Chapter 1
Introduction

1.1 Diffusion process

The term ”diffusion” originates from the Latin language, meaning ”to spread out.” It’s a fundamental process driven by the random collision of solute molecules, resulting in the movement of solute particles from areas of higher concentration to areas of lower concentration. This concept was articulated by Bear in the year 1979 [1]. Moreover, Bear and Bachmat [2] highlighted that the coefficients of molecular diffusion in a uniform medium depend on the diffusion coefficient of the solute in water and the tortuosity of the medium. Unlike mechanical dispersion, which is significant in scale, the rates of molecular diffusion remain constant regardless of groundwater velocity, and diffusion can occur even when there’s no fluid movement. If only the diffusion process is responsible for the movement of the solute particle, then its governing equation take the following form:

$$\frac{\partial u}{\partial t} = \nabla.(D\nabla u). \tag{1.1}$$

Diffusion is a process that occurs in many different situations, from mixing ingredients in cooking to the exchange of gases in the lungs. It plays a crucial role in biology, chemistry, physics, and many other fields of science.

Let's explore a unique example of diffusion: the process of perfume spreading in a room. This everyday phenomenon offers a perfect illustration of how diffusion works in action. Imagine being in a room where someone has just sprayed some perfume. At first, the perfume smell might only be strong near the person who sprayed it, as the perfume molecules are concentrated around them. However, as time passes, something interesting happens—the smell starts to spread out and fill the entire room, reaching your nose even if you're far away. When the perfume is sprayed, tiny perfume molecules are released into the air, constantly moving, bouncing, and colliding with each other and with the air molecules in the room. Initially, the perfume molecules are concentrated near the person who sprayed it, creating a high concentration area. However, due to Brownian motion the random movement of molecules, the perfume molecules start to spread out from areas of high concentration to areas of low concentration, gradually moving away and spreading throughout the room. This movement continues until the perfume molecules are evenly distributed throughout the entire room, eventually reaching your nose and allowing you to smell the perfume no matter where you are. This spreading out of the perfume smell is a perfect example of diffusion.

1.2 Reaction-advection-diffusion equation

When pollutants enter an aquifer, those form a contaminant plume that spreads widely due to the dispersion of particles and water flow, known as the plume front. This phenomenon is analyzed using solute transport modeling, an essential tool in environmental research that mathematically models the movement of pollutants through groundwater. Employing various advanced methods, this approach addresses and resolves issues related to groundwater contamination, enabling scientists and engineers to effectively predict and control the dispersion of pollutants. When the conditions influencing pollutant transport remain relatively constant, the reaction-advection-dispersion equation (RADE) is used, providing information on pollutant concentration changes over time and distance from the source. This is achieved by incorporating data on groundwater velocity, dispersion rates, reaction speeds, initial pollutant levels, and the physical boundaries of the groundwater flow. This modeling is vital for understanding and safeguarding water resources.

Over the years, lots of mathematical models have been developed by the engineers and scientists to tackle the complex nature of solute transport in groundwater. These models have become essential tools for hydrologists and researchers, helping them assess the potential of water resources and predict the environmental impacts of various scenarios. Groundwater modeling, in particular, has been spotlighted in several significant publications. For instance, Anderson and Woessner [3] discussed the use of groundwater models and the simulation of flow and advective transport in their detailed study. Similarly, Charbeneau [4] has shed light on the hydraulics of groundwater and how pollutants navigate through it, while Kehew [5] has brought attention to the chemical aspects of hydrology. In 2005, Rausch [6] made notable contributions by modeling solute transport and offering analytical solutions to these complex problems. In practical applications, the advection-diffusion equation is used to describe heat transfer in a draining film [7], unsteady fluid flow in porous media [8], transportation of pollutant in river [9]. Moreover, mathematical models which describe the groundwater contamination can be found in [10, 11, 12, 13, 14] etc.

