Chapter 1

Introduction

1.1 A brief background

Calculus, a fundamental mathematical discipline, serves as a significant tool that forges interdisciplinary connections across a wide spectrum of scientific, engineering, economic, demographical, and rheological fields. Its utility is manifest in the diverse practical applications it offers, ranging from solving real-world problems like elucidating Newton's second law of motion, exploring Einstein's theory of general relativity, to deducing the rates of radioactive decay [12]. Nonetheless, the world is replete with natural phenomena exhibiting a memory effect, a characteristic that classical calculus is ill-suited to represent. Examples of such phenomena include human behavior, business dynamics, and the complex properties of viscoelastic materials, all of which remain beyond the purview of classical calculus [55]. Consequently, the emergence of fractional calculus became a significant development. In the subsequent part, we will provide insights into the origins and historical development of fractional calculus.

1.1.1 Fractional calculus

Fractional calculus introduces a theory that encompasses derivatives and integrals of arbitrary order, unifying and broadening the classical concept of differentiation and multiple integrations based solely on integer orders. It has gained significant attention in recent decades due to its applicability in a wide range of scientific, engineering, and mathematical disciplines. This emerging field represents a paradigm shift in classical calculus, offering a powerful framework for modeling and understanding complex systems exhibiting memory, non-locality, and hereditary properties. As we delve deeper into the realm of fractional calculus, we uncover a rich tapestry of theory and applications that have the potential to revolutionize the way we approach problems in science and engineering.

The roots of fractional calculus can be traced back to the late 17th century. However, during that period, most scientists and researchers were primarily engrossed in classical calculus, resulting in fractional calculus receiving relatively less attention. Its emergence in mathematical history is as old as classical calculus itself. September 30th holds significance as it marks the "birthday" of fractional calculus, dating back to 1695 when Leibnitz introduced notations $\frac{d^n}{dx^n}f(x)$ and $\int f(x)dx$. It was during this time that L'Hôpital posed a pivotal question to Leibnitz: *"What does the notation $\frac{d^n}{dx^n}f(x)$ mean when n equals $1/2$?"* In a letter bearing the date of September 30, 1695, Leibniz wrote to L'Hôpital, *"This is an apparent paradox from which, one-day useful consequences will be drawn"*.

The tautochrone (isochrone) problem posed by Abel [3], marked the earliest known instance of a problem formulated using fractional operators. Over time, fractional calculus has been established on solid theoretical ground by a cadre of celebrated mathematicians, among them Liouville, Grunwald, Riemann, Euler, Lagrange, Heaviside, and Fourier. The inaugural work entirely devoted to the study of fractional calculus was published by Oldham and Spanier in 1974 [84]. Podlubny's book [87], played a pivotal role in advancing the fundamental theory of fractional differential equations and its practical applications. For a more comprehensive understanding of this subject, inquisitive readers are encouraged to explore additional resources available in references [55, 60, 78].

1.1.2 Fractional partial differential equation

Partial differential equations (PDEs) play a pivotal role across numerous fields due to their ability to mathematically capture complex natural phenomena. These equations are employed in the modeling of diverse subjects, including the spread of waves and heat, fluid dynamics, population dynamics, financial instrument valuation, and even medical imaging. PDEs find applications in a wide spectrum of domains, from physics and engineering to economics, biology, and beyond, making them an indispensable tool for understanding and solving real-world problems.

A fractional partial differential equation (FPDE) is a specialized type of partial differential equation that involves fractional derivatives, encompassing non-integer orders. The non-local nature of fractional operators is of great interest in fractional calculus, benefiting diverse fields like biology [75], viscoelastic fluid [116], finance [29], signal processing [9, 98], electrochemical process [111], and others. Unlike traditional PDEs, FPDEs deal with derivatives of fractional order, often represented using fractional Laplacians. They are essential for modeling and understanding complex phenomena with anomalous diffusion behavior and power-law scaling. FPDEs are particularly useful in situations where standard integer-order derivatives are insufficient to describe intricate, non-Gaussian patterns of diffusion and transport. These equations find application in diverse fields, including physics, biology, finance, and materials science, providing a valuable framework for addressing intricate real-world problems [105]. The FPDEs presented here serve as the foundation for this thesis and contribute to the study of various other FPDEs.

1.1.2.1 Fractional reaction-diffusion equations

Reaction-diffusion equations (RDEs) are a class of partial differential equations that describe how the distribution of one or more chemical species changes over time due to two fundamental processes: diffusion, which causes the species to spread or disperse, and reaction, which accounts for the transformation of species when they interact with each other. These equations are used to model a wide range of natural phenomena, including chemical reactions [102], population dynamics [6], pattern formation in biological systems [115], and the behavior of complex systems like ecosystems, chemical reactors, and biological tissues. They have applications in various scientific and engineering fields, including chemistry, biology, ecology, and material science etc [6, 13, 77, 102, 115]. The general form of a one-dimensional reaction-diffusion equation is often represented as

$$\frac{\partial u(x,t)}{\partial t} + q(t)R(u(x,t)) = p(t)\frac{\partial^2 u(x,t)}{\partial x^2}, \tag{1.1}$$

where

- $\frac{\partial u}{\partial t}$ represents the rate of change of the concentration u with respect to time t.
- $q \geq 0$.
- $R(u)$ represents the reaction term, which may be either linear or non-linear, describing the effects of chemical reactions on the concentration u at a given point in space.
- $p > 0$ is the diffusion coefficient, governing the rate of diffusion.
- $\frac{\partial^2 u}{\partial x^2}$ is the second spatial derivative, indicating the spatial diffusion of u.

Fractional reaction-diffusion equations are a specialized class of partial differential equations that incorporate fractional derivatives to describe phenomena with non-integer order diffusion and chemical reactions. These equations are used to model complex processes where the behavior of a species or quantity is influenced by both fractional-order spatial diffusion and chemical reactions. Fractional derivatives of non-integer order are introduced to account for anomalous diffusion behavior, which may exhibit sub-diffusion or super-diffusion. These equations are particularly valuable for understanding phenomena with intricate spatial patterns, such as anomalous transport in porous media [6, 23], biological pattern formation [85], or the dynamics of complex systems. The specific form and behavior of fractional reaction-diffusion equations depend on the nature of the reactions involved and the fractional order of the derivatives used. They find applications in various scientific and engineering fields [6, 14, 23, 85, 97].

1.1.2.2 Fractional convection-diffusion equations

The convection-diffusion equation is a partial differential equation that combines two fundamental processes: convection, which represents the transport of a quantity by a moving fluid or medium, and diffusion, which accounts for the spreading or mixing of that quantity due to molecular or random motion. This equation is commonly used to describe various physical phenomena, such as the transport of heat, mass, or chemical species in fluid dynamics, environmental science, and engineering [10, 11, 44, 110]. The one-dimensional convection-diffusion equation is typically expressed as

$$\frac{\partial u(x,t)}{\partial t} + r(t)\frac{\partial u(x,t)}{\partial x} = p(t)\frac{\partial^2 u(x,t)}{\partial x^2}, \tag{1.2}$$

where

- $\frac{\partial u}{\partial t}$ represents the rate of change of the quantity u with respect to time t.
- r is the convection or advection velocity, indicating the speed and direction of the fluid flow.
- $\frac{\partial u}{\partial x}$ represents the spatial gradient of u in the x-direction.
- $p > 0$ is the diffusion coefficient, governing the rate of diffusion or spreading of u.
- $\frac{\partial^2 u}{\partial x^2}$ is the second spatial derivative, indicating the spatial diffusion of u.

This equation can be extended to higher dimensions, and it is frequently used in various fields to model the advection and diffusion of quantities such as heat, concentration of substances, or pollutants in fluid flow.

The fractional convection-diffusion equation is a partial differential equation that incorporates fractional derivatives to describe the combined effects of convection and diffusion in the transport of a quantity, where the fractional derivatives account for non-integer order behavior in the diffusion process.

The fractional convection-diffusion equation, with its numerous real-world applications, has led to groundbreaking research developments in a multitude of disciplines. In the field of environmental science, it facilitates precise modeling of the dispersion of pollutants in both air and water systems, playing a crucial role in the formulation of efficient pollution control strategies [21, 39]. In biomedical research, it contributes to our comprehension of drug diffusion in tissues and the dynamics of disease propagation among populations. [41, 48]. Furthermore, it serves a purpose in materials engineering by enhancing the optimization of heat and mass transfer in complex media, including porous materials and composite structures [53, 63, 125]. By using fractional derivatives, this equation becomes a valuable tool for understanding complex dynamics and anomalous diffusion behavior.

1.2 Mathematical preliminaries

Within this section, we provide a concise introduction to several crucial mathematical definitions that will serve as foundational concepts throughout the course of this study. Fractional derivatives, unlike their integer-order counterparts, exhibit a wide range of definitions used to characterize fractional differentiation. While these definitions often vary, they all share the common objective of preserving classical calculus properties. Further details on specific fractional derivative definitions can be found in references [55, 87].

Definition 1.2.1. Gamma function [87]

The Gamma function is defined by the integral

$$\Gamma(\mathcal{Z}) = \int_0^\infty t^{\mathcal{Z}-1} \exp(-t) dt. \tag{1.3}$$

The Gamma function exhibits several noteworthy properties, including

- It is denoted as $\Gamma(\mathcal{Z})$, defined, and exhibits analytic behavior within the domain where $Re(\mathcal{Z}) > 0$.
- $\Gamma(\mathcal{Z}+1) = \mathcal{Z}\Gamma(\mathcal{Z})$.
- $\Gamma(n+1) = n!$, for $n \in \{0\} \cup \mathbb{N}$.

- The complex analytical continuation of $\Gamma(\mathcal{Z})$ extends its meromorphic behavior across the entire plane, marked by the presence of simple poles at non-positive integer values.

Definition 1.2.2. Prabhakar function

For any $\mathcal{Z} \in \mathbb{C}$, the Prabhakar function or the three-parameter Mittag-Leffler function is defined as

$$E^{\eta}_{\beta,\alpha}(\mathcal{Z}) = \sum_{k=0}^{\infty} \frac{\Gamma(\eta + k)\mathcal{Z}^k}{\Gamma(\eta)\Gamma(\beta k + \alpha)k!}, \tag{1.4}$$

where β, α, $\eta \in \mathbb{C}$, and Re$(\beta)> 0$.

- When η is set to 1, it simplifies into the two-parameter Mittag-Leffler function as follows

$$E^{1}_{\beta,\alpha}(\mathcal{Z}) = \sum_{k=0}^{\infty} \frac{\Gamma(1 + k)\mathcal{Z}^k}{\Gamma(\beta k + \alpha)k!} = \sum_{k=0}^{\infty} \frac{\mathcal{Z}^k}{\Gamma(\beta k + \alpha)} = E_{\beta,\alpha}(\mathcal{Z}). \tag{1.5}$$

- When η and α are set to 1, it simplifies into the one-parameter Mittag-Leffler function as follows

$$E^{1}_{\beta,1}(\mathcal{Z}) = \sum_{k=0}^{\infty} \frac{\Gamma(1 + k)\mathcal{Z}^k}{\Gamma(\beta k + 1)k!} = \sum_{k=0}^{\infty} \frac{\mathcal{Z}^k}{\Gamma(\beta k + 1)} = E_{\beta}(\mathcal{Z}). \tag{1.6}$$

- When all the three parameters η, α and β are set to one then it simplifies into the exponential function as follows

$$E^{1}_{1,1}(\mathcal{Z}) = \sum_{k=0}^{\infty} \frac{\Gamma(1 + k)\mathcal{Z}^k}{\Gamma(k + 1)k!} = \sum_{k=0}^{\infty} \frac{\mathcal{Z}^k}{k!} = \exp(\mathcal{Z}). \tag{1.7}$$

The Prabhakar function exhibits several noteworthy properties, including

- For $k \in \mathbb{N}$
$$\frac{d^k}{dt^k}\left[t^{\alpha-1}E^{\eta}_{\beta,\alpha}\left(\kappa t^{\beta}\right)\right] = t^{\alpha-k-1}E^{\eta}_{\beta,\alpha-m}\left(\kappa t^{\beta}\right), \tag{1.8}$$
where $\beta, \alpha, \kappa, \eta \in \mathbb{C}$, and $t \in \mathbb{R}^+$.

- $$\int_0^t \tau^{\alpha-1}E^{\eta}_{\beta,\alpha}\left(\kappa\tau^{\beta}\right)d\tau = t^{\alpha}E^{\eta}_{\beta,\alpha+1}\left(\kappa t^{\beta}\right), \tag{1.9}$$
where $\beta, \alpha, \kappa, \eta \in \mathbb{C}$, and $t \in \mathbb{R}^+$.

1.2.1 Basic definitions of fractional operators

Let $[t_0, T] \subset \mathbb{R}$ be a finite interval, and function $f \in L^1[t_0, T]$.

Definition 1.2.1.1. Riemann–Liouville fractional integral

For the function f, the left and right Riemann–Liouville integrals with a fractional order $\alpha \in \mathbb{R}^+$ can be defined as follows

$$ {}^{RL}_{t_0}D^{-\alpha}_{t}f(t) = \frac{1}{\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}f(\tau)d\tau, \quad t > t_0, \tag{1.10}$$

and

$$ {}^{RL}_{t}D^{-\alpha}_{T}f(t) = \frac{1}{\Gamma(\alpha)}\int_{t}^{T}(\tau-t)^{\alpha-1}f(\tau)d\tau, \quad t < T, \tag{1.11}$$

respectively, where $\Gamma(.)$ denotes the Gamma function.

Definition 1.2.1.2. Riemann–Liouville fractional derivative

For the function f, the left and right Riemann–Liouville derivatives with a fractional order $\alpha > 0$ can be defined as follows

$$\begin{aligned} {}^{RL}_{t_0}D^{\alpha}_{t}f(t) &= \frac{d^k}{dt^k}\left({}^{RL}_{t_0}D^{-(k-\alpha)}_{t}f(t)\right) \\ &= \frac{1}{\Gamma(k-\alpha)}\frac{d^k}{dt^k}\int_{t_0}^{t}(t-\tau)^{k-\alpha-1}f(\tau)d\tau, \quad t > t_0, \end{aligned} \tag{1.12}$$

and

$$
\begin{aligned}
{}_{t}^{RL}D_T^{\alpha} f(t) &= (-1)^k \frac{d^k}{dt^k}\left({}_{t}^{RL}D_T^{-(k-\alpha)} f(t)\right) \\
&= \frac{(-1)^k}{\Gamma(k-\alpha)} \frac{d^k}{dt^k} \int_t^T (\tau - t)^{k-\alpha-1} f(\tau) d\tau, \quad t < T,
\end{aligned} \tag{1.13}
$$

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

Definition 1.2.1.3. Caputo fractional derivative

For the function f, the left and right Caputo derivative with a fractional order $\alpha > 0$ can be defined as follows

$$
\begin{aligned}
{}_{t_0}^{C}D_t^{\alpha} f(t) &= {}_{t_0}^{RL}D_t^{-(k-\alpha)} \left(\frac{d^k f(t)}{dt^k}\right) \\
&= \frac{1}{\Gamma(k-\alpha)} \int_{t_0}^t (t - \tau)^{k-\alpha-1} f^{(k)}(\tau) d\tau, \quad t > t_0,
\end{aligned} \tag{1.14}
$$

and

$$
{}_{t}^{C}D_T^{\alpha} f(t) = \frac{(-1)^k}{\Gamma(k-\alpha)} \int_t^T (\tau - t)^{k-\alpha-1} f^{(k)}(\tau) d\tau, \quad t < T, \tag{1.15}
$$

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

In the subsequent subsections, additional significant definitions of fractional operators are provided.

1.2.1.1 Generalized fractional operators

Generalized fractional operators incorporate two key components: a scale function denoted as $z(t)$ and a weight function represented as $\omega(t)$. These derivatives can be described in following ways [4, 5]:

Definition 1.2.1.1.1. Generalized fractional integral

For the function $f(t) \in (t_0, T)$, the left/forward generalized fractional integral of order $\alpha > 0$, with respect to the scale function $z(t)$ and weight function $\omega(t)$ is as follows

$$ {}_{t_0}D^{-\alpha}_{t;[z;\omega]}f(t) = \frac{[\omega(t)]^{-1}}{\Gamma(\alpha)} \int_{t_0}^{t} \frac{\omega(\tau)z'(\tau)f(\tau)}{[z(t)-z(\tau)]^{1-\alpha}} d\tau, \quad t > t_0, \tag{1.16} $$

provided the integral exists.

Definition 1.2.1.1.2. Generalized fractional derivative

For the function $f(t) \in (t_0, T)$, the left/forward generalized fractional derivative of order k, with respect to a scale function $z(t)$ and a weight function $\omega(t)$, is defined as

$$ {}_{t_0}D^{k}_{t;[z;\omega]}f(t) = [\omega(t)]^{-1} \left[\left(\frac{1}{z'(t)} \frac{d}{dt} \right)^{k} (\omega(t)z(t)) \right], \quad t > t_0, \tag{1.17} $$

under the condition that the equation's right side remains finite, with k representing a positive integer.

Definition 1.2.1.1.3. Generalized fractional derivative of Riemann-Liouville type

For the function $f(t) \in (t_0, T)$, the left/forward generalized fractional derivative of Riemann type, of order $\alpha > 0$ is defined as

$$ {}^{R}_{t_0}D^{\alpha}_{t:[z,\omega]}f(t) = {}_{t_0}D^{k}_{t;[z;\omega]}\,{}_{t_0}D^{-(k-\alpha)}_{t;[z;\omega]}f(t), \tag{1.18} $$

under the condition that the equation's right side remains finite, with $k-1 < \alpha < k$, $k \in \mathbb{Z}^{+}$.

Definition 1.2.1.1.4. Generalized fractional derivative of Caputo type

For the function $f(t) \in (t_0, T)$, the left/forward generalized fractional derivative of Caputo type, of order, $\alpha > 0$ is defined as

$$ {}^{C}_{t_0}D^{\alpha}_{t:[z,\omega]}f(t) = {}_{t_0}D^{-(k-\alpha)}_{t;[z;\omega]}\,{}_{t_0}D^{k}_{t;[z;\omega]}f(t), \tag{1.19} $$

under the condition that the equation's right side remains finite, $k-1<\alpha<k$, $k\in\mathbb{Z}^+$.

The Definitions 1.2.1.1.1-1.2.1.1.4 provided above exclusively pertain to the "left/-forward" interpretation of generalized fractional integrals and generalized fractional derivatives. Just as in the case of classical fractional integrals and fractional derivatives, it's worth noting that these can also be defined in the "right/backward" context.

