Chapter 1

Introduction

Fractional calculus (FC) is the branch of applied mathematics in which we deal with non-integer order derivatives in place of integer order derivatives or integration [8, 9, 10, 11, 12, 13, 12]. These derivatives or integration may be real or complex numbers. The origin of fractional calculus is considered in the 17^{th} century. It's was first noticed in the correspondence between G.A. de L'Hôpital and G.W. Leibniz, in 1695. In this communication, Leibniz wrote a letter commenting the posibility of the order of derivatives to a fractional number. L'Hôpital was curious to know the answer of this question and replied on September 30, 1695 that it will lead to a paradox from which one-day useful consequences will be drawn. Since then many applications of FC were presented by the researcher using different types of fractional derivatives such as Riemann, Caputo, Liouville, Grunwald, Letnikov, Weyl, Hadamard etc. Further, FC was studied by Abel in [16]. In [16], the derivatives are used in the form of fractional order differentiation and integration, and showing mutually reverse relationship between them. The unified operation of integration and differentiation of arbitrary order is considered in [15] and [16]. In [17, 18], Liouville studied the foundation of FC in 1832. The extension in theory as well as application of fractional calculus were increased rapidly during 19^{th} and 20^{th} century. The applications of FC are not only in mathematics but also found in other fields such as physics [19], engineering [20], biophysics [21], fluids mechanics and bioengineering [22, 23], control theory [24], viscoelasticity [25] and many more can be seen in literature [26, 27, 28, 29]. Introductory overview of fractional order derivatives and recent developments are presented in [8].

1.1 Definition of Fractional Integral and Fractional Derivative

In this section, we give basic definitions and properties of fractional calculus. More details can be found in [2, 12].

Definition 1.1.1 ([6]). The Caputo derivative of a function $u(\tau)$ whose n^{th} derivative is absolute continuous in $[a, b]$ $(AC^n[a, b])$ of order γ defined as,

$$(\mathcal{D}^{\gamma}_{0+;}u)(\tau) = \frac{1}{\Gamma(n-\gamma)} \int_0^{\tau} (\tau - s)^{n-\gamma-1} u^{(n)}(s) ds, \ \tau > 0, \tag{1.1}$$

where $n - 1 < \gamma \leq n$ *, and* $n \in \mathbb{Z}^+$.

Definition 1.1.2 ([6]). Generalized fractional derivative of order n of a function $u(\tau) \in AC^n[a, b]$ with weight function $\omega(\tau)$ and scale function $z(\tau)$ is defined as,

$$(\mathcal{D}^{n}_{0+;[z;\omega;L]}u)(\tau) = [\omega(\tau)]^{-1} \left[\left(\frac{D_t}{z'(\tau)} \right)^n (\omega(\tau) f(\tau)) \right]. \tag{1.2}$$

Definition 1.1.3 ([6]). The forward/left generalized fractional integral of a function $u(\tau) \in AC^n[a, b]$ of fractional order $\gamma > 0$ is given as,

$$(\mathcal{I}^{\gamma}_{0+;[z;\omega]}u)(\tau) = \frac{[\omega(\tau)]^{-1}}{\Gamma(\gamma)} \int_0^{\tau} \frac{\omega(s)z'(s)u(s)}{[z(\tau)-z(s)]^{1-\gamma}}ds, \tag{1.3}$$

provided the integral on the right-hand side exists.

Definition 1.1.4 ([6]). The forward/left generalized Caputo fractional derivative of order γ and of type 2 of function $u(\tau) \in AC^n[a,b]$ with respect to scale function $z(\tau)$ and weight function $\omega(\tau)$ is given by,

$$(\mathcal{D}^{\gamma}_{0+;[z;\omega;2]}u)(\tau) = (\mathcal{I}^{n-\gamma}_{0+;[z;\omega]}\mathcal{D}^{n}_{0+;[z;\omega;L]}u)(\tau) = \frac{[\omega(\tau)]^{-1}}{\Gamma(n-\gamma)} \int_0^{\tau} \frac{[\omega(s)u(s)]^{(n)}}{(z(\tau)-z(s))^{\gamma}}ds, \tag{1.4}$$

where $n-1 \leq \gamma < n, \ n \in \mathbb{N}$.

Definition 1.1.5. [30] The K operator is defined by

$$K^{\gamma}_{P}u(x) = r\int_a^x w_{\gamma}(x,t)u(t)\ dt + s\int_x^b w_{\gamma}(x,t)u(t)\ dt, \quad \gamma > 0, \tag{1.5}$$

where, $x \in [a,b], \ P =< a,b,r,s >$ denote the all parameters, $w_{\gamma}(x,t)$ is a kernel defined on the space $I \times I$. We assume that $w_{\gamma}(x,t)$ and $u(t)$ both are square integrable function such that Eq. (1.5) exists. K operator satisfies the linearity properties, i.e. for any two functions $u_1(t)$ and $u_2(t)$, then

$$K^{\gamma}_{P}(u_1(x)+u_2(x)) = K^{\gamma}_{P}u_1(x) + K^{\gamma}_{P}u_2(x). \tag{1.6}$$

Define, A and B-operators [30] as follows,

$$A^{\gamma}_{P}u(x) = D^n K^{(n-\gamma)}_{P}u(x), \tag{1.7}$$

$$B^{\gamma}_{P}u(x) = K^{(n-\gamma)}_{P}D^n u(x). \tag{1.8}$$

by using Eq. (1.5) and Eq. (1.8) can be written as,

$$B_P^{\gamma}u(x) = r\int_0^x w_{m-\gamma}(x,t)D^n u(t)\,dt + s\int_x^1 w_{m-\gamma}(t,x)D^n u(t)\,dt, \quad \gamma > 0, \tag{1.9}$$

where, $m-1<\gamma<m$, m is an integer and $P=<a,b,r,s>$ and $D^n u(t)$ denote the n^{th} derivative of the function $u(t)$. In the definition of B-operator, we assume that $D^n u(x)$ is integrable once on domain I. More details about these operators can be found in [30].

1.2 Fractional Integro-Differential Equations

In recent years, fractional integro-differential equations (FIDEs) are used to investigate the physical phenomena in various fields such as electromagnetic [31], viscoelasticity [32] etc. For handling different types of physical models, some state-of-the-art fractional derivatives are being used e.g. Riemann-Liouville fractional derivative, Caputo fractional derivative, Riesz fractional derivative, etc. In [6], Agrawal discussed a new generalized fractional derivative (GFD) which unifies all above-stated derivatives by using weight and scale functions. Here, scale functions can be used to compress and enlarge the domain for the observation of the diffusion phenomena closely while weight functions provide flexibility to the researchers for assessing the physical events at different times. Due to vast real life application of scale and weight functions, several fractional PDEs were studied using GFD. As the analytical solutions for such FPDEs/FPIDEs were difficult to obtain so several authors have investigated the numerical methods for solving such equations. We cite here a few of them [33, 34, 35, 36, 37, 38].

In this thesis, we define FIDE in terms of B operator [30] with homogeneous boundary conditions. Now, we define GFIDEs using B-operator as follows

$$(B_P^{\gamma}u)(x) = (Hu)(x), \quad 0 < \gamma < 1, \tag{1.10}$$

$$u(0) = u_0, \tag{1.11}$$

where

$$(Hu)(x) = \phi(x) + g(x)u(x) + \int_0^x \rho(x,t)G(u(t))dt, \quad 0 < \gamma < 1, \quad x \in I = [0,1], \tag{1.12}$$

$$(B_P^{\gamma}u)(x) = r\int_0^x w_{m-\gamma}D^n u(t)dt + s\int_x^1 w_{m-\gamma}(t,x)D^n u(t)dt, \quad \gamma > 0, \tag{1.13}$$

where, function $\phi(x)$ and $g(x)$ are square integrable functions in I with, $g(x) \neq 0$, and $u(x)$ is unknown. This problem is considered in the interval $[0,1]$ and kernel $\rho(x,t)$ is weakly singular of the form

$$\rho(x,t) = (x-t)^{-v}, \quad 0 < v < 1. \tag{1.14}$$

1.3 Fractional Sub-Diffusion Equations

Diffusion equations are used to describe the change in the concentration of matter with respect to time. This diffusion process can be studied by diffusion equations. The problem of solving advection diffusion equation obtained from energy or mass transportation by the movement of fluid is thoroughly studied in recent years. A wide range of applications of ADEs can be seen in biological, chemical and physical sciences, such as transport occur in fluids [39], probability distribution for Markov processes [40, 41], porous media [7], chemical transport [42], modelling of suspended sediments [43], evolution of conditional dispersal [44], reactions and chemotaxis [45], water dynamics [46] etc. Fractional diffusion equations are also used to study the anamolous behaviour of diffusion equations. Basically it arises where there is non-linear relationship between the mean square distance (MSD) and time i.e.

$$MSD \propto t^{\alpha}. \tag{1.15}$$

It is classified into three types 1) $\alpha > 1$ called the super diffusion, 2) $\alpha = 1$ shows the Brownian motion of the particles, 3) $\alpha < 1$ which shows the sub diffusion behavior. In this thesis, we will study the sub-diffusion behavior of anamoluos diffusion equations. It can be observed where the medium of the flow is inhomogeneous. Such type of equation has a lot of physical applications in the real world such as random walk [47], particle tracking [48], diffusion of gases in the environment under gravity [49] etc.

1.4 Motivation

In FC, we study non-integer order derivatives and integration which may be real or complex in place of the integer order derivatives [50, 51]. In last few decades, FC has become an attractive topic of research due to its applications in various fields of science and engineering. Fractional order derivatives of a given function involve the entire function history where the state of a fractional order system is not only dependent on its current state but also on all its ast states [52, 19]. It is also used in the modeling of several natural and mathematical problems or describing the behavior of modeling phenomena. Applications of FC in different fields like science, physics, engineering, biology, economics, finance can be found in Refs. [55, 56, 57, 58]. Another important application of FC in memory process can also be seen in

[59, 60]. In literature, some definitions have been introduced to find the derivative and integration of fractional order such as Riemann-Liouville, Caputo, Hadamard, Weyl etc. Recently the generalization of there derivatives are presented in [6] and named as B-operator. The B-operator allows the kernel to be arbitrary and reduces to other derivatives in special case.

In this thesis, we explore the solution method for fractional integro-differential equations and fractional diffusion equations defined in terms of B-operator and generalized fractional derivatives.

1.5 Literature Review

This section includes the summary of the current work and past work done on the FIDE, FDE, and their applications along with the proposed numerical method for solving such type of problems.

1.5.1 Literature Review on the Fractional Integro-Differential Equations

During 17^{th} century after origin of fractional calculus, the applications of FIDE increased very rapidly in modeling of various real world problems. Several researchers have been concentrating on the development of numerical and analytical techniques for FIDEs. For example, Angell and Olmstead [61] solved integro-differential equation modeling filament stretching using by singular perturbation method. Khosro et al. [62] presented a numerical technique based on Bernstein's operational matrix for a family of FIDEs utilizing the trapezoidal rule. Bounds, the convergence and error analysis were also established. Kilbas et al. [63] developed some basic concepts for solving FIDEs. Also provided the existence and uniqueness theorem. In [64], a new set of function is constructed to obtain the numerical solution of FIDEs called fractional-order Euler function, which is based on Euler function. By using the property of the fractional-order Euler function, the approximate solution was obtained using operational matrix approach. Saddatmandi and Dehghan [65] developed a numerical method for solving the linear and non-linear FIDEs by defining the fractional derivative in the Caputo sense. The approximate solution was found by Legendre approximations. The property of Legendre polynomials together with the Gaussian integration method were utilized to convert the problem into system of algebraic equations. In [66], two numerical approximations such as linear and quadratic scheme for solving the generalized Abel integral have been presented. The error and convergence of schemes were also discussed. It was found that the quadratic scheme achieves the convergence order up to three. In [68, 69], Adomian's decomposition method for solving the system of the nonlinear FIDEs are discussed. In [70, 71, 72, 73, 32, 1], the authors used the collocation method for solving the fractional differential equation. Odibat [74] presented the analytical study on a linear system of fractional differential equations with constant coefficient and briefly described the existence and uniqueness for systems of the differential equation of fractional order. There are many other methods to solve FIDEs such as the finite difference method, finite–element methods [75]. Kamal et al. [76] applied the spectral Tau method for solving general fractional-order differential equations. In [77], we can see that system of fractional differential equations is solved by the homotopy analysis method. Hassani et al. [78] proposed a method for solving a system of non-linear fractional-order partial differential equations with initial conditions. First, they expand the solution by using the operational matrix method, and then the unknown coefficients are evaluated by the optimization technique.

1.5.2 Literature Review on the Time Fractional Diffusion Equations

Some diffusion process occur in nature in non-homogeneous medium whose study is not possible using normal diffusion process. The study of the diffusion equations in in-homogeneous medium is classified by sub-diffusion equation and the various researchers are finding numerical solution by applying various methods. Lin and Xu [79] solved time-fractional diffusion equation (TFDE) using spectral method and finite difference method (FDM). In [80], Murio solved time-fractional advection-diffusion equation (TFADE) by using implicit FDM. Sweilam et al. [81] developed the Crank-Nicolson FDM to solve linear TFDE defined in terms of Caputo fractional derivative. In [82], Luchko solved initial and boundary value multi terms TFDE based on an appropriate maximum principle. Dubey et al. [83] proposed a residual power series method to obtain the solution of homogeneous and non-homogeneous nonlinear fractional order partial differential equations. In [84], the authors presented the perturbed Sumudu transform technique to solve the fractional equal width equation. Li and Wong [85] constructed an efficient numerical scheme to find the solution to the generalized sub-diffusion equation. The authors used the generalized Grunwald-Letnikov approximation method for numerical approximation. In the past few years, several methods are proposed for finding the solution of FADEs. In [86, 87], authors developed a numerical method for solving space-time FADE by using Chebyshev collocation method. Safdari et al. [88] used compact finite difference scheme to solve the space-time FADE and also discussed their convergence analysis. A tau method is presented for the space fractional diffusion equation by Saadatmandi and Dehghan [89]. In [90], Mesgarani et al. solved the space fractional advection dispersion equation with Caputo fractional derivative using compact finite difference and fourth kind shifted Chebyshev polynomials in temporal direction and spatial direction respectively. The convergence order and unconditional stability are also investigated via the energy method. Tajadodi [91] proposed a novel approach consisting Atangana-Baleanu-Caputo derivative for solving the time fractional ADEs using operational matrix method. Wang et al. [92, 93] used the Petrov-Galerkin method to find the solution of ADE with the help of Jacobi polynomials. Kumar et al. [94] analyzed the modified homotopy analysis transform method to find solution of one-dimensional space fractional ADEs. For solving space fractional ADEs, Khader et al. [95] demonstrated an efficient numerical method with the help of Legendre approximations.

Some other numerical methods for solving FADEs include radial basis function-finite difference technique [96], finite difference approximation [97], Legendre spectral element method [98], homotopy analysis method [99] and shifted fractional Jacobi spectral algorithm [100]. Readers can go through [101, 102, 10, 103, 104] few more numerical techniques for solving space-time FADEs.

Most of the above discussed works are either based upon Riemann Liouville fractional derivative or Caputo fractional derivative. Recently, Agrawal [6] presented a more generalized form of fractional derivative consisting weight and scale functions knows as a new generalized fractional derivative (GFD). For particular choices of weight and scale functions, it reduces to Caputo, Riemann as well as other fractional derivatives. The scale functions allow us to study both faster and slower physical phenomena by stretching and contracting time domain, respectively. Weight function helps us to extend the kernel in fractional integral to provide more flexibility in modelling real problems. In [33], the numerical solution of generalized fractional Burgers equation is studied by direct finite difference method. In [33], both the analytical and numerical solutions of diffusion equation equipped with such new GFD are investigated. The dependence of dynamics of solutions on scale function and weight function are graphically illustrated via fruitful numerical simulations. For more work, we refer to [105, 106, 107, 108].

1.6 Problem Statement and Thesis Objectives

In this thesis, we study the numerical methods for solving linear and non-linear FIDE, FDE, and FADE defined in terms of B-operators and generalized Caputo derivatives. Many research works have been carried out on such problems defined using generalized Caputo derivative but still there is scope of contribution in developing the stable numerical methods.

The purpose of the thesis is to propose a numerical method to solve the FIDE and FADE defined using generalized derivatives applicable for linear or non-linear cases. For checking its numerical applicability and comparison to other existing methods, we have used descritization based finite difference methods (FDM).

The objectives of the thesis are

1. To propose the stable numerical method to solve the linear/non-linear FIDE in higher dimension with known and unknown exact solutions.
2. To develop the convergent stable numerical method for generalized fractional diffusion equations in 1D and 2D.
3. To study the behavior of the numerical solutions under the effect of weight and scale function of different choices involved in the generalized Caputo derivatives.

1.7 Outline of the Thesis

In this thesis, we discuss convergent and stable numerical methods for solving FIDE and fractional sub-diffusion equations. This thesis contains five chapters.

Chapter 1 is the introduction which describes fractional integro-differential equation, the historical background of the problem. This chapter includes definition and some basic properties of shifted Jacobi poly-fractonomials, Legendre polynomials and fundamental descriptions of the Jacobi polynomials. The basic idea of B operator and collocation method are also demonstrated in this chapter. Definition of generalized Caputo fractional derivative and its properties, utilized in this thesis, are given in the last section of the chapter.

Chapter 2 describes the problem based on the FIDE which is defined in terms of B operator. The B operator contains some integration and differentiation terms in its expression. Further, we define our problem using B operator. Numerical solution of FIDE is based on the approximation method, and for the function approximation we have used the Jacobi poly-fractonomials. Jacobi poly-fractonomials are the eigenfunction of fractional Sturm-Livouille problem. So, we write our considered function in the summation form of infinite series by taking basis as Jacobi-poly-fractonomials. Further, we use collocation method for finding numerical solutions. The convergence and error analysis of the problem is discussed analytically and numerically. We make the comparison of numerical solution to exact solution graphically. Also, we compare our result with other results available in the literature and we find that results obtained by our proposed method provide better accuracy than other existing methods.

Chapter 3 explores the problem given in Chapter 2 for two-dimensional bounded domain including the fractional order derivative on the space and time both variables.

This problem is defined into summation form in terms of B operators together with some function. In this problem, the Dirichlet type of boundary condition is taken into account and in some examples, we have taken Neummann boundary condition. The application of the problem given in Chapter 3 are shown in various other fields likewise for specific choice of the parameters and function, the considered problem reduces to 1) space time fractional diffusion equations, 2) time fractional telegraph equations, and 3) fractional diffusion equations. We also present an approximate approach based on spectral shifted Jacobi collocation method to solve the problem. We also discuss its convergence, error, and stability analysis mathematically and numerically. From this study, it can be seen that the approximate results are adequately accurate.

In Chapter 4, we discuss the time fractional diffusion equation considering time derivative as generalized Caputo derivative. We study this equation in a bounded domain by taking Dirichlet type boundary conditions. For the Numerical solution, we have applied finite difference scheme on the time derivative to discretize the time domain and further on the space variable, we use collocation method. The approximate solution is based on the collocation method with Jacobi polynomials as basis functions. Then an approximate approach based on collocation method with shifted second kind Jacobi polynomials is used to find a numerical solution of the obtained boundary value problem. Further, we discuss its convergence, order of convergence, stability analysis and show that the proposed scheme is unconditionally stable. For accuracy of the scheme, we compare our results with available analytical solutions.

In Chapter 5, a numerical method is discussed to solve fractional advection diffusion equations in which derivative is defined in terms of generalized Caputo derivatives. The approximate solution of this problem is obtained by shifted Legendre collocation method in a bounded domain with Dirichlet boundary conditions. This can also be reduced to the explored problem defined in the Chapter 4 by taking advection term zero. In order to get numerical results, a suitable value for the auxiliary parameter is determined optimally and the obtained results are presented through figures. For accuracy of our results, comparisons are made between the exact analytic solution and the approximate solution obtained by the presented method. It is found that the collocation method is valid and feasible technique to study the diffusion problems.

Chapter 6 presents the conclusion of the thesis and explains possible outcomes for solving FIDE and fractional sub-diffusion equations defined using generalized derivatives.

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