The transport of fluid is governed by the RADE, it is used to figure out how pollutants move around in bodies of water. This equation helps to predict where pollutants will go by considering three main factors: how the water carries pollutants along its flow, how these pollutants spread out over time, and how they react chemically with the water and other substances. This makes it an essential tool for understanding and managing pollution in water environments. Mathematically, it is written as

$$\frac{\partial u}{\partial t} + \nabla \cdot (\nu u) = D\nabla^2 u + R(u). \tag{1.2}$$

If transport of solute is due to the combined effect of advection and diffusion then it is described by the advection-diffusion equation (ADE). In this case, the above equation take the following form

$$\frac{\partial u}{\partial t} + \nabla \cdot (\nu u) = D\nabla^2 u, \tag{1.3}$$

and if the transport of solute is due to the combined effects of reaction and diffusion, then it is described by reaction-diffusion equation (RDE), which is mathematically represented by

$$\frac{\partial u}{\partial t} = D\nabla^2 u + R(u), \tag{1.4}$$

where u describes the species concentration for mass transfer problem and temperature for heat transfer problem. The term $\frac{\partial u}{\partial t}$ represents the rate of change of concentration with respect to time, accounting for reactions occurring over time. The term $\nabla \cdot (\nu u)$ represents the advection of the substance, where ν is the velocity vector of the fluid medium. This term describes how the substance is transported through the medium due to bulk fluid flow. The first term on right hand side $D\nabla^2 u$

represents diffusion, where D is the diffusion coefficient and ∇^2 is the Laplacian operator. This term accounts for the spreading out of the substance due to random molecular motion and the term $R(u)$ represents any reaction or transformation that the substance undergoes, which can be a function of concentration u. This term captures chemical reactions or other processes that change the concentration of the substance over time.

1.3 Fractional calculus

Fractional calculus is a branch of mathematical analysis that extends the concepts of differentiation and integration to non-integer orders. The origin of fractional calculus can be traced in the end of 17th century from a conversation between Gottfried Leibniz and Guillaume de l' Hôpital. Leibniz introduced the concept of successive differentiation i.e. $\frac{d^n y}{dx^n}$. In a letter dated September 30, 1695, L'Hospital wrote to Leibniz and asked him, what would the result be if $n = \frac{1}{2}$. Leibniz replied, "This is an apparent paradox from which, one day, useful consequences will be drawn." Since then, the question raised by L'Hôpital and Leibniz has sparked considerable research interest among mathematicians. Over the years, numerous esteemed mathematicians, including Leonhard Euler, J-L Lagrange, P-S Laplace, S.F. Lacroix, J. Fourier, N.H. Abel, J. Liouville, O. Heaviside, B. Riemann, H. Weyl, G. Leibniz, A. K. Grunwald, and A.V. Letnikov, have made invaluable contributions to the field of fractional calculus.

From the late 17th century through the 18th century, there is a notable absence of significant work in the field of fractional calculus in the literature. While mathematicians like Leonhard Euler and Joseph Fourier briefly mentioned the concept of derivatives of arbitrary order during this time, they did not delve further into its exploration or application in their subsequent work. It wasn't until the early 19th century that significant advancements in the understanding of derivatives of arbitrary order began to emerge. In particular, S.F. Lacroix [15] made a notable contribution in 1819 by defining the derivative of arbitrary order. Lacroix introduced this concept using the Gamma function as a fundamental tool, marking a significant milestone in the development of fractional calculus.

$$D^n x^m = \frac{\Gamma(m+1)}{\Gamma(m+1-n)} x^{m-n}, \quad m \geq n. \tag{1.5}$$

Using above definition, he obtained

$$D^{1/2} x^m = \frac{\Gamma(m+1)}{\Gamma(m+1/2)} x^{m-1/2}. \tag{1.6}$$

In 1822, Joseph Fourier [16] was among the early mathematicians to discuss derivatives of arbitrary order. His contributions to fractional operations stemmed from his integral representation of any function $f(x)$, wherein he provided insights into the fractional derivatives of functions. He wrote

$$\frac{d^\alpha}{dx^\alpha} f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(z) dz \Big(\int_{-\infty}^{\infty} n^\alpha \cos \Big[n(x-z) + \frac{n\pi}{2} \Big] dn \Big). \tag{1.7}$$

Fourier asserted that the parameter α appearing in the aforementioned expression could be interpreted as any quantity, whether positive or negative.

Niels Henrik Abel was the first person to use fractional operations in 1823. He used them to solve a tricky math problem called the tautochrone problem. This was a big deal because it showed that fractional calculus could be really useful in solving practical problems, proving how important it is in math. In 1832, Joseph Liouville conducted the first major study into fractional calculus and presented two different definitions for fractional derivatives. Building upon the Fourier fractional integral and Abel's solution in potential theory, Liouville assumed the expansion of a function $f(x)$ in series form to explore the arbitrary derivative. He extended the concept of ordinary derivatives to fractional derivatives. He assumed that the arbitrary function $f(x)$ may be expressed as a series expansion as,

