CHAPTER 1

Introduction

This chapter contains a brief illustration of objective, approach, and arrangement of the thesis. Sect. 1.1 contains the history of fractional calculus (FC) and fractional partial differential equations (FPDEs). Some basic definitions that are thorougly used in the entire thesis are inclusively provided in Sect. 1.2. Sect. 1.3 presents a detailed review on the generalized time-fractional diffusion equations (GTFDEs). Sect. 1.4 presents some mathematical preliminaries. Sect. 1.5 presents some results based on the proposed numerical methods that are used in the thesis. The challenges and the motivation behind the works are discussed in Sect. 1.6. Sect. 1.7 defines the aim and outline of the thesis.

1.1 Background

1.1.1 Fractional calculus

Calculus, also called as “infinitesimal analysis” is the vital branch of mathematics that deals with the calculation of instantaneous rates of change (known as differential calculus) and the addition of infinitely many small components to determine the whole (known as integral calculus). The idea of calculus lies in the concept of derivative. In 1666, Isaac Newton defined the instantaneous velocity with a physical or geometrical view point of derivative i.e. the first derivative of displacement is called velocity and the second order derivative is acceleration. The classical calculus using ordinary differential equations has been extensively used to model many physical phenomena in science, engineering, demography, economics etc. However, there are many real world problems with memory effect, for example, signal and image processing [1, 2], finance [3], fluid dynamics [4–6], behavior of real materials [7–9] that cannot be modeled by the classical calculus, hence revealing the requirement of fractional differential equations.

Fractional calculus owes its origin to a question of whether the meaning of a derivative to an integer order can be extended to still be valid when is not an integer. Two well-known examples of such extension in mathematical formulae are the extension of real numbers to complex numbers and integer factorials to complex factorials. The question of generalization of an integer order derivative was raised for the first time by L’Hopital to Leibniz through a letter dated September 30th, 1695. In this letter, L’Hopital curiously asked about What would be the result if $n = 1/2$ in the notation $d^n y/dx^n$ for a derivative? Leibniz replied, “This is an apparent paradox, from which, one day, useful consequences can be drawn ”. In 1816, for the first time, a French mathematician, S.F. Lacroix [10] gave the concept of an arbitrary order derivative. He started with $y = x^m$, m being a positive integer, and defined the n^{th} order derivative as:

$$\frac{d^n y}{dx^n} = \frac{m!}{(m-n)!} x^{m-n}.$$

Using the concept of the Gamma function (Γ), that represents generalized factorial, he designed the following formula where n is replaced by 1/2 and m by any positive real number a,

$$\frac{d^{1/2} y}{dx^{1/2}} = \frac{\Gamma(a+1)}{\Gamma(a+1/2)} x^{a-1/2},$$

which denotes the 1/2 order derivative of the function x^a. For example, consider $y = x$ that yields

$$\frac{d^{1/2} y}{dx^{1/2}} = \frac{2\sqrt{x}}{\sqrt{\pi}}$$

It is noteworthy that the present Riemann-Liouville derivative has the same definition as the above formula. After this many scientists like Euler, Laplace and Fourier mentioned about the arbitrary order derivative, but no applications were given. Hence the honor goes to Niels Henrik Abel for making the first application in 1823 [11]. For the first time, using the theory of fractional calculus, Abel solved an integral equation arising from the formulation of tautochrone problem, sometimes also called as isochrone problem [12]. The problem is to find the geometry of a frictionless wire lying in a vertical plane such that the time taken by a bead placed on the wire to slide down to its lowest position is same, irrespective of the position of the bead on the wire. The problem for finding the shortest time of the slide is known as brachistochrone problem. Oldham and Spanier did the first work on fractional calculus, which was published in 1974 [13]. Many renowned mathematicians including N.H. Abel, B. Riemann, J. Liouville, G.W. Leibniz, H. Weyl, A.V. Letnikov, and J. Caputo, contributed remarkably for the development of fractional calculus.