The functions $z(t)$ and $\omega(t)$ are sufficiently effective for the purpose. The scale function $z(t)$ enables adjustments within the given domain. Sometimes there are situations where the results are temporary and only last for a period of time. In those cases we use a stretching scale function. Conversely, there are also situations where the process unfolds over the course of several decades, and in these cases, a contracting scale function becomes necessary. However, by incorporating the weight function $\omega(t)$, one can effectively expand the kernel in fractional operators, resulting in a greater scope for flexibility in the modeling process. When it comes to modeling the memory of specific diffusion processes, there can be a demand for a significant focus on the current time point, while other diffusion processes might necessitate a stronger emphasis on past events. Utilizing a weight function can be advantageous when tackling these tasks. By choosing alternative scale and weight functions, it's possible to derive a range of diverse generalized fractional derivatives and integrals. The incorporation of generalized fractional derivatives and integrals in fractional differential equations serves to elevate the model's attractiveness and utility [4, 5].

1.2.1.2 Prabhakar fractional operators

Prabhakar fractional operators are characterized by the inclusion of the Mittag-Leffler function, as given in equation (1.4), featuring three parameters.

Definition 1.2.1.2.1. Prabhakar integral

Prabhakar integral of a function $f \in L^1[t_0, T]$ $(-\infty < t_0 < t < T < \infty)$ of order α is defined as

$$I^{\eta}_{\beta,\alpha,\kappa,t_0} f(t) = \int_{t_0}^{t} (t-\tau)^{\alpha-1} E^{\eta}_{\beta,\alpha}\{\kappa(t-\tau)^{\beta}\} f(\tau) d\tau, \tag{1.20}$$

where $\beta, \alpha, \kappa, \eta \in \mathbb{C}$, and $\mathrm{Re}(\beta)$, $\mathrm{Re}(\alpha) > 0$.

Definition 1.2.1.2.2. Riemann-Liouville Prabhakar derivative

The Riemann-Liouville Prabhakar derivative of a function $f \in L^1[t_0, T]$, $(-\infty < t_0 < t < T < \infty)$ of order α $(k-1 < \mathrm{Re}(\alpha) < k)$ is defined as

$${}^{RLP}_{\quad t_0}D^{\eta}_{\beta,\alpha,\kappa} f(t) = \frac{d^k}{dt^k} \int_{t_0}^{t} (t-\tau)^{k-\alpha-1} E^{-\eta}_{\beta,k-\alpha}\{\kappa(t-\tau)^{\beta}\} f(\tau) d\tau, \tag{1.21}$$

where $\beta, \alpha, \kappa, \eta \in \mathbb{C}$.

Definition 1.2.1.2.3. Caputo-Prabhakar derivative

The Caputo-Prabhakar derivative of a function $f \in AC^k[t_0, T]$, $(-\infty < t_0 < t < T < \infty)$ of order α $(k-1 < \mathrm{Re}(\alpha) < k)$ is defined as

$${}^{CP}_{\ t_0}D^{\eta}_{\beta,\alpha,\kappa} f(t) = \int_{t_0}^{t} (t-s)^{k-\alpha-1} E^{-\eta}_{\beta,k-\alpha}\{\kappa(t-\tau)^{\beta}\} f^k(\tau) d\tau, \tag{1.22}$$

where $\beta, \alpha, \kappa, \eta \in \mathbb{C}$.

1.3 Literature review

This section offers a summary of the research findings found in the existing literature pertaining to the numerical handling of fractional derivatives and different classes of fractional partial differential equations, which will be elaborated upon in the forthcoming chapters of this thesis.

1.3.1 Generalized fractional derivative and generalized fractional differential equations

In the literature, various definitions of fractional derivatives exist, including the Riemann-Liouville derivative, Grunwald-Letnikov derivative, Caputo derivative, Riesz derivative, and the regularized Ψ-Hilfer fractional derivative, etc. [45, 55, 78]. These definitions have held a prominent position within the field of fractional calculus and have been effectively applied to simulate many physical phenomena. Various methods used for generalizing fractional integrals (or derivatives) from their integer counterparts can lead to non-uniqueness. In order to bring together the various procedures, Agrawal introduced a new derivative known as the Generalized Fractional Derivative (GFD) [4]. This GFD unifies well-known fractional derivatives, including the Riemann-Liouville, Caputo, modified Erdélyi-Kober, and Hadamard derivatives. Analytical solutions for problems involving GFDs are challenging, except for a small class of problems [56, 119]. Xu et al. offer both numerical and analytical solutions for a novel generalized fractional diffusion equation [119]. Several groundbreaking studies [66–68, 118, 120] have made significant contributions to the numerical solution of various generalized fractional problems.

The majority of previous studies have focused on the diffusion model problem without the inclusion of a reaction term and with the assumption of a constant diffusion coefficient. Hence, it becomes necessary to explore a more generalized problem that includes variable coefficients. Additionally, they employed a second-order central difference scheme to discretize the spatial variable. Therefore, the fully discrete schemes produced are of lower-order accuracy. As a result, there is a clear need to develop high-order numerical schemes for addressing these problems.

1.3.2 Prabhakar fractional derivative and fractional differential equations defined in Prabhakar sense

Swedish mathematician Mittag-Leffler introduced the Mittag-Leffler function while working on summation techniques for divergent series [79, 80]. In 1953, Humbert et al. expanded the definition with an additional parameter [42, 43]. Prabhakar [88] introduced an extension of the Mittag-Leffler function with three parameters, and this function has come to be known as the "Prabhakar function", bearing his name.

The Prabhakar function was employed as a kernel by Kilbas et al. [55], Garra et al. [31], and Prabhakar [88] to extend the fractional Caputo (or Riemann-Liouville) derivative and Riemann-Liouville integral to Prabhakar fractional derivatives and integrals. In the modern era, these fractional order operators have become a focal point of interest, offering versatile solutions to address real-world problems in a variety of scientific domains. These operators can elucidate phenomena such as the fractional Poisson process [31], generalized Langevin equations [96], and the anomalous relaxation behavior observed in Havriliak-Negami models [76, 86], as well as the fractional Maxwell model in linear viscoelasticity [33], etc. For an in-depth exploration of the extensive history and practical applications of Prabhakar fractional calculus, we recommend readers to refer to the survey paper [34]. Theoretical aspects of these operators have received extensive attention in the literature. Although there are a few studies offering numerical approximations for such equations [8, 27, 28, 101], their availability remains limited. Hence, there is a pressing need to devise new approximation techniques for Prabhakar derivatives and employ them to tackle fractional differential equations that incorporate these derivatives.

1.3.3 Caputo time-fractional reaction–diffusion equations with smooth and non-smooth solutions

The study of numerical approximation methods for solving time-fractional reaction-diffusion equations (TFRDE) has been widely acclaimed among researchers. Numerous studies, including the residual power series method, domain decomposition method, and exponential B-spline collocation method [35, 36, 47, 109], have been employed to solve TFRDE. Several alternative approaches are also available for approximating the TFRDE, including the meshless method, the mixed finite element method, and the operational matrix method [1, 2, 26, 59, 72, 94]. But in these studies, the initial layer at $t = 0$ is often neglected, and convergence analyses are conducted with the assumption that the solution exhibits smooth behavior across the entire closed domain. To address this challenge and enhance the effectiveness of numerical methods, the use of time-graded meshes has been explored in [103]. The authors applied the central difference scheme in the spatial direction. However, it's worth noting that the bound derived in the convergence theorem is termed "α-nonrobust" because the right-hand side becomes infinite as α approaches 1. Furthermore, graded meshes have been employed in prior studies [15, 17, 19, 49] to enhance the performance and obtain better results for different classes of fractional differential equations. Consequently, there is a necessity to devise numerical schemes for the TFRDE that take into account the non-smooth characteristics of the solution while also achieving α-robust convergence analysis.

1.3.4 Non-linear Caputo time-fractional reaction–diffusion equations with smooth and non-smooth solutions

Non-linear time-fractional reaction diffusion equations (TFRDE) have been a focal point of research for numerical approximation techniques. Li and Zhang [61] introduced a linearized finite difference scheme for non-linear time-fractional parabolic problems with second-order spatial accuracy and first-order temporal accuracy. Li et al. [62] introduced a linearized Galerkin finite element method for the solution of non-linear TFRDE. Their method achieved a temporal accuracy of the first order. Additional methodologies have also been employed to tackle non-linear time-fractional diffusion models [37, 74, 112, 122]. These mentioned schemes, which rely on uniform meshes, might encounter challenges when dealing with the singularity that emerges in the solution at $t = 0$. So, we need to design a numerical scheme that can perform well in real-world situations, even when the solution isn't perfectly smooth. In [103], the utilization of a time-graded mesh was introduced in overcoming this challenge, leading to notable improvements in the efficiency of numerical techniques for non-smooth data. This approach has been subsequently adopted in [18, 32, 99, 107]. Nevertheless, it is worth noting that studies dedicated to the numerical approximations of non-linear TFRDE with non-smooth solutions remain relatively scarce. In [92], a linearized scheme is described that combines L1 time discretization with finite element spatial discretization, achieving second-order spatial convergence and α-order temporal convergence. Jin et al. [46] presented two finite element schemes: one utilizing the L1 method and the other employing convolution quadrature via a backward difference scheme in time. Both schemes demonstrated α-order accuracy in time and second-order accuracy in space. Therefore, it should be noted that the existing numerical schemes for solving non-linear TFRDE with non-smooth solutions lack a satisfactory order of convergence in both space and time. Consequently, this presents an opportunity to develop a numerical method that can surpass the spatial and temporal convergence orders of the current ones [46, 92, 126].