$$f(x) = \sum_{m=0}^{\infty} a_m e^{s_m x}, \quad Re\ s_m > 0, \tag{1.8}$$

and derivative of arbitrary order α will be

$$D^\alpha f(x) = \sum_{m=0}^{\infty} a_m s_m^\alpha e^{s_m x}. \tag{1.9}$$

This formula is called Liouville's first definition, and while it had some problems, it was a big step forward in fractional calculus. To overcome these problems, Liouville came up with a second definition. He did this by changing an integral into the gamma function and then came up with a new formula for finding derivatives of arbitrary order, given by

$$D^\beta x^\alpha = (-1)^\beta \frac{\Gamma(\beta + \alpha)}{\Gamma(\alpha)} x^{-\alpha-\beta}. \tag{1.10}$$

The problem with the second definition is that it doesn't work well with many types of functions.

Between 1835 and 1850, mathematicians had a big argument about how to define fractional-order derivatives. The problem was that two famous mathematicians, Lacroix and Liouville, had different ideas. Lacroix said that when you take the fractional derivative of a constant number, you get a non-zero answer. But Liouville thought it should be zero. This caused a lot of discussion and debate among mathematicians at that time about which definition was the right one.

The biggest progress in fractional calculus came from G.F. Bernhard Riemann's work when he was still a student in 1853. He was trying to make a more general version of the Taylor series. Riemann came up with a new way of looking at integrals, using definite integrals in a different way. This new method was a game-changer in math and helped solve many tough problems. He derived the following definition for fractional integration:

$$D_c^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_c^x (x-t)^{\alpha-1} f(t)dt + \psi(x). \tag{1.11}$$

Because there was some confusions about the lower limit of the integration, Riemann included a "complementary" function $\psi(x)$ in his definition. Nowadays, this definition is widely accepted for fractional integration, but the complementary function is usually set to zero, and the lower limit of integration c is often taken as zero as well, i.e.,

$$_0D_x^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t)dt, \quad Re(\alpha) > 0. \tag{1.12}$$

This type of fractional integral is often called the Riemann-Liouville fractional integral. In the latter part of the 19th century, several mathematicians, including A.K. Grunwald, A.V. Letnikov, H. Laurent, A. Krug, O. Heaviside, and others, made significant contributions to the advancement of fractional calculus. In 1967, M. Caputo made the most significant contribution to the fractional calculus in the modern era to deal with the main drawback of Riemann-Liouville's definition of fractional derivative. The first conference on fractional calculus, titled "The First Conference on Fractional Calculus and its Applications," took place in 1974 in New Haven. In the same year, the first book on fractional calculus was published by Oldham and Spanier [17]. This has attracted researchers from various backgrounds, leading to the publication of numerous books on fractional calculus thereafter. Some notable authors include Nishimoto [18], Miller and Ross [19], Kiryakova [20], Rubin [21], Podlubny [22], Hilfer [23], Kilbas et al. [24], etc.

1.4 Special functions

The Gamma function, Mittag-Leffler function and the Wright function play the most important role in the theory of fractional calculus. Some results about these functions are given in this section.

1.4.1 Euler's Gamma function

The Gamma function, denoted by $\Gamma(x)$, is a special function that generalizes the factorial function to non-integer and complex numbers. Mathematically, the gamma function is defined as

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt, \qquad \text{for } x > 0, \tag{1.13}$$

This integral converges for all complex numbers x with positive real part. In other words, the Gamma function is defined for all x in the complex plane except for negative integers where it has simple poles.

1.4.2 Mittag-Leffler function

The Mittag-Leffler function holds significant importance in the realm of fractional calculus, extensive applications. Similar to how the exponential function emerges as a solution to differential equations of integer order, the Mittag-Leffler function assumes a parallel significance in resolving differential equations of non-integer order.

One-parameter Mittage-Leffler function is denoted by $E_\alpha(z)$ and defined as

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha + 1)}, \tag{1.14}$$

and two-parameter Mittage-Leffler function is denoted by $E_{\alpha,\beta}(z)$ and defined by

$$E_{\alpha,\beta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha + \beta)}, \qquad \alpha > 0,\ \beta > 0, \tag{1.15}$$

where z is a complex number.

The Mittag-Leffler function generalizes the exponential function, providing a solution to fractional differential equations and playing a crucial role in fractional calculus. It is characterized by its entire function property, which means it is analytic for all complex values of z.

1.4.3 Wright function

The Wright function is a special kind of function that is an extension of the exponential function. This function play an important role in the solution of fractional differential equation. The Wright function is defined as

$$W(z;\alpha,\beta) = \sum_{n=0}^{\infty} \frac{z^n}{n!\ \Gamma(n\alpha + \beta)}. \tag{1.16}$$

The Wright function is an entire function, meaning it is analytic for all complex values of z.

1.4.4 Error function and complementary error function

Error function denoted by $erf(x)$ and defined as

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \tag{1.17}$$

The error function arises in various areas of mathematics and physics, particularly in probability theory, statistics, and the theory of random processes. It is often encountered in problems involving probability distributions, random variables, and the propagation of errors in measurements.
The complementary error function is denoted by $erfc(x)$ and defined as

$$erfc(x) = 1 - erf(x) = \int_x^\infty e^{-t^2} dt. \tag{1.18}$$

1.5 Fractional order reaction-advection-diffusion equation

The fractional versions of reaction-advection-diffusion equations have not been widely studied yet. In this study, the focus is given on numerical solutions for FRADE and explores the characteristics of these solutions. FRADE is increasingly being recognized for its fascinating applications in various fields like electromagnetics, robotics, acoustics, viscoelastic damping, electrochemistry, and materials science. This interest is due to FRADE's ability to more accurately describe how solutes move through complex environments like porous aquifers. The fractional-order derivatives used in FRADE allow it to account for more history or memory effects than the standard RADE, making it useful in engineering, physics, economics, and more for addressing issues like anomalous diffusion and signal processing. The study of FRADE is gaining attention because it provides more flexibility and detailed insights into how materials behave in non-uniform conditions. In last few years, there has been intense research into fractional calculus due to its significant applications across various fields, including chemistry, physics, biology, geology, and finance. For example, Heydari et al. [25] introduced orthonormal shifted discrete Legendre polynomials and collocation method for nonlinear reaction-advection-diffusion equation of variable-order having Caputo-Fabrizio derivative and Chen et al. [26] found the numerical solution of space fractional order reaction-adevction-diffusion equation. Cartea and Negrete [27] developed a fractional order diffusion model to better predict option prices in markets characterized by jumps. Oqielat et al. [28] introduced fractional reaction-diffusion model for bacteria growth, researchers in [29, 30, 31, 32] have modeled reaction-diffusion system for biological pattern formation. Scientists and researches of [33, 34, 35, 36, 37] have used reaction-advection-diffusion equation to modeled problem arising in chemistry and the RADE model arising in physics can be seen in [38]. Gul et al. [39] has developed a computational method to deal with fractional order partial reaction-diffusion equation, Owolabi [40] has solved the Riesz space fractional-order reaction-diffusion equations. A nonlinear fourth order fractional reaction diffusion equation is approximated by [41] using finite difference/ finite element method, Roul and Goura [42] have developed a numerical scheme for non-homogeneous reaction diffusion equation of fractional order etc.

1.6 Basic definitions of fractional calculus

There are various versions of the definition of fractional order derivative and integral. In this section, only those definitions are discussed, which have been used in the forthcoming chapters.

1.6.1 Riemann-Liouville fractional integral

The Riemann-Liouville fractional integral $I^{\alpha}f(x)$ of a locally integrable function $f(x)$ of order α is defined as

$$I^{\alpha}f(x) = \begin{cases} \frac{1}{\Gamma(\alpha)}\int_0^x (x-t)^{\alpha-1} f(t)dt, & \alpha > 0,\ x > 0, \\ f(x), & \alpha = 0, \end{cases} \tag{1.19}$$

where $x, \alpha \in \mathbb{R}$, and $\Gamma(.)$ denotes the Gamma function.

Some of the properties of I^{α} are as follows.

- $I^{\alpha}I^{\beta}f(x) = I^{\alpha+\beta}f(x)$,
- $I^{\alpha}I^{\beta}f(x) = I^{\beta}I^{\alpha}f(x)$,
- $I^{\alpha}x^{\vartheta} = \frac{(\vartheta+1)}{\Gamma(\vartheta+1-\alpha)}x^{\vartheta+\alpha}$

1.6.2 Riemann-Liouville fractional derivative

The Riemann-Liouville fractional derivative ${}_aD_x^{\alpha}f(x)$ of a locally integrable function $f(x)$ is defined by

$${}_aD_x^{\alpha}f(x) = \frac{1}{\Gamma(1-\alpha)}\frac{d}{dx}\int_a^x \frac{f(t)}{(x-t)^{\alpha}}dt,\ \alpha \in (0,1). \tag{1.20}$$

In general,

$${}_aD_x^{\alpha}f(x) = \frac{1}{\Gamma(n-\alpha)}\frac{d^n}{dx^n}\int_a^x \frac{f(t)}{(x-t)^{\alpha-n+1}}dt, \tag{1.21}$$

where $n-1 < \alpha < n$, n is the smallest integer greater than α.

1.6.3 Caputo derivative

Definition The fractional order Caputo derivative of the function $f(x)$ of order α with respect to the variable x is given by

$$ {}_{0}^{c}D_x^{\alpha} f(x) = \begin{cases} \frac{1}{\Gamma(n-\alpha)} \int_0^x (x-s)^{n-\alpha-1} \frac{\partial^n f(s)}{\partial s^n} ds, & n-1 < \alpha < n, \\ \frac{d^n f(x)}{dx^n}, & \alpha = n. \end{cases} \tag{1.22} $$

Also from the definition of Caputo derivative, we have

$$ {}_{0}^{c}D_x^{\alpha} x^k = \begin{cases} \frac{\Gamma(k+1)}{\Gamma(k+1-\alpha)} x^{k-\alpha}, & k \in \mathbb{N}_0, \text{ and } k \geq \lceil \alpha \rceil \text{ or} \\ & k \notin \mathbb{N}_0, \text{ and } k > \lfloor \alpha \rfloor, \\ 0, & \text{else} . \end{cases} $$

The Riemann-Liouville non-integer derivative of a constant is non-zero. That is Riemann-Liouville fractional derivative of a constant C is

$$ {}_{a}D_x^{\alpha}\, C = \frac{Cx^{-\alpha}}{\Gamma(1-\alpha)}. \tag{1.23} $$

For all orders $\alpha > 0$, the Caputo fractional derivative of constant is zero. Because of this fact, the Caputo fractional derivative seems to be more favored in the physical sciences.

Properties of fractional operators

- ${}_{a}D_x^{\alpha}\Big(I^{\alpha} f(x)\Big) = f(x),$

- $I^{\alpha} f(x)\Big({}_{a}D_x^{\alpha} f(x)\Big) = f(x) - \sum_{i=1}^{k} \Big[{}_{a}D_x^{\alpha-i} f(x)\Big]_{x=a} \frac{(x-a)^{\alpha-i}}{\Gamma(\alpha-i+1)}, \quad k-1 \leq \alpha < k,$

- ${}_0^cD_x^\alpha(\lambda f(x) + \mu g(x)) = \lambda({}_0^cD_x^\alpha f(x)) + \mu(({}_0^cD_x^\alpha g(x))$

1.7 Mathematical preliminaries

In this section, some notations and definitions are given which have been used in the thesis.

1.7.1 Lucas polynomials

The Lucas polynomial is the series solution of Lucas differential equation [43]

$$(t^2+4)\frac{d^2L}{dt^2} + t\frac{dL}{dt} - n^2L = 0. \tag{1.24}$$

The recurrence relation of the Lucas polynomial is given by

$$L_{n+2}(x) = L_n(x) + xL_{n+1}(x), \;\; n \geq 0, \tag{1.25}$$

with the conditions

$$L_0(x) = 2, \;\; L_1(x) = x.$$

From the above relation series form of Lucas polynomial obtained as

$$L_n(x) = n\sum_{m=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(n-2m+1)_{m-1}}{m!} x^{n-2m}, \tag{1.26}$$

where the notation $\lfloor x \rfloor$ represent the largest integer less than or equal to x, and $(k)_m$ is the pochhammer notation which is defined by $(k)_m = \frac{\Gamma(k+m)}{\Gamma(k)}$.

Every polynomial x^m for $m \geq 1$, can be written in combination of Lucas polynomials as

$$x^m = \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} \frac{(-1)^k \delta_{m-2k} (m-k+1)_k}{k!} L_{m-2k}(x), \tag{1.27}$$

where δ_s is defined by

$$\delta_s = \begin{cases} 1 & s > 0, \\ \frac{1}{2}, & s = 0. \end{cases} \tag{1.28}$$

First few Lucas polynomials are

$$\begin{aligned} L_0(x) &= 2, \\ L_1(x) &= x, \\ L_2(x) &= x^2 + 2, \\ L_3(x) &= x^3 + 3x, \\ L_4(x) &= x^4 + 4x^2 + 2. \end{aligned}$$

1.7.2 Vieta-Fibonacci polynomials

Several properties of Vieta-Fibonacci polynomials have been discