$ approximation formula to solve fractional reaction-diffusion equation and second order error bound discussed on non-uniform time meshes. Alikhanov [100] constructed $L2 - 1_{\sigma}$ formula to approximate Caputo derivative and then used this derived scheme in solving time fractional diffusion equation with variable coefficients. Abu Arqub [101] considered reproducing kernel algorithm for approximate solution of the nonlinear time-fractional PDEs with initial and Robin boundary conditions. Li and Yan [102] discussed the idea of [103] (i.e. L_2 approximation formula for time discretization), also derived a new time discretization method with

OC $\mathcal{O}(\tau^{3-\alpha})$ and finite element method for spatial discretization. Cao et al. [4] presented a high-order approximation formula based on the cubic interpolation to approximate the Caputo derivative for the time fractional advection-diffiusion equation. Xu and Agrawal [104] used the finite difference method (FDM) to approximate the GCFD for solving the generalized fractional Burgers equation. Kumar et al. [105] presented $L1$ and $L2$ methods to approximate the generalized time fractional Caputo derivative. Yadav et al. [106] discussed Taylor expansion for the approximation of the generalized time-fractional derivative to solve generalized fractional advection-diffusion equation. In [107], the authors used the generalized weighted and shifted Grünwald–Letnikov difference operator to approximate the generalized Caputo fractional derivative and then adopt it to solve the generalized fractional diffusion equation.

1.5 Motivation and Objectives of the Thesis

1.5.1 Motivation

Many research articles have taken into account finite difference methods (FDMs) for the numerical solution of sub-diffusion and super-diffusion equations on uniform temporal meshes [73, 79, 100]. Although, the sub-diffusion equation has an initial layer at $t = 0$ in the solution and is studied in the literature (see [108] related are in this). The solution behavior at initial singularity $t = 0$ in Caputo derivative remains to be addressed for super-diffusion, and mixed diffusion and diffusion-wave equations.

The initial singularity in TFCD of order $\beta \in (0, 1)$ is addressed in some research studies that are available in the literature [99, 109, 110]. However, the solution layer at initial singularity $t = 0$ for the TFCD of order $\alpha \in (1, 2)$ remains to be addressed. It has been shown that the current approximation techniques [64, 111, 112] provide better accuracy on nonuniform meshes as compared to uniform meshes for $0 < \beta < 1$. In addition, the numerical methods for solving TFDW [113, 113, 114, 115, 116, 117, 118, 119, 120] and TFMDW [70, 76, 82] equations are done on uniform temporal meshes by taking smooth exact solution under some restrictive regularity conditions with smooth initial data. However, these articles ignored the presence of weak singularity in solution at the initial time $t = 0$ for both TFDW and TFMDW equations. The main purpose of this thesis is to deal with the initial singularity of the TFCD of order $\alpha \in (1, 2)$. To tackle the singularity in both derivatives together of order $\beta \in (0, 1)$ and $\alpha \in (1, 2)$ remains to be marked. Our main interest in this thesis is to handle the weak initial singularity in the solution of the linear/nonlinear TFDW and TFMDW equations with constant/variable coefficients. To overcome the low accuracy caused by nonsmooth exact solutions of TFDW and TFMDW equations, this thesis includes the discretization of TFCDs on nonuniform time mesh. While existing numerical methods for solving TFDW and TFMDW equations are discussed in one dimension [113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125], another objective of this thesis is to extend these methods by providing difference schemes capable of solving the considered model problems in two dimensions.

1.5.2 Objectives

In this thesis, we mainly interested to tackle the weak singularity at $t = 0$ in nonsmooth solutions of TFDW equation and TFMDW equation. To overcome the low accuracy caused by nonsmooth exact solutions of linear/nonlinear TFDW problem, this thesis includes the discretization of TFCD of order $\alpha \in (1, 2)$ on nonuniform time mesh. In conclusion, the primary objectives of this thesis can be outlined as:

- To develop approximation methods based on linear and quadratic interpolation polynomials for the discretization of both TFCDs of order $\beta \in (0,1)$ and $\alpha \in (1,2)$ on nonuniform temporal grids to tackle the initial singularity.
- To solve the 1D and 2D linear/nonlinear TFDW equations and TFMDW equations using finite difference method and analyze the behavior of nonsmooth solutions near the singular point $t = 0$.
- To analyze the error bound in approximating the Caputo derivative by assuming weak initial singularity at $t = 0$ and stability analysis of the proposed finite difference scheme.
- To verify the effect of nonuniform temporal meshes on nonsmooth solutions of governing problems, graphical representation of error, and numerical description of the nonsmooth solutions.

1.6 Outline of the Thesis

The main objective of this thesis is to study the numerical solutions of time-fractional PDEs in bounded domain. The original contribution of this thesis is listed in six chapters. The summaries of these chapters are outlined in the following.

In **Chapter 2**, we proposed two numerical schemes to achieve the desired accuracy near the initial singularity $t = 0$ in solving 2D TFDW equation, where the Caputo fractional derivative of order α $(1 < \alpha < 2)$ is used. The Nonuniform $L1$ (single-step) and Nonuniform Crank-Nicolson $L1-2$ (multi-step) methods are utilized to approximate the TFCD. These methods $L1$ and $L1-2$ have order of convergence (OC) $\min(3-\alpha, \gamma\alpha)$ and second-order, respectively where γ is the mesh grading parameter used in construction of the nonuniform mesh. The nonuniform temporal meshes are considered to compensate the lack of smoothness caused by the presence of singularity in TFCD near $t = 0$. Further, the central difference operator for the spatial derivative discretization and the proposed TFCD approximation methods ($L1$ and $L1-2$) are adopted to obtain the system of equations for governing problem. Then, the Alternating Direction Implicit (ADI) approach is used to generate the two fully discrete difference schemes in solving the 2D TFDW equations. Stability analysis for the discussed schemes are provided. To validate the accuracy of ADI schemes, two numerical examples are given by choosing the smooth and non-smooth exact solutions for 1D and 2D TFDW equations. The numerical results show that both schemes have second-order spatial accuracy, and in temporal direction the schemes achieve $\min(3-\alpha, \gamma\alpha)$ and second order convergence, respectively for all $1 < \alpha < 2$. The corresponding absolute error is plotted to see the advantage of nonuniform time meshes near the initial singularity $t = 0$.

In **Chapter 3**, we established a difference scheme to tackle the weak initial singularity in the solution of nonlinear time-fractional mixed diffusion-wave (TFMDW) equation. The considered problem involved two time-fractional derivatives terms diffusion and wave of order β $(0 < \beta < 1)$ and α $(1 < \alpha < 2)$, respectively. The nonuniform linearized $L1$ method is used to discretize both the time-fractional Caputo derivatives (TFCDs). Further, the considered model will convert to an equivalent system of equations by approximating TFCDs with the proposed $L1$ method and central difference operator for the space derivative approximation. The ADI approach is developed to get the numerical solutions of 2D TFNMDWE. The stability analysis of the presented scheme is proved. Finally, the numerical examples are describe the convergence rate of established method for 1D and 2D nonlinear TFMDW equations with smooth and non-smooth exact solutions. The shown examples verify that the method has OC is $\min(2-\alpha, 3-\beta, \gamma\alpha, \gamma(\beta-1))$ in the time direction and second-order accuracy in space, where γ is the mesh grading parameter. The corresponding absolute error is plotted to see the advantage of nonuniform time meshes at the initial singularity $t = 0$.

Chapter 4 presented an efficient discretization in dealing with the discontinuous initial data and nonsmooth exact solution of the nonlinear time-fractional diffusion-wave (TFDW) equation with variable coefficients to achieve the optimal convergence rate. The half point discretization $L1$ approach is used to obtain the desired temporal accuracy in approximation of the Caputo fractional derivative of order $\alpha \in (1, 2)$. The error analysis in approximation of the Caputo derivative is proved by assuming the weak singularity at $t = 0$. Next, the considered model is converted into a system of equations by utilizing the second order approximation of the space derivatives and the proposed nonuniform $L1$ approach. Two linearized finite difference schemes are constructed to solve the nonlinear single-term and multi-term TFDW equations with $\min(3-\alpha, \gamma(\alpha-1))$ and $\min(3-\alpha_r, \gamma(\alpha_r-1))$, $r = 0,\ 1,\ 2$ convergence order, respectively where parameter $\gamma \geq 1$ is used in formation of nonuniform temporal grids. The ADI process is used in solving the two-dimensional nonlinear TFDW equation with variable coefficients. Further, we discussed the Von Neumann stability analysis for the developed scheme. To demonstrate the theoretical findings, four numerical examples are given in 1D and 2D with smooth, nonsmooth and also discontinuous initial data. The presented numerical results confirm that the suggested method agrees with theoretical accuracy for both cases nonsmooth solutions and discontinuous initial data.

In **Chapter 5**, a high-order approximation formula based on cubic interpolation polynomials is examined to approximate the generalized Caputo fractional derivative (GCFD) of order $\beta \in (0, 1)$. Additionally, the local truncation error bound is shown. Next, we utilized the central difference for spatial derivatives and the proposed

GCFD approximation approach to generate a difference scheme for the numerical solution of the generalized fractional advection–diffusion equation with Dirichlet boundary conditions. Furthermore, the stability and convergence of the difference scheme are also discussed. To investigate the theoretical claims, numerical examples are given. The numerical analysis reveals that the difference scheme has second-order convergence in space and $(4-\alpha)$ in temporal direction.

In **Chapter 6**, the key conclusions from the research work are summarized and the contributions of the thesis work are highlighted. This thesis concludes with some suggestions for additional future investigation of the work that has been presented.

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