1.1 Background

1.1.1 Fractional calculus

Calculus is a fundamental branch of mathematics concerned with the calculation of instantaneous rates of change (differential calculus) and the accumulation of infinitely small quantities to determine a whole (integral calculus). This powerful area of study was independently developed in the 17th century by Isaac Newton and Gottfried Wilhelm Leibniz. Over time, calculus has become a cornerstone in nearly every scientific and engineering discipline, including economics, demography, and rheology. Its applications are vast ranging from modeling radioactive decay to explaining Newton's second law of motion and even underpinning Einstein's theory of general relativity. However, many natural phenomena-such as human behavior, business trends, and viscoelastic materials-exhibit memory effects that traditional calculus cannot effectively model. This is where fractional calculus becomes essential. Fractional calculus extends classical calculus by generalizing its concepts, much like how real numbers are extended to complex numbers or factorials to non-integer values. The meaning of the extension in generalized integration and differentiation is that: Can we extend the meaning of derivatives of integral order $d^n y/dx^n$, where n is an integer, to the derivatives of non-integral order *i.e.* $d^n y/dx^n$, where n is any number fractional, irrational or complex? Leibniz was the first to propose this extension. It may have begun as a clever manipulation of symbols when L'Hospital posed the question to Leibniz, "What if n equals 1/2?" In 1695, Leibniz responded, "It will lead to a paradox." However, he insightfully added, "From this apparent paradox, useful results will one day emerge."

Referring to Wallis's infinite product for $\pi/2$, in 1697, Leibnitz used the notation $d^{1/2}y$ and noted that the same outcome could have been obtained through the use of differential calculus. The concept of a derivative of arbitrary order was mentioned for the first time in a text in 1816 by S. F. Lacroix, [2], a French mathematician, in his 700-page text on differential and integral calculus, he dedicated less than two pages to this topic. Lacroix started with $y = x^n$, n being a positive integer, and found the m^{th} derivative as

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

Lacroix used Legendre's symbol Γ denoting the generalized factorial, and replaced m by $1/2$ and n by any positive real number a, following the typical classical formalists of the period, established the below formula:

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

which represents the derivative of arbitrary order $1/2$ of the function x^a. For an example with $y = x$, obtained

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

This corresponds to the result obtained using the current Riemann–Liouville definition of a fractional derivative. It was 279 years after L'Hospital first raised the question before a dedicated text on the topic appeared [3]. Although eminent mathematicians like Fourier and Euler discussed arbitrary-order derivatives, they did not present any concrete examples or practical uses. Niels Henrik Abel deserves recognition for the first application made in 1823 [4]. For the first time, Abel employed fractional calculus to solve an integral equation that emerged in the formulation of the tautochrone problem, also referred to as the isochrone problem [5]. This problem

involves determining the shape of a frictionless wire in a vertical plane such that a bead sliding along it always takes the same amount of time to reach the lowest point, regardless of its starting position. In contrast, the brachistochrone problem seeks the path that minimizes the time of descent. The first major work on fractional calculus was carried out by Oldham and Spanier and published in 1974 [3]. The development of fractional calculus has been significantly shaped by the contributions of several renowned mathematicians, including N. H. Abel, B. Riemann, J. Liouville, H. Weyl, G. W. Leibniz, A. K. Grünwald, A. V. Letnikov, and J. Caputo.

Fractional calculus (FC) is widely applied in physics [6, 7], finance [8, 9], statistics [10], hydrology [11, 12], Brownian motion, entropy etc. It is now well known that several fractional derivatives e.g. Caputo derivative, Riemann Liouville (RL) derivative, Riesz derivative, Atangana-Baleanu fractional derivative, Caputo-Fabrizio derivative etc. are used to analyze various physical, chemical and biological phenomena. The most frequently used derivatives are the Riemann-Liouville and the Caputo derivatives, and which commonly employed to describe various physical processes into time-fractional partial differential equations (TFPDEs) [13]. Compared to the integer-order derivatives, the fractional derivative, which simultaneously possesses memory, can describe various nonlinear phenomena more effectively [14, 15]. In consideration of this, the FC is an effective tool to simulate complicated dynamical systems [16, 17]. Readers can refer to [18–20] for a detailed discussion.

1.1.2 Fractional partial differential equation

Partial differential equations (PDEs) play a fundamental role in modeling natural phenomena and appear across nearly all scientific disciplines, including finance, biology, ecology, medicine, sociology, aerospace and naval engineering, nuclear reactors,

combustion processes, electricity production and distribution, and traffic control. Derivatives of non-integer (arbitrary) order are commonly referred to as fractional derivatives (FDs). Partial differential equations that involve fractional derivatives are known as fractional partial differential equations (FPDEs). FPDEs are partial differential equations that involve FDs. The nonlocal nature of fractional operators has generated significant interest in the field of fractional calculus, as it offers a powerful framework for modeling complex natural phenomena. Applications include biological systems [21], control theory [22], finance [23], signal and image processing [24, 25], sub-diffusion and super-diffusion process [26], viscoelastic fluid [27], electrochemical process [28], and many more. The primary advantage of fractional differential equations (FDEs) lies in their ability to effectively model systems with memory, long-range interactions, and hereditary properties-capabilities that are difficult to achieve using classical differential equations [29, 30].

Ludwig Boltzmann was the first to mathematically describe processes with memory in 1874 and 1876 [31, 32]. In this context, 'memory' refers to the property of a system where the output depends not only on the current input but also on the history of input changes over a finite or infinite time interval. Such behavior can be characterized using memory functions, which serve as the kernel of integro-differential operators-specifically, the power-law memory functions used in fractional calculus. This highlights a key advantage of fractional differential equations (FDEs) over classical integer-order differential equations, which are only locally defined and thus inadequate for modeling systems with memory. In contrast, non-integer-order derivatives, despite violating the classical Leibniz rule, allow for the representation of memory effects. As a result, fractional integro-differential equations are widely used in continuous-time models across various areas of physics to describe memory-dependent processes. Various applications of FDEs in real-world problems across

different fields are discussed in [33].

1.1.3 Variable-order fractional derivatives and its applications

The constant-order fractional calculus framework is capable of modeling various important physical phenomena. However, certain complex behaviors cannot be accurately captured using constant-order models—particularly when the fractional order depends on independent variables. For example, protein reaction kinetics have shown relaxation mechanisms that are best described by a temperature-dependent fractional order. Similarly, diffusion processes in porous media may require variable-order formulations, as the structure of the medium or external fields can evolve over time. The one-dimensional diffusion equation with a constant fractional order can be expressed as follows [34]. Let $L > 0,\ T > 0,$

$$D_0^{\alpha} C(\xi,\eta) = \frac{\partial^2 C(\xi,\eta)}{\partial \xi^2} + f(\xi,\eta), \qquad 0 < x < L, 0 < t \leq T, \tag{1.1}$$

with initial and boundary conditions

$$\begin{cases} C(\xi,0) = G(\xi), \quad 0 < \xi < 1, \\ C(0,\eta) = C(L,\eta) = 0, \quad 0 \leq \eta \leq T, \end{cases} \tag{1.2}$$

where $0 < \alpha < 1$ and D_{η}^{α} denotes the constant order time-fractional derivatives. In many diffusion processes, the diffusion behavior evolves over time. As an alternative modeling approach, a time-dependent variable-order model is more suitable for capturing such dynamics. The time-fractional diffusion equation with variable order

can be expressed as follows [35]:

$$D_0^{\alpha(\xi,\eta)} C(\xi,\eta) = \frac{\partial^2 C(\xi,\eta)}{\partial \xi^2} + f(\xi,\eta), \qquad 0 < x < L, 0 < t \leq T, \tag{1.3}$$

with initial and boundary conditions

$$\begin{cases} C(\xi,0) = G(\xi), \quad 0 < \xi < 1, \\ C(0,\eta) = C(L,\eta) = 0, \quad 0 \leq \eta \leq T, \end{cases} \tag{1.4}$$

where, $D_0^{\alpha(\xi,\eta)} C(\xi,\eta)$ denotes the variable-order time-fractional derivative in variable $\alpha(\xi,\eta)$. In science and engineering, many physical problems exist that are governed by variable-order fractional operators [36] such as anomalous diffusion models [37], viscoelastic mechanics [38], control systems [39], petroleum engineering [40, 41], and many others.Many dynamic processes exhibit fractional-order behavior that varies with time or space, making variable-order calculus a natural and effective mathematical framework for modeling complex dynamical systems. To address such cases, the concept of constant-order fractional derivatives is extended to space- and time-dependent fractional derivatives, leading to the formulation of variable-order (VO) Caputo fractional derivatives. Several definitions of VO derivatives have been proposed in the literature, including the VO Caputo derivative, Coimbra derivative, Caputo–Fabrizio derivative, and the Grunwald–Letnikov derivative [36]. Several numerical methods are extensively utilized for solving the VO PDEs like the Crank-Nicolson difference scheme [42], Operational Matrix method [43–46], Finite difference method, Collocation method [47], Galerkin method [48, 49] and so on. The optimal order finite difference/ local discontinuous Galerkin method presented by L. Wei [49]. G. Diaz et al. [50] investigated the dynamics and control of nonlinear viscoelastic oscillators using VO operators. Similarly, Ingman et al. [51] employed time-dependent

VO operators to model viscoelastic deformation. These fractional differential operators are essential for formulating both constant-order and VO mathematical models. We have outlined several key foundational concepts in the introduction section in order to set the stage for the objectives of this thesis.

1.1.3.1 Variable-order reaction sub-diffusion equations

In 1993, Samko and Ross [52] introduced the concept of the VO integral and differential and some basic properties of these operators. The outcomes of the VO fractional operators research were summarized by Lorenzo and Hartley [53, 54] and they looked into the various definitions of VO fractional operators. The order of the VO fractional derivatives either depends on space [37] or time [52, 55] or both [56, 57]. Recently, several scholars have investigated the accuracy of the variable order fractional calculus in describing complex physical models as compared to constant-order types [58, 59]. Coimbra has discussed the VO differential operators [38]. In [60], the authors derived the Feller semigroups using VO subordination. In [61], VO generating Feller semigroups have been used to investigate the pseudo-differential operators. The Markov processes have been classified by Kikuchi and Negoro [62] with this kind of VO pseudo-differential operator. In [63], Leopold talked about the merging of VO function spaces of differentiation into VO function spaces of integration.

Furthermore, the nonlocal characteristics of VO fractional operators reduce the cost of calculation and boost computation accuracy. Consequently, it is preferred to create some practical techniques to tackle such nonlinear systems involving the VO fractional derivatives, such as optimal control problems, diffusion equations and integro-differential equations [57]. However, up to now, only a few researchers have taken into consideration the numerical analysis of variable-order differential equations [64–68]. Since analytical solution of these variable order fractional differential

equations (VOFDE) are typically very challenging, we seek for the numerical solutions for VOFDE. This chapter consider a particular VOFDE called Variable order reaction-subdiffusion equation (VORSDE).

1.1.3.2 Variable order sub-diffusion partial differential equation

The number of scientific and engineering problems involving fractional calculus is growing and constantly rising. The fractional derivative is an efficient technique for describing memory and some transmitted properties of various materials and processes. This is one of the key advantages of fractional calculus. Many scientists have discovered a wide range of significant dynamical problems that exhibit fractional order characteristics that may vary over time or space. Due to non-local property and weak singularity of fractional derivatives, it is quite problematic or impossible to obtain analytical solutions for several fractional differential equations (FDEs). This motivates many researchers to develop some efficient and higher order numerical methods for solving FDEs [13, 22, 69]. In the past decades, several numerical methods have been developed for solving FDEs via finite difference method [11, 70–75], finite element method [76], operational matrix method [77–80] etc..

A new paradigm in science, the idea of a variable order (VO) operator is a considerably more recent innovation. The variable-order fractional calculus offers amazing capabilities to model transdisciplinary processes. VO operators are logically analytical extension of constant-order operators. As a function of either dependent or independent integration (or differentiation) factors, such as time, space, or even an independent external variable, the order can change frequently in VO operators [38, 52–54, 60–63, 81, 82]. Even though it seems natural to extend from constant-order operators to VO operators, the first definitions of these operators were provided by Samko and Ross [52] in 1993. They directly generalised the Riemann-Liouville

and Marchaud fractional integration and differentiation of the case of VO, then demonstrated some properties and an inversion formula.

Recently, Lorenzo and Hartley [53, 54], and Coimbra [38] proposed the mathematics of variable-order fractional calculus in perspective by discussing possible applications of variable-order fractional calculus in mechanics. Later, so many other authors proposed multiple definitions of these operators, such as Coimbra, Caputo [83], Grunwald-Letnikov and Heydari Hasseininia. Numerous other researchers have given different definitions of variable order differential operators. The variable exponent cannot be used with the variable order operators because of their complicated kernel. Therefore, it is highly appealing to obtain the numerical solutions of variable order fractional differential equations (VO-FDEs). The research on numerical methods for VO-FDEs is very limited in number. Some important numerical methods for solving these VO-FDEs are given in [1, 49, 64, 66, 84–87]. In the next subsection, we will consider variable order sub-diffusion equation.

1.1.4 Mathematical model based on fractional PDEs

1.1.4.1 Multi-term time-fractional electromagnetic wave model

Fractional differential equations (FDEs) are used to describe electromagnetic fields and waves in extensive regions of dielectric media. Their emergence and applications play a significant role in electromagnetic theory [88, 89] and have drawn the attention of researchers in recent years. In [90, 91], the authors illustrate the use of FDEs to model electromagnetic fields and waves across a broad spectrum of dielectric media. In real life, the electromagnetic waves equation is applied in a dielectric media, such as in microwave heating systems, which are frequently employed in the food service and processing industries for quick heating. The topic of electromagnetic

waves and their application to food preparation and microwave heating are covered in [92]. On the other hand, commercial or industrial microwave systems users face several challenges. Uneven heating is one of the most significant problems they encounter. The authors discussed the elements contributing to unequal heating in [92]. Additionally, how the food's dielectric quality affects microwave characteristics is discussed in [92]. In 2011, Tarasov proposed the electromagnetic wave model in fractional integro-differential terms [93].

In this thesis, we have considered the following multi-term time-fractional wave model (MT-TFWM) [93]

$$\begin{cases} \lambda_{1_0}{}^{C}\mathrm{D}_{\mathfrak{t}}^{\alpha}\mathfrak{U}(\mathrm{x},\mathfrak{t}) + \lambda_{2_0}{}^{C}\mathrm{D}_{\mathfrak{t}}^{\beta}\mathfrak{U}(\mathrm{x},\mathfrak{t}) = \mathfrak{U}_{\mathrm{xx}}(\mathrm{x},\mathfrak{t}) + \mathfrak{f}(\mathrm{x},\mathfrak{t}), \quad (\mathrm{x},\mathfrak{t}) \in \Omega = [\mathrm{x_l},\mathrm{x_r}] \times [0,T], \\ I.C. : \mathfrak{U}(\mathrm{x},0) = \phi_1(\mathrm{x}), \quad \partial_{\mathfrak{t}}\mathfrak{U}(\mathrm{x},0) = \phi_2(\mathrm{x}), \\ B.C. : \mathfrak{U}(\mathrm{x_l},\mathfrak{t}) = \psi_1(\mathrm{x}), \quad \mathfrak{U}(\mathrm{x_r},\mathfrak{t}) = \psi_2(\mathrm{x}), \end{cases} \tag{1.5}$$

where $1 < \beta < \alpha < 2$, and the Caputo fractional derivatives are defined as

$${}_{0}^{C}\mathrm{D}_{\mathfrak{t}}^{\alpha}\mathfrak{U}(x,\mathfrak{t}) = \frac{1}{\Gamma(2-\alpha)} \int_{0}^{\mathfrak{t}} \frac{\mathfrak{U}''(\cdot,s)}{(\mathfrak{t}-s)^{\alpha-1}} ds, \quad \alpha \in (1,2). \tag{1.6}$$

1.1.4.2 Time-fractional Black-Scholes model

In financial markets, a derivative is a financial instrument whose value is derived from the performance of an underlying asset. Among the various types of derivatives, options are widely regarded as both popular and significant. Options are divided into two primary types: call options and put options. A call option grants the holder the right, but not the obligation, to purchase the underlying asset at a predetermined

price (known as the strike price, K) at a specified future date, typically at maturity. The holder of a call option benefits when the market price of the asset rises above the strike price, enabling them to buy the asset at a lower cost than its current value. Exercising the call option at maturity is profitable when the stock price (S) exceeds the strike price (K). In contrast, a put option grants the holder the right, but not the obligation, to sell the underlying asset at the strike price (K) at the time of maturity. The holder of a put option benefits when the stock price declines, allowing them to sell the asset for more than its market value. A put option becomes profitable if exercised at maturity when the stock price is below the strike price. If an option is exercised before its maturity date, it is referred to as an American option. Consequently, from both theoretical and practical standpoints, determining the correct price of an option presents a significant challenge. In 1973, Black and Scholes introduced the Black-Scholes (B-S) model to describe the behavior of underlying assets. While the option prices generated by the B-S model are often very close to actual market prices, the model has certain limitations. Notably, it fails to account for key market phenomena such as the 'volatility smile' and sudden price jumps over short time intervals. [94]. Following the discovery of fractal structures in stochastic processes, fractional calculus has increasingly been used to model financial systems [10]. In this context, two forms of fractional derivatives—space-fractional and time-fractional derivatives—play a crucial role in modeling financial processes. Utilizing the space-fractional derivative, Carr & Wu introduced the Finite Moment Log Stable (FMLS) model, employing the Fourier transform method to calculate option values [95]. The authors in [96] derived three popular space-fractional B-S models in which they established an essential connection between FMLS, CGMY, and KoBoL processes. Using the time-fractional derivative, [97] priced a European call option by a time-fractional Black-Scholes model for pricing the European vanilla

options. [98] modeled the European-style option by time-fractional partial differential equation utilizing tick-by-tick data via a non-explosive market point process. The author uses the Caputo derivative as a non-local operator in terms of time-to-maturity. A time-space fractional B-S model is derived by [99] using fractional order Taylor formula and Ito's lemma, which is later applied to Merton's optimal portfolio [100]. Based on this idea, [101] introduced a bi-fractional B-S model assuming that the underlying asset follows a fractional Ito's process, and the change in the option price with time is a fractional transmission system. In the same way, pricing an American option is also an essential task in finance. A greedy algorithm for the partition of unity collocation method is used in pricing American option by [102]. Recently, [103, 104] have discussed the B-S model in distributive order.

1.2 Definition of some fractional derivatives

Unlike the classical derivative, which has a single definition, fractional derivatives have multiple formulations. Among these, the Riemann-Liouville and Caputo derivatives are the most commonly used. In this section, we introduce several types of fractional-order and variable-order derivatives.

Definition 1.1. (Caputo fractional derivative) The left and right Caputo fractional derivatives with order $\alpha > 0$ of the given function $u(t)$, $t \in (a, b)$ are defined as [13, 19]:

$$ {}_a^C\mathcal{D}_t^\alpha u(t) = \frac{1}{\Gamma(m-\alpha)} \int_a^t (t-s)^{m-\alpha-1} u^{(m)}(s) ds, \tag{1.7}$$

and

$$ {}_{t}^{C}\mathcal{D}_{b}^{\alpha}u(t) = \frac{(-1)^{m}}{\Gamma(m-\alpha)}\int_{t}^{b}(s-t)^{m-\alpha-1}u^{(m)}(s)ds, \tag{1.8} $$

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

Definition 1.2. (VO Caputo fractional derivative) The left and right Caputo fractional derivatives with order $\alpha(t) > 0$ of the given function $u(t)$, $t \in (a,b)$ are defined as [13, 19]:

$$ {}_{a}^{C}\mathcal{D}_{t}^{\alpha(t)}u(t) = \frac{1}{\Gamma(m-\alpha(t))}\int_{a}^{t}(t-s)^{m-\alpha(t)-1}u^{(m)}(s)ds, \tag{1.9} $$

and

$$ {}_{t}^{C}\mathcal{D}_{b}^{\alpha(t)}u(t) = \frac{(-1)^{m}}{\Gamma(m-\alpha(t))}\int_{t}^{b}(s-t)^{m-\alpha(t)-1}u^{(m)}(s)ds, \tag{1.10} $$

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

Definition 1.3. (Riemann-Liouville fractional derivative) The left and right Riemann-Liouville fractional derivatives with order $\alpha > 0$ of the given function $u(t)$, $t \in (a,b)$ are defined as [13, 19]:

$$ {}_{a}^{RL}\mathcal{D}_{t}^{\alpha}u(t) = \frac{1}{\Gamma(m-\alpha)}\frac{d^{m}}{dt^{m}}\int_{a}^{t}(t-s)^{(m-\alpha-1)}u(s)ds, \tag{1.11} $$

and

$$ {}_{t}^{RL}\mathcal{D}_{b}^{\alpha}u(t) = \frac{(-1)^{m}}{\Gamma(m-\alpha)}\frac{d^{m}}{dt^{m}}\int_{t}^{b}(s-t)^{(m-\alpha-1)}u(s)ds, \tag{1.12} $$

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

Definition 1.4. (VO Riemann-Liouville fractional derivative) The left and right Riemann-Liouville fractional derivatives with order $\alpha(t) > 0$ of the given function $u(t)$, $t \in (a, b)$ are defined as [13, 19]:

$$ {}^{RL}_{a}\mathcal{D}_{t}^{\alpha(t)}u(t) = \frac{1}{\Gamma(m-\alpha(t))}\frac{d^m}{dt^m}\int_a^t (t-s)^{(m-\alpha(t)-1)}u(s)ds, \tag{1.13} $$

and,

$$ {}^{RL}_{t}\mathcal{D}_{b}^{\alpha(t)}u(t) = \frac{(-1)^m}{\Gamma(m-\alpha(t))}\frac{d^m}{dt^m}\int_t^b (s-t)^{(m-\alpha(t)-1)}u(s)ds, \tag{1.14} $$

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

Definition 1.5. (Grünwald-Letnikov fractional derivatives) The left and right Grünwald-Letnikov derivatives with order $\alpha > 0$ of the given function $u(t)$, $t \in (a, b)$ are defined as [13, 19]:

$$ {}^{\mathrm{GL}}_{a}\mathcal{D}_{t}^{\alpha}u(t) = \lim_{\substack{h\to 0 \\ Nh=t-a}} h^{-\alpha}\sum_{j=0}^{N}(-1)^j\binom{\alpha}{j}u(t-jh), \tag{1.15} $$

and

$$ {}^{\mathrm{GL}}_{t}\mathcal{D}_{b}^{\alpha}u(t) = \lim_{\substack{h\to 0 \\ Nh=b-t}} h^{-\alpha}\sum_{j=0}^{N}(-1)^j\binom{\alpha}{j}u(t+jh), \tag{1.16} $$

respectively. For more information about the role of Grünwald and Letnikov to derive the above formulae (1.15) and (1.16) one can see [22].

Definition 1.6. (Riesz fractional derivative) The Riesz fractional derivative with order $\alpha > 0$ of the given function $u(t)$, $t \in (a, b)$ is defined as [13, 19]:

$$ {}^{RZ}\mathcal{D}_{t}^{\alpha}u(t) = c_\alpha\left({}^{RL}_{a}\mathcal{D}_{t}^{\alpha}u(t) + {}^{RL}_{t}\mathcal{D}_{b}^{\alpha}u(t)\right), \tag{1.17} $$

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

1.3 Literature review

The theory of integrals and derivatives of fractional order has achieved much popularity and importance due to its applications in science and engineering. Mathematical models based on arbitrary order integrals and derivatives provide a powerful and flexible tool for describing the behavior of real materials [105], viscoelastic fluid [27, 106, 107], finance [108–111], signal and image processing [112–115], electrochemical process [69, 116], biological systems [21, 117], control theory [28, 118, 119], electromagnetic waves [88, 93, 120] and so on. We now present a brief literature review for some classes of variable order and fractional order mathematical models that are considered in this thesis.

1.3.1 Literature review on variable-order time-fractional reaction sub-diffusion equation

In this section, we have discussed some of the important literature on variable-order time-fractional reaction sub-diffusion equation. In 2012, Chen et al. [56] proposed a numerical approximation method to find the solution behavior of variable-order nonlinear reaction sub-diffusion equations. They have analyzed stability and convergence using the Fourier analysis. In the same year, Yang et al. [121] proposed

a computationally effective method for solving variable order fractional reaction-subdiffusion equations with the finite difference scheme. The shifted Jacobi collocation approach was developed in 2018 by Hafez and Youssri [122] to solve the variable-order fractional linear sub-diffusion and nonlinear reaction-subdiffusion equations. They have also established convergence and stability of the numerical scheme. In 2018, Yang et al. [123] constructed the orthogonal spline collocation scheme in space and the weighted-shifted Grünwald difference (WSGD) approximation in time. The proposed scheme is proved to be unconditionally stable and converges with the order $O(\tau^2 + \Delta\alpha^2 + h_x^{r+1})$, where τ, $\Delta\alpha$, h_x and r are the step lengths in time, space, and polynomial degree of space respectively. In 2019, Hajipour et al. [55] proposed a discretization method to solve the problems with variable-order reaction diffusion equation. They discretized problem in spatial direction using a compact finite difference operator and in the temporal discretization a WSGD formula is applied. The stability and convergence of the proposed scheme are also discussed with $O(\tau^3 + h_x^4)$, where h_x and τ are step sizes in spatial and temporal direction, respectively. In 2021, Adel and Elsaid [124] presented numerical solutions for the linear and nonlinear variable-orde reaction-diffusion equation which is based on the Hermite formula. They have also discussed stability by the Von-Neumann method. A higher-order efficient numerical scheme for one and two dimensional variable order temporal fractional advection reaction-subdiffusion equations was proposed by Kheirkhah et al. [57] in 2022. In the spatial and temporal directions, they used a third order WSGD formula and a fourth order compact finite difference operator, respectively. The authors have also addressed convergence and stability of their proposed numerical scheme.