1.3.5 Two-dimensional time-fractional convection-diffusion equations with smooth and non-smooth solutions

A diverse array of numerical methods has been developed for solving two-dimensional time-fractional convection-diffusion equations (TFCDE). Cui [24] introduced a compact exponential ADI scheme that solves two-dimensional TFCDE numerically. Chen and Liu [20] proposed a novel technique for solving the two-dimensional fractional advection-dispersion equation, employing a combination of the ADI-Euler method and extrapolation method. Several other approaches are also available to approximate the TFCDE, including the Padé approximation, compact scheme, meshless method, and mixed finite element method [108, 113, 117, 123]. The previously mentioned methods, which are constructed using uniform grids, might not effectively handle the singularity in the solution occurring at $t = 0$. As a result, there is a pressing requirement to develop a numerical approach that can operate effectively in real-world situations where the solution may not exhibit the expected level of smoothness. The use of fitted meshes has become a potent tool for successfully addressing the singularity displayed by the solution. This powerful method has brought about a revolution in the field by elevating the precision and efficiency of numerical techniques when dealing with problems featuring singularities [15, 17–19, 99, 103].

Although nonuniform graded meshes have been explored in certain studies [89, 93], the attained temporal convergence order continues to be somewhat low. Crucially, we have not encountered any numerical technique that achieves high orders of convergence in both spatial and temporal dimensions for two-dimensional TFCDE with non-smooth solutions.

1.4 Challenges and motivations

The definition of fractional derivatives is notably less straightforward than that of classical calculus. For the past few decades, both theoretical and experimental research have been ongoing to establish a precise definition that aligns with the fundamental principles of derivatives. The Caputo derivative and Riemann-Liouville derivative are widely recognized and extensively utilized definitions in the field of fractional calculus [87]. Recently, these definitions have been broadened by researchers to encompass a range of important scientific phenomena, including viscoelasticity and electromagnetic systems.

In 2012, Agrawal made notable contributions by offering generalized definitions for fractional integrals and derivatives [4, 5]. The introduction of these new definitions relied on the utilization of scale functions and weight functions. Consequently, the development and analysis of high-order numerical methods for fractional problems that incorporate these derivatives pose a significant challenge. Furthermore, Kilbas et al. in their work [55], along with Garra et al. [31], and Prabhakar [88], made use of the Prabhakar function as a fundamental component, leading to the development and exploration of Prabhakar fractional derivatives. These derivatives have garnered the attention of researchers, prompting further investigation and exploration. Theoretical investigations into these derivatives have received considerable attention, but their numerical treatment has been comparatively less explored and utilized due to their somewhat intricate structure. There appears to be limited research in the numerical treatment of the Caputo-Prabhakar derivative, with only a single paper addressing this specific topic [101]. This motivation drives us to focus on this direction and introduce novel approximations for such derivatives.

Continuing ahead, as observed previously, the extensive incorporation of the Caputo time fractional derivative in numerous FPDEs is well-documented in the literature. However, it is important to highlight that the literature often falls short in adequately capturing a crucial behavior of the solution of such FPDEs. In these FPDEs, the presence of a Caputo time-fractional derivative with a fractional order between 0 and 1 introduces a distinctive feature known as an "initial layer". It means the solution near $t = 0$ exhibit non-smooth or singular behavior. In 2017, Stynes et al. have noted that solution v to these FPDEs exhibit the following derivative bound [103]

$$\left|\frac{\partial v}{\partial t}(x,t)\right| \leq c(1+t^{\alpha-1}), \quad \text{for all } t \in (0,T]. \tag{1.23}$$

It is evident from equation (1.23) that the derivative of the solution with respect to time blows up as $t \to 0^+$. Therefore, the presence of an initial layer makes it challenging to obtain a satisfactory numerical solution for these FPDEs using traditional numerical methods, as they often require a very fine mesh near the initial time $t = 0$ to resolve the layer. To address this challenge, the utilization of a time-graded mesh was first introduced in [103], leading to significant improvements in the efficiency of numerical techniques for handling non-smooth data. However, it is worth noting that studies dedicated to the numerical approximation of FPDEs incorporating Caputo time-fractional derivative with an initial singularity often exhibit relatively smaller convergence orders, both in the temporal and spatial directions.

High-order methods are always the center of attraction of the mathematics community as they produce good approximations with minimal computational cost. With numerous real-world applications, there is a growing demand for the development and analysis of high-order methods for many exciting and challenging time-fractional problems with non-smooth solution. Considerable efforts have been made in constructing and analyzing high-order methods for time-fractional problems with smooth solution. However, constructing and analyzing high-order methods for time-fractional problems with non-smooth solution is relatively less common. So, it is interesting and challenging to construct and analyze high-order methods based on non-uniform graded meshes for time-fractional problems.

1.5 Objective of the thesis

The literature review underscores a significant gap in research concerning new numerical approximations of Caputo Prabhakar time-fractional operator and high-order methods for solving linear and non-linear time-fractional partial differential equations, particularly when dealing with non-smooth solutions. In many complex real-world phenomena, fractional models provide accurate descriptions. However, in realistic scenarios, it is not always feasible to assume that the solutions of such models exhibit sufficient smoothness. This challenge underscores the need for advanced high-order numerical methods capable of handling fractional partial differential equations with both smooth and non-smooth solutions. While numerous research papers are available in which fractional partial differential equations have been solved numerically, they often rely on unrealistic assumptions, assuming that the solution is mostly smooth. Moreover, the work, where non-smooth behavior has been considered lacks high-order convergence in both time and space directions. These gaps in literature have spurred our motivation to contribute to this area.

To fulfill this purpose, we have systematically considered the following important classes of fractional partial differential equations throughout the thesis.

(i) Generalized variable coefficients fractional reaction–diffusion equations.

(ii) Time-fractional reaction-diffusion equation defined in Caputo Prabhakar sense.

(iii) Caputo time-fractional reaction-diffusion equations with smooth and non-smooth solutions.

(iv) Non-linear Caputo time-fractional reaction-diffusion equations with non-smooth solutions.

(v) Two-dimensional time-fractional convection-diffusion equations with non-smooth solutions.

Overall, the primary objective of this thesis is to develop and analyze high-order numerical methods for various classes of fractional problems, encompassing both smooth and non-smooth solutions. In brief, in the first two upcoming chapters, our focus is on smooth solutions, while in the following chapters, we shift our attention to exploring the non-smooth behavior of the solutions. Moreover, the thesis will not only focus on the formulation of these numerical methods but also on their theoretical analysis, which includes a thorough discussion of stability and convergence of developed methods. In addition, numerical outcomes support the theoretical findings.

1.6 Outline of the thesis

We continue with a few words about the structure of the thesis. The thesis is structured into six chapters, each containing distinct components of the research work. Now, let us briefly describe the material included in the thesis.

Chapter 1 serves as the introduction to the thesis. Fundamental definitions, used consistently in the thesis, are brought together in this chapter. This chapter also provides an in-depth review of the historical progress made in the field of fractional problems and their numerical treatment. It also includes a concise literature survey related to the problems addressed in the thesis, along with a presentation of the thesis objectives.

Chapter 2 focuses on developing and analyzing two high-order schemes, $\text{CFD}_{g-\sigma}$ and $\text{PQS}_{g-\sigma}$, for solving generalized variable coefficients fractional reaction-diffusion equations. These schemes use the $(3-\alpha)$th order Generalized Alikhanov's formula $(gL2-1_\sigma)$ to approximate the generalized time-fractional derivative of Caputo type, with α representing the order of the GFD. $\text{CFD}_{g-\sigma}$ employs a fourth-order compact difference operator, while $\text{PQS}_{g-\sigma}$ utilizes a parametric quintic spline scheme for spatial discretization. The stability and convergence analysis of both schemes are demonstrated thoroughly using the discrete energy method in the $\mathcal{L}_2$-norm. Numerical results align well with the proposed theory.

Chapter 3 is devoted to constructing and analysing two new approximations (CPL2-1_σ and CPL-2 formulas) for the Caputo-Prabhakar fractional derivative. The newly developed approximations are then used in the numerical treatment of a reaction-diffusion problem with variable coefficients defined in the Caputo-Prabhakar sense. Moreover, the space variable in the developed numerical schemes, CFD_1 and CFD_2, is discretized using a fourth-order compact difference operator. Both schemes' stability and convergence analysis are demonstrated thoroughly using the discrete energy method. Numerical results are consistent with our theoretical findings.

Chapter 4 aims to develop and analyze a robust fully discrete scheme for solving time-fractional reaction-diffusion equations with both smooth and non-smooth solutions. The method combines the L1 scheme for time discretization on uniform or graded meshes with a cubic spline difference scheme on a uniform mesh for spatial discretization. It incorporates a graded mesh in time to address the initial layer at $t = 0$. The chapter provides separate stability and convergence analyses for both smooth and non-smooth solutions. Two test problems are presented to validate the proposed method, one featuring a smooth solution and the other a non-smooth solution.

Chapter 5 introduces a high-order non-polynomial spline method for non-linear time-fractional reaction-diffusion equations with non-smooth solutions. This method combines the L2-1_σ scheme on a graded mesh to approximate the Caputo fractional derivative and utilizes a parametric quintic spline for spatial discretization. The chapter demonstrates the solvability, stability, and convergence of the scheme and provides numerical results supporting the theory.

Chapter 6 introduces an innovative high-order numerical method for solving the two-dimensional time-fractional convection-diffusion equation with non-smooth solutions. This approach combines Alikhanov's high-order scheme (L2-1_σ) for Caputo time-fractional derivative discretization on a non-uniform fitted mesh with a high-order two-dimensional compact difference operator on a uniform mesh for spatial discretization. The system is efficiently solved using a robust two-step Alternating Direction Implicit (ADI) approach. The chapter includes a comprehensive theoretical analysis, focusing on convergence and stability, employing Fourier analysis.

It also presents numerical results, in the form of graphs and tables, validating the proposed theory.