1.1.2 Fractional partial differential equations

Partial differential equations play a fundamental role in the modeling of natural phenomena; that occur in diverse field of science (e.g. biology, ecology, medicine, nuclear reactors, sociology, electricity production and distribution, traffic control, aerospace projects etc). The abbreviation for arbitrary order derivatives is fractional derivatives (FDs). The PDEs conatining FDs are called FPDEs. Due to the non-local nature of fractional derivatives, they provide a more powerful tool in order to deal with the complex natural phenomena such as control theory [14], biological systems [15], finance, signal processing, sub-diffusion and super-diffusion process [16], image processing [17], viscoelastic fluid [5], electrochemical process [6], and so on. The major benefit of FDEs is that they provide an effective method for representing the memory based systems and hereditary properties of several materials in contradiction to the classical differential equations in which it becomes difficult to include such effects [7, 18]. Boltzmann described the process with memory for the first time in 1874 and 1876 [19, 20]. Memory means that the existence of output of any process will depend not only on current time but also on the history of change of input on a finite or infinite time interval. It can be described by functions called memory functions. These functions are the kernel of an integro-differential operator known as power-law memory in fractional calculus. This can also be seen as an advantage of FDEs over integer-order differential equations as the latter has the property of being differentiable only in an infinitesimal neighbourhood of the considered point. So, it cannot describe the processes with memory. Since the non-integer order derivatives violate the Leibnitz rule, it allows us to represent memory. A wide range of functions with memory in continuous time models of physics actively uses fractional integro-differential equations. Some of the real-world problem based applications of FDEs are discussed in [21].

1.1.2.1 Generalized time-fractional diffusion equations (GTFDEs)

It is well-known that various fractional derivatives like Riemann-Liouville, Caputo derivative, Riesz derivative, Caputo-Fabrizio derivatve, etc, are used to model several physical phenomena [22, 23]. Among all the derivatives, the advantage of Caputo derivative is that it allows traditional initial and boundary conditions to be incorporated in the problem. Also, the derivative of a constant is zero in this derivative which encourages the study of this operator on a broader aspect. Hence, Caputo derivatives are extensively used to model many physical processes into time-fractional diffusion equations (TFDEs) and time-fractional wave equations (TFWEs) [22, 23]. TFDEs are derived by substituting the first-order time derivative of the classical diffusion equations with α-order $(0 < \alpha < 1)$ Caputo derivative, and TFDWEs are derived by substituting the second-order time derivative of the standard diffusion or wave equations with α-order $(1 < \alpha < 2)$ FD.

In the present thesis, we are interested to study the generalized Caputo derivative which is obtained by adding a non-unity weighting function $\omega(t)$ to the classical α-order $(0 < \alpha < 1)$ Caputo derivative. The definition of generalized Caputo fractional derivative reads as follows [24]:

$$\partial_{0,t}^{\alpha,\omega(t)}\zeta(t) = \frac{1}{\Gamma(1-\alpha)}\int\limits_0^t \frac{\omega(t-\xi)}{(t-\xi)^{\alpha}}\zeta'(\xi)\mathrm{d}\xi,\ \ 0 < \alpha < 1,\ \ \omega(t) > 0. \tag{1.1}$$

The kernel function of the generalized Caputo FD defined in (1.1) is $\frac{\omega(t)t^{-\alpha}}{\Gamma(1-\alpha)}$ with $\omega(t)$ being the weight function. It can be easily noted that using $\omega(t) = 1$ in equation (1.1) quickly reduces to the classical Caputo derivative case. The weighting function has both mathematical and practical applications. One of the commonly used variants of (1.1) is obtained by using the function $\omega(t) = e^{-bt},\ b > 0$, known as the tempered FD [25], and has immense applications in the field of geophysics [26, 27] and finance [28]. The PDEs with generalized Caputo derivative are widely used for representing dynamical systems with anomalous subdiffusion. Besides the case of tempered kernel, using different weighting functions in (1.1) may generate various significant physical models available in literature. For instance, using $\omega(t) = \omega_0 + \omega_1 t^{\alpha-\alpha_1} + \omega_2 t^{\alpha-\alpha_2} + \ldots + \omega_t^{\alpha-\alpha_m}$, where $0 < \alpha_m < \alpha_{m-1} < \alpha_{m-2} \ldots < \alpha_1 < \alpha < 1$ and $\omega_0, \omega_1, \ldots, \omega_m$ and m are positive constants in equation (1.1) reduces to the multi-term time-fractional diffusion equation (TFDEs) discussed in [29]. Thus, GTFDEs play a significant role in diverse field of science and engineering. But, due to the non-local nature of these fractional derivatives, it becomes difficult to find their analytical solution. Hence, it is necessary to develop stable numerical schemes with higher accuracy to solve such FDs.

1.2 Definitions

In contrary to the classical one, there are several definitions of the FDs. The two most commonly used derivatives are the Riemann Liouville derivative and the Caputo derivative. Here, we present the definitions of some of the fractional order derivatives.

Definition 1.1. Grünwald-Letnikov derivatives: The left and right Grünwald-Letnikov derivatives with order $\alpha > 0$ of a function $\zeta(t),\ t \in (a, b)$ are defined as

[30, 31]:

$$ {}_{a}^{\mathrm{GL}}\mathcal{D}_{t}^{\alpha}\zeta(t) = \lim_{\substack{h\to 0\\ h=\frac{t-a}{N}}} h^{-\alpha}\sum_{j=0}^{N}(-1)^{j}\binom{\alpha}{j}\zeta(t-jh), \tag{1.2} $$

and,

$$ {}_{t}^{\mathrm{GL}}\mathcal{D}_{b}^{\alpha}\zeta(t) = \lim_{\substack{h\to 0\\ h=\frac{b-t}{N}}} h^{-\alpha}\sum_{j=0}^{N}(-1)^{j}\binom{\alpha}{j}\zeta(t+jh), \tag{1.3} $$

respectively. For further details of derivation of the above formulae (1.2) and (1.3) one can refer to [8].

Definition 1.2. Riemann-Liouville fractional derivative: The definition of left and right Riemann-Liouville FDs with order $\alpha > 0$ of the given function $\zeta(t)$, $t \in (a, b)$ are defined as [30, 31]:

$$ {}_{a}^{RL}\mathcal{D}_{t}^{\alpha}\zeta(t) = \frac{1}{\Gamma(m-\alpha)}\frac{d^{m}}{dt^{m}}\int_{a}^{t}(t-s)^{(m-\alpha-1)}\zeta(s)ds, \tag{1.4} $$

and,

$$ {}_{t}^{RL}\mathcal{D}_{b}^{\alpha}\zeta(t) = \frac{(-1)^{m}}{\Gamma(m-\alpha)}\frac{d^{m}}{dt^{m}}\int_{t}^{b}(s-t)^{(m-\alpha-1)}\zeta(s)ds, \tag{1.5} $$

respectively, where $m \in \mathbb{Z}^{+}$ satisfying $m-1 \leq \alpha < m$.

Definition 1.3. Caputo fractional derivative: The left and right Caputo FDs with order $\alpha > 0$ of the given function $\zeta(t)$, $t \in (a, b)$ are defined as [30, 31]:

$$ {}_{a}^{C}\mathcal{D}_{t}^{\alpha}\zeta(t) = \frac{1}{\Gamma(m-\alpha)}\int_{a}^{t}(t-s)^{m-\alpha-1}\zeta^{(m)}(s)ds, \tag{1.6} $$

and,

$$ {}_{t}^{C}\mathcal{D}_{b}^{\alpha}\zeta(t) = \frac{(-1)^m}{\Gamma(m-\alpha)} \int_t^b (s-t)^{m-\alpha-1} \zeta^{(m)}(s)ds, \tag{1.7} $$

respectively, where $m \in \mathbb{Z}^+$ satisfying $m-1 < \alpha \leq m$.

Definition 1.4. Riesz fractional derivative: The Riesz FD with order $\alpha > 0$ of the given function $\zeta(t)$, $t \in (a,b)$ is defined as [30, 31]:

$$ {}^{RZ}\mathcal{D}_{t}^{\alpha}\zeta(t) = c_\alpha \left({}_{a}^{RL}\mathcal{D}_{t}^{\alpha}\zeta(t) + {}_{t}^{RL}\mathcal{D}_{b}^{\alpha}\zeta(t) \right), \tag{1.8} $$

where $c_\alpha = -\dfrac{1}{2\cos(\alpha\pi/2)}$, $\alpha \neq 2k+1,\ k = 0, 1, \ldots$. ${}^{RZ}\mathcal{D}_{t}^{\alpha}\zeta(t)$ is sometimes expressed as $\dfrac{\partial^\alpha \zeta(t)}{\partial |t|^\alpha}$.

1.3 Literature review

In recent years, mathematicians have constantly upgraded and enhanced the algorithms to find the analytical solutions of fractional differential equations. But, due to the presence of a singular kernel in most of the fractional operators, computation of their analytical solution is not easy. Therefore, some effective numerical methods are required to solve such types of singular problems. In this section, we present a brief literature review of several numerical approximations for the fractional mathematical models used in this thesis.

1.3.1 Review on numerical approximation of Caputo derivatives and time-fractional diffusion equation

Numerous researchers have developed different numerical techniques for the approximation of the Caputo derivatives for $\alpha \in (0, 1)$. The two main techniques for the discretization of subdiffusion equation are: The L1 type approximation [32–37] and the Grünwald-Letnikov approximation [38–40]. The traditional L1 technique [34, 41–43] is one of the most commonly used method to find a discrete analog of the Caputo FD defined in (1.6)-(1.7). The basic approach of this method is to use a piecewise linear polynomial for the interpolation of the function $\zeta(t)$ resulting in a convergence order (CO) of $2-\alpha$. Lin and Xu [33] developed the L1 scheme for the derivative in Caputo sense and a method of Legendre spectral in space and examined the convergence and stability with local truncation error of order $\mathcal{O}(\tau^{2-\alpha})$. Another form of the L1 scheme was investigated in [44] for $\mathcal{C}^3$ solutions and attained a convergence rate of $\mathcal{O}(\tau^2)$. In continuation to that, Gao et al. developed a new type of L1 scheme [37] based on quadratic interpolation formula with a convergence rate of order $\mathcal{O}(\tau^{3-\alpha})$ for smooth solutions. Later, in [45], the higher order $L1-2$ formula was designed with $3-\alpha$ order of approximation. On a similar note, using a piecewise quadratic interpolating polynomial $L2-1_\sigma$ formula was invented in [46] with an accuracy of $\mathcal{O}(\tau^{3-\alpha})$. The new L2 formula was proposed in [47, 48] that uses quadratic interpolation of the function $\zeta(t)$ in whole domain resulting in CO of $(3-\alpha)$.

Many works have been done considering the L1 formula for the subdiffusion equation. But, most of those work, except a few, assumed the solution to be sufficiently smooth, even for a homogeneous problem with smooth initial data, the solution may be nonsmooth in a closed interval due to the singularity of derivatives of $\zeta(x, t)$ at $t = 0$ as shown in [49, 50].

- In [51], the analysis for the case of the non-smooth source term for the inhomogeneous time-fractional diffusion equation (TFDEs) was done. Then, in [52], the convergence rate of $\mathcal{O}(\tau)$ was established for smooth as well as non-smooth initial data.

- Authors of [53] utilized the FDM technique on non-uniform mesh for solving non-linear fractional PDEs and the results were proved to be better than the results obtained for uniform mesh.

- Ford et al. [54] used a very interesting method to tackle non-smooth solutions by modifying the initial steps of time discretization schemes to capture the singularity of such non-smooth solutions. It used the L1 scheme and its modification, Lubich's fractional multistep methods, discontinuous Galerkin methods, etc.

- In [55], Stynes et al. proved that the rate of convergence of the L1 scheme on a uniform mesh was $\mathcal{O}(N^{-\alpha})$ and on a non-uniform grid was $\mathcal{O}(N^{\alpha-2})$. After that, in [56], it was shown that the same scheme for uniform grid has the order of convergence (CO) as $\mathcal{O}(N^{-1})$ on any subdomain that is bounded away from t=0.

- Yan et al. [57] established an improved version of the L1 scheme for smooth and non-smooth initial data for homogeneous as well as inhomogeneous cases. The rate of convergence has been validated to be $\mathcal{O}(\tau^{2-\alpha})$ for both the cases where τ is the time step size. Also, error estimates were obtained for the improved version of the L1 scheme in an inhomogeneous case for smooth and non-smooth initial data.

- In [58], Galerkin finite element methods and spectral methods were used for space-fractional, time-fractional, and time-space fractional partial differential equations with 1D, 2D, and 3D variables in space. Also, rapid algorithms were found because of the high complexity cost in the implementation of these numerical schemes.

- Chen and Stynes [59] used Alikhanov's high-order scheme [45] for classical Caputo FD on non-uniform mesh for temporal direction and a spectral method in space, attaining a CO of $3 - \alpha$ order in time.

- Huang and Stynes did many recent works based on this scheme as given in [60–62].

- A two-grid algorithm was designed in [63] to solve the time-fractional transport model and theoretical analysis was investigated in L_2-norm. Stable multistep schemes were designed in [64] for both 1-D and 2-D non-linear time-fractional wave models.

- Zhang et al. [65, 66] designed different temporal spectral methods with second order accuracy for solving non-linear subdiffusion problems. The theoretical analysis has been established in the L_2-norm in [65] and in the H^1-norm in work [66], respectively.

1.3.2 Review on approximation for generalized Caputo derivatives

Due to the immense physical significance of the generalized Caputo derivative, GTFDEs attracted researchers and several numerical techniques have been developed to solve these PDEs in the past few years. Some of them are as follows:

- A. Alikhanov [24] developed the L1 method for GTFDEs on the uniform grid for smooth solutions and non-smooth solutions by splitting into two parts: one smooth but unknown, and the other known but non-smooth as done in [67]. By using this method for non-smooth solutions, convergence order of $2-\alpha$ is attained at the final time, and CO of 1 in the domain. For smooth solutions, it attained a convergence order of $2-\alpha$.

- In [68], Khibiev develpoed the L1 method for multi-term GTFDEs on the uniform grid for smooth solutions. Afterward in [69, 70], a modified version of the L1 formula was presented on a non-uniform mesh that improved the order of convergence significantly for non-smooth solutions.

- The Caputo FD with a generalized memory kernel has a non-local property, increasing the complexity and cost of computation. Hence, fast and parallel algorithms were discovered in [71–73] for easy and fast implementation of the scheme.

- Sandev et al. studied diffusion equation and Fokker-Planck-Smoluchowski equations with generalized memory kernel in [74]. Here, the Laplace transform of the generalized diffusion equation with a general memory kernel, is a completely monotonic function, due to which a broad range of examples was considered, namely, distributed order kernels, power-law function, a combination of Dirac delta, etc.

- Khibiev and Alikhanov [75] developed an $L2-1_{\sigma}$ formula for equation (1.1) on a uniform grid resulting in second order of convergence in time. .

1.4 Preliminaries

Here, we define some mathematical prerequisites that are essential for achieving the aim of our thesis.

1.4.1 Taylor's theorem

Taylor's theorem gives an approximation of a n-times differentiable function near a given point by a nth degree polynomial.
Let $f : [a, b] \to \mathbb{R}, f, f', f'', ..., f^{(n-1)}$ be continuous on $[a, b]$ and suppose $f^{(n)}$ exists on (a, b). Then there exists $c \in (a, b)$ such that

$$f(b) = f(a) + f'(a)(b-a) + \frac{f''(a)}{2}(b-a)^2 + ... + \frac{f^{(n-1)}a}{(n-1)!}(b-a)^{n-1} + \frac{f^{(n)}(c)}{n!}(b-a)^n.$$

1.4.2 Gamma and Beta function

1.4.2.1 Gamma function

Gamma function is a frequently used extension of the factorial function to complex numbers. It is defined for all the complex numbers except for the non-positive integers. For every positive integer k, the Gamma function is defined as

$$\Gamma(k) = (k-1)!,$$

and for complex numbers with a positive real part, it is defined by a convergent improper integral,

$$\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}dt, \qquad \Re(z) > 0.$$

Gamma function has significant applications in the field of calculus. While the function behaves like a factorial in the case of natural numbers, which is a discrete set, its extension to positive real numbers, which is a continuous set, makes this function helpful in the modeling of various phenomena which are changing continuously.

1.4.3 Beta function

The Beta function, which is also known as the Euler integral of the first kind, is defined by the following integral,

$$B(z_1, z_2) = \int_0^1 t^{z_1-1}(1-t)^{z_2-1}dt$$

for complex numbes z_1, z_2 such that $\Re(z_1), \Re(z_2) > 0$. The Beta function and the Gamma function has the following relation:

$$B(z_1, z_2) = \frac{\Gamma(z_1)\Gamma(z_2)}{\Gamma(z_1 + z_2)}.$$

1.4.4 Mittag-Leffler function

The Mittag-Leffler function is a direct generalization of the exponential function e^x, and plays an important role in the theory of fractional calculus. It is named after a Swedish mathematician Gösta Mittag-Leffler who defined and studied it in 1903

[76–78].

The one parameter Mittag-Leffler function can be defined in terms of power series as:

$$E_{\alpha}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\alpha k + 1)}, \ \alpha > 0.$$

The two-parameter representations of Mittag-Leffler function is a generalization of the one-parameter function which was first introduced in 1953 by R.P. Agarwal [79]. It is defined as:

$$E_{\alpha,\beta}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\alpha k + \beta)}, \alpha > 0, \beta > 0.$$

1.4.5 Error function and complementary error function

Error function is represented by $erf(t)$ and defined as:

$$erf(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-x^2} dx,$$

with $erf(-\infty) = -1$ and $erf(\infty) = 1$.

The complementary error function $erfc(t)$ is defined in the following manner:

$$erfc(t) = 1 - erf(t) = \frac{2}{\sqrt{\pi}} \int_t^{\infty} e^{-x^2} dx.$$

1.5 Approximation methods

In this thesis, we utilized the finite difference method (FDM) to design the numerical schemes for solving the fractional order mathematical models.

1.5.1 Finite difference method

The finite difference method (FDM) is one of the oldest technique for finding the approximate solutions to the differential equations. It has been used extensively to solve a wide range of problems including linear, non-linear, time dependent and space dependent problems. It was first used by Euler apparently in the year 1768. The basic idea of FDM is to replace the derivatives present in the differential equations by finite differences formulae. These difference formulae are based on the values of the function itself at discrete points. The original ordinary or partial differential equation is then converted to a finite set of algebraic equations. The numerical solution to the original boundary value problem can then be obtained by solving these simultaneous equations. This technique requires use of a regular grid and to enhance explanation of the procedure, and it will be considered that it is uniform, although this is not essential. The grid must be constructed so that the nodal points are located at the intersection of either curved lines or rectilinear [80]. Among numerous difference approximation methods used, Taylor's series expansion is one of the most common one used to derive difference aproximations of DEs. Several applications of FDM in FDEs are elaborated in details in the works [80–83]. Based on FDM, the numerical solution, provides the values of dependent variables at discrete nodal points in the domain.

Consider the space-time domain such that the space variable $x \in [0, L]$ and temporal variable $t \in [0, T]$. Let M & N be any two positive integers, and the discretization parameters $h = L/M$ and $\tau = T/N$ represent the uniform spatial and temporal step size, respectively. Here both the space and time discretization are uniform, however it is not always necessary. In order to achieve higher accuracy, one has to refine the mesh by taking more number of mesh points. Let $\Omega_h = \{x_i : x_i = ih,\ i =$

$0, 1, \ldots, M\}$ and $\Omega_\tau = \{t_j : t_j = j\tau,\ j = 0, 1, \ldots, N\}$, then the spatial and time domain $[0, L]$ & $[0, T]$ are covered by $\Omega_{\Delta x}$ & $\Omega_{\Delta t}$, respectively. At the nodal points (x_i, t_j), u_i^j denote the approximate value of $u(x_i, t_j)$.

The forward difference schemes for space and time are

$$\frac{\partial u}{\partial x}(x_i, t_j) \approx \frac{u_{i+1}^j - u_i^j}{h}, \tag{1.9}$$
$$\frac{\partial u}{\partial t}(x_i, t_j) \approx \frac{u_i^{j+1} - u_i^j}{k}, \tag{1.10}$$

and the backward space and time difference schemes are given by

$$\frac{\partial u}{\partial x}(x_i, t_j) \approx \frac{u_i^j - u_{i-1}^j}{h}, \tag{1.11}$$
$$\frac{\partial u}{\partial t}(x_i, t_j) \approx \frac{u_i^j - u_i^{j-1}}{k}. \tag{1.12}$$

The difference approximations given in (1.9)-(1.12) are of first-order accuracy in space and time direction. Second-order central difference schemes in space direction are given by the relations:

$$\frac{\partial u}{\partial x}(x_i, t_j) \approx \frac{u_{i+1}^j - u_{i-1}^j}{2h},$$
$$\frac{\partial^2 u}{\partial x^2}(x_i, t_j) \approx \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2}.$$

The same approach can be made to generate finite difference approximation of higher order derivative (see [84]).

1.6 Challenges and motivation

The significance of the generalized Caputo derivative defined in (1.1) lies in the fact that using different values of the weight function $\omega(t)$ may generate various known mathematical models available in literature, thus resulting in a unified study of different physical problems through a single model. For example, the tempered FDs ($\omega(t) = e^{-bt},\ b > 0$) exhibit the behavior of both the subdiffusion and the normal diffusion motions at different time limits. The mathematical model with such tempered kernel is also known as *transient anomalous diffusion*. The significance of tempered fractional Brownian motion in the field of stochastic process has been discussed in [25]. Thus, GTFDEs has great physical significance and is an interesting topic of research. But these fractional derivatives have memory effect and non-local property which creates complexity in finding the analytical solutions of these FDEs. Numerous researchers have developed different numerical techniques such as Finite Difference Methods (FDMs) [34, 80–83, 85], spectral methods [33, 35, 86–89], collocation methods [90–92], finite element methods [93–98], finite volume methods [99, 100], to solve FDEs of different kind. But, the major challenge in these numerical methods is to find a stable numerical solution with higher order of accuracy and higher order of convergence. This motivates us to develop stable and efficient numerical schemes with higher order of accuracy and higher order of convergence. In this thesis, we have considered three different models of GTFDEs, viz. linear GTFDEs model with Dirichlet boundary conditions, Non-linear GTFDEs with Dirichlet boundary conditions and linear GTFDEs model with Robin boundary conditions. We have designed unconditionally stable non-uniform L1 schemes for both the linear and non-linear GTFDEs models having smooth and non-smooth solutions. We have also designed a stable and robust L2 scheme with higher order of convergence for the linear GTFDEs model.

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1.7 Aim and outline

The aim of the thesis are:

- To develop stable and efficient higher order numerical schemes based on FDM technique for the generalized time-fractional diffusion equations having smooth and non-smooth solutions.
- To improve the order of convergence for non-smooth solutions by using non-uniform mesh grading such that the mesh is refined near $t = 0$ to handle the singularity near $t = 0$.
- To investigate the theoretical stability and convergence analysis for all the developed schemes in L_2-norm and L_∞-norm.
- To develop robust non-uniform L1 schemes for both the linear and non-linear GTFDEs with smooth and non-smooth solutions. In addition, to develop a higher order convergence L2 scheme for the linear GTFDEs model.

1.7.1 Outline

The main theme of this thesis is the development, analysis and the implementation of robust finite difference schemes for the GTFDEs problems. The work incorporated in this thesis is divided into five chapters.

- Chapter 1, consists of introduction to fractional calculus and generalized time-fractional diffusion equations. Then we give a brief literature review of the TFDEs and GTFDEs models. It also provides the motivation, objectives and the outline of the thesis.

- In Chapter 2, we designed the modified version of the L1 formula for the linear GTFDEs model with smooth and non-smooth solutions, on a non-uniform grid, and it is shown that for non-smooth solutions, this scheme presents a better or equivalent result than the uniform mesh.

- In Chapter 3, higher order L2 scheme is developed for the linear GTFDEs model with smooth solutions considering different classes of weighting function. The theoretical stability and convergence are established in the L_2-norm.

- In Chapter 4, we study, for the first time, the numerical solution for the non-linear GTFDEs model with smooth and non-smooth solutions. We use Taylor's series approximation method to linearize the non-linear reaction term.

- In Chapter 5, our goal is to design stable finite difference scheme for the GTFDEs model with Robin boundary conditions. The mesh refinement technique is used to handle the singularity of the non-smooth solutions.

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