1.3.2 Literature review on variable-order time-fractional sub-diffusion equation

In this section, we will review some of the essential literature for variable-order time-fractional sub-diffusion equation (VOTFSDE) For the variable-order anomalous subdiffusion equation, Chen et al. in 2010 [64] established a numerical scheme with great spatial precision. A compact difference scheme of Crank-Nicolson type was introduced by J. Cao et al. [1] in 2016 for the variable-order sub-diffusion equation. They have demonstrated second-order accuracy in time and fourth-order accuracy in space direction. Chen et al. [84] in 2019 provide a multi-term time-space variable-order fractional advection-diffusion model to account for transient dispersion. In this study, the traditional finite difference method is used to create a fully discrete numerical framework. The authors also demonstrated convergence and the unconditional stability of the proposed method. In the same year, Heydari et al. [85] presented a computational method to solve the non-linear variable order fractional diffusion wave equation by using the Chebyshev cardinal function. In 2020, Du et al. [86] devised temporal second order numerical scheme for the multi-dimensional VOTFSDE with second order precision in time and fourth order in space. The authors have also used the discrete energy approach to discuss the solvability, stability, and convergence of the provided difference schemes. A quick approach for variable-order Caputo fractional derivative with applications to time-fractional diffusion equations was established by Fang et al. [87] in the same year 2020. The energy approach examines the suggested scheme's convergence and stability in the discrete H1-norm. Wei and Yang introduced a fully discrete local discontinuous Galerkin method for solving a class of variable-order fractional differential equation in 2021, [49]. The locally discontinuous Galerkin method in space and the finite

difference approach in time form the idea's foundation. The proposed technique converges to $O(h^{k+1} + \tau)$ and is unconditionally stable, where h and τ are the spatial and temporal step sizes, respectively, and k is the degree of the polynomial.

1.3.3 Literature review on Multi-term time-fractional wave model

In 2015, Ren and Sun [125] presented a numerical scheme for one dimensional and two dimensional multi-term time-fractional diffusion-wave equations. The authors also gave unconditional stability and convergence for the numerical scheme. For the numerical solution of multi-term time fractional partial differential equations, Dehghan et al [126] introduced a high order difference scheme and Galerkin spectral technique in 2015. The authors proved the unconditional stability of the compact scheme by the coefficient matrix property and discussed L_∞ convergence of the compact scheme has been proved by the energy method and also obtained an error estimate for the Galerkin spectral method. In 2017, Meng Li et al. [127] analyzed the multi-term time-fractional diffusion equations and diffusion-wave equations using the finite-element approach and the finite difference analogue of the Caputo fractional derivative. The authors have also discussed unconditional stability and convergence. In 2018 [128], In one and two dimensions on nonuniform grids, Z Soori et al. proposed a high-order technique for numerically solving the multiterm time fractional diffusion-wave equation.

In the same year, Liu et al. [129] developed a novel finite difference discrete scheme for the diffusion wave equation involving a Caputo fractional derivative of order $\alpha \in (1, 2)$ in time. The authors proved unconditional stability and convergence orders $O(\tau^{3-\alpha} + h^2)$ both in L_2 and L_∞ are derived, where τ and h are the temporal and spatial mesh sizes.

In 2018, Sarvestani et al. [130] established the Galerkin method (based on the second kind Chebyshev wavelets) for the solution of the multi-term time fractional diffusion-wave equation. The authors also provided theoretical error and convergence analysis. In 2020, Rashidinia et al. [131] developed a numerical scheme for one and two dimensional multi-term time fractional diffusion and diffusion-wave equations (smooth and nonsmooth solutions). They have also talked about the convergence analysis of the Legendre collocation spectral method. In 2020, Maurya et al. [132] developed multistep finite difference schemes for solving one and two dimensional fractional differential models of electromagnetic waves that are arising in dielectric media. They have also investigated Theoretical unconditional stability, convergence analysis and error bounds. In 2023, in a dielectric medium, Devi et al. [133] proposed the semi-discretization technique with an operational matrix approach to solve the fractional order wave equation that arises. And authors have also shown the efficiency and accuracy of the proposed method.

1.3.4 Literature review on time fractional Black-Scholes model govering the European option

Due to the importance of fractional-order derivatives, the fractional Black-Scholes model has gained much interest amongst researchers to find its solution. To find the analytical solution, some of the researchers have used the homotopy perturbation method [134], the homotopy analysis method [135], and the integral transform method [97, 100, 101, 136] for the fractional B-S model. But the problem with these solutions lies in the fact that they are of the form of convolution of some special functions or an infinite series with integrals [108]. Therefore, developing a numerical approximation for the solution of TFBSM becomes more crucial. In the past few years, only a few reports have been available on the numerical solution of TFBSM

using different approaches. In 2022, Kamran Kazmi [137] has designed an efficient method for solving the time fractional Black-Scholes model which is transformed into an equivalent integro differential equation. In the same year, Pradip Roul [138] presented a numerical scheme for one dimensional and two dimensional multi-term time fractional diffusion-wave equation. The author also showed unconditional stability and global convergence. In 2022 Srivastava et al. [77] constructed a computational approach based on the combination of finite difference with the operational matrix for the time fractional Black-Scholes model. Theoretical unconditional stability and convergence of the numerical scheme are established for $\alpha \in (0, \bar{\alpha}]$. In 2023, Kaur et al. [139] developed a new numerical scheme on uniform mesh for the time fractional Black-Scholes partial differential equation governing European option. They have also analyzed stability and convergence of the numerical scheme.

1.4 Mathematical preliminaries

1.4.1 Lagrangian polynomials

Let $x_0, ..., x_N$ be $N+1$ distinct node points in given closed interval $[a, b]$, where $x_0 < x_1 < ... < x_N$ and N is a positive integer. Then the Lagrangian polynomials are defined as [140]:

$$L^k(x) = \prod_{\substack{j=0 \\ j \neq k}}^{N} \frac{(x - x_j)}{(x_k - x_j)}; \qquad k = 0, ..., N, \tag{1.18}$$

and satisfy the Kronecker property $L^k(x_j) = \delta_{kj}$.

1.4.2 Newton interpolating polynomials

Let $x_0, ..., x_N$ are $N+1$ distinct node points in $[a, b]$ and $f \in C^{n+1}[a, b]$. Then, the general Newton's interpolation formula with divided differences are defined as [140]:

$$f(x) = f(x_0) + (x - x_0)f[x_0, x_1] + \cdots + (x - x_0)\dots(x - x_n)f[x_0, \dots, x_n] + R_n,$$

where, $R_n = \dfrac{f^{(n+1)}(\xi(x))}{(n+1)!}(x - x_0)\dots(x - x_n)$, and $\xi(x) \in (x_0, x_n)$.

1.4.3 Legendre polynomials

Legendre polynomials were discovered in 1782 by Adrien-Marie Legendre, which form a system of complete and orthogonal polynomials in the domain $[-1, 1]$, with a vast number of mathematical properties, and numerous applications with the orthogonality property as:

$$\int_{-1}^{1} P_n(x)P_m(x)dx = \frac{2}{2n+1}\delta_{nm},$$

where δ_{nm} is the Kronecker delta. We can define the Legendre polynomials using different aspects. Let us define Legendre polynomials as follows.

Definition 1.7. The Legendre polynomials can be defined as the coefficients in a formal expansion in powers of t of the generating function

$$\frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} P_n(x)t^n.$$

The coefficients of each t^n is a polynomial of degree n.

Definition 1.8. The Legendre polynomial is the series solution of Legendre's differential equation

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_n(x)}{dx}\right] + n(n+1)P_n(x) = 0.$$

Some of the Legendre polynomials are

$$P_0(x) = 1,$$
$$p_1(x) = x,$$
$$P_2(x) = \frac{1}{2}(3x^2 - 1),$$
$$P_3(x) = \frac{1}{2}(5x^3 - 3x),$$
$$P_4(x) = \frac{1}{2}(35x^4 - 30x^2 + 3).$$

1.5 Numerical methods

1.5.1 Operational matrices

Orthogonal functions and polynomials are fundamental to the development of operational matrices, which serve as key tools for constructing numerical methods aimed at solving both linear and nonlinear fractional mathematical models. Over the past three decades, they have significantly contributed to the advancement of techniques for addressing challenges such as system identification, analysis, and optimal control.

Operational matrices are derived by approximating the derivatives or integrals of functions using orthogonal functions. In numerical analysis, this technique serves as a powerful tool for approximating solutions to integral and fractional differential

equations (FDEs) (see [26, 141–143]). Many equations, including partial differential equations (PDEs) and fractional partial differential equations (FPDEs), involve singularities that make them unsolvable by classical methods. However, operational matrix techniques are well-suited for addressing such singularities. These methods simplify singularity-related problems, enhance computational efficiency, and reduce error.

The theory of operational matrices primarily relies on two fundamental operators: differentiation and integration. The corresponding operational matrices can be constructed as follows:

$$\begin{aligned} \frac{d\Psi(t)}{dt} &\approx D\Psi(t), \\ \int_a^t \Psi(x)dx &\approx I\Psi(t), \end{aligned}$$

where, D and I are the operational matrices of differentiation and integration, respectively of dimension $N+1$ and $\Psi(t) = [\psi_1(t), \psi_2(t), \ldots, \psi_{N+1}(t)]$ is an orthonormal basis defined over a specific interval. More broadly, the mathematical formulations of the operational matrices are presented below as:

$$\begin{aligned} \frac{d^k\Psi(t)}{dt^k} &\approx D^k\Psi(t), \\ \int_a^t \cdots \int_a^t \Psi(x)\,(dx)^k &\approx I^k\Psi(t). \end{aligned}$$

The operational matrix approach is widely favored for its straightforward implementation, rapid convergence, and adaptability to higher-dimensional problems. Some key advantages are such as it can be seamlessly extended to higher dimensions through the use of the Kronecker product. This method transforms complex equations (such as PDEs and FPDEs) into systems of algebraic equations that can be efficiently solved using established techniques. Moreover, the solution remains

convergent even with relatively large step sizes. Because of these advantages, operational matrices for differentiation and integration have been widely adopted by researchers. Various types of orthogonal basis functions, such as Legendre polynomials, have been employed in constructing differentiation operational matrices. [144–146], Berstein polynomials [147], Fourier series [148], Chebyshev wavelets [149] and Bernoulli wavelets [150]. Similarly, the operational matrix of integration has been developed for various types of orthogonal basis functions, including Chebyshev wavelets [151, 152], Legendre wavelets [153, 154], Haar wavelets [155], Fourier series [156], Berstein polynomials [157] and Bessel functions [158].

1.5.1.1 Kronecker Product

Definition 1.9. Let P and Q be two matrices of orders $m \times n$ and $p \times q$, respectively. Then the Kronecker product $P \otimes Q$ of matrices P and Q is defined as the following $mp \times nq$ order block structure [159]:

$$P \otimes Q = \begin{bmatrix} p_{11}Q & p_{12}Q & \cdots & p_{1n}Q \\ \vdots & \vdots & \ddots & \vdots \\ p_{i1}Q & p_{i2}Q & \cdots & p_{in}Q \\ \vdots & \vdots & \ddots & \vdots \\ p_{m1}Q & p_{m2}Q & \cdots & p_{mn}Q \end{bmatrix},$$

where

$$P = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ p_{i1} & p_{i2} & \cdots & p_{in} \\ \vdots & \vdots & \ddots & \vdots \\ p_{m1} & p_{m2} & \cdots & p_{mn} \end{bmatrix}, \qquad Q = \begin{bmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ q_{i1} & q_{i2} & \cdots & q_{in} \\ \vdots & \vdots & \ddots & \vdots \\ q_{m1} & q_{m2} & \cdots & q_{mn} \end{bmatrix}.$$

1.5.2 Finite difference method

The finite difference method (FDM) is well understood and among the first approaches applied to approximate the derivative operators. Euler first utilized it, probably in 1768 [160]. There are many ways to derive the finite difference approximation of the given differential equations (DEs). One way is the Taylor series expansion to approximate the derivative terms of DEs. Some of the applications of FDM in FDEs are described in detail in the articles [108, 129, 161, 162].

FDM replaces the derivative terms from the differential equations with difference quotients, which require the values of the solution at discrete mesh points in the domain under study. By this replacement, the method converts the DEs into an algebraic system of equations in terms of unknown grid point values. Additionally, unknown terms are considered only at discrete grid points.

This method requires the use of a regular grid and to facilitate explanation of the approach, and it will be considered that it is uniform, although this is not essential. The grid must be constructed such that the nodal points are located at the intersection of either curved lines or rectilinear lines. These lines appear as a set of numerical coordinates, which is illustrated in one dimension.

1.5.2.1 Construction of the method

Among various difference approximations methods, Taylor's series expansion is one of the most popular ones to derive difference approximations of DEs. The numerical solutions, based on FDM, provide 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 time variable $t \in [0, T]$. Let us assume that the discretization in spatial direction is uniform and given by Δx. Likewise, the discretization in the temporal direction is also uniform and given by Δt. Neither discretization parameter must be uniform; one or both may be non-uniform The basic philosophy of FDMs is to replace the derivatives of the governing equations with algebraic difference quotients. This will result in a system of algebraic equations that can be solved at each and every internal grid point by using the given initial and boundary conditions. FDM requires more grid points to achieve reasonable accuracy.

1.5.2.2 Finite difference approximation of derivatives

In the finite difference approximations, let M & N be any two positive integers, and the discretization parameters $\Delta x = L/M$ and $\Delta t = T/N$ stand for the uniform spatial and temporal mesh points, respectively. Let $\Omega_{\Delta x} = \{x_i : x_i = i\Delta x,\ i = 0, 1, \ldots, M\}$ and $\Omega_{\Delta t} = \{t_j : t_j = k\Delta t,\ j = 0, 1, \ldots, N\}$, 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

$$\frac{\partial u}{\partial x}(x_i, t_j) \approx \frac{u_{i+1}^j - u_i^j}{h}, \tag{1.19}$$

$$\frac{\partial u}{\partial t}(x_i, t_j) \approx \frac{u_i^{j+1} - u_i^j}{k}, \tag{1.20}$$

and the backward space and time difference schemes are given by

$$\frac{\partial u}{\partial x}(x_i, t_j) \approx \frac{u_i^j - u_{i-1}^j}{h}, \tag{1.21}$$

$$\frac{\partial u}{\partial t}(x_i, t_j) \approx \frac{u_i^j - u_i^{j-1}}{k}. \tag{1.22}$$

The difference approximations given in (1.19)-(1.22) 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 [163]).

1.6 Challenges and motivations

The definition of FDs is not as straightforward as it is in classical calculus. For the past few decades, theoretical and experimental efforts have been made to provide a precise definition that satisfies the basic rules of derivatives. Riemann-Liouville and Caputo derivatives are the most common and widely used definitions [22]. Certain

researchers have lately extended these definitions to simulate several fundamental scientific phenomena such as viscoelasticity, electromagnetic systems, and so on. Katugampola [164] proposed new definitions for generalizing the fractional integrals and derivatives of Riemann-Liouville and Hadamard into a single form. Jarad et al. [165] proposed a generalized proportional fractional derivative.

The thesis aim is to understand the nature of different types of fractional mathematical models proposed by Abel and generated by the Caputo FD in time. Non-integer order derivatives make the differential equations too complex to be solved analytically, so numerical simulation is required. It is a challenge to provide more accurate numerical results. FDM [108, 129, 161, 162, 166, 167], spectral methods [34, 168–172], collocation methods [173–175], finite element methods [176–181], finite volume methods [182, 183] are some methods that are being used to solve FPDEs.

1.7 Problem statement and thesis objectives

The key objectives of the thesis are:

1. To develop stable and efficient numerical schemes for variable-order time-fractional reaction sub-diffusion equations.

2. To develop higher-order convergence schemes for variable-order time-fractional sub-diffusion equations.

3. To design a difference scheme for multi-term time-fractional electromagnetic wave model arising in dielectric medium.

4. To develop a semi-discrete scheme for the financial mathematical model governing European options with the help of L-123 approximation of the Caputo derivatives and operational matrix method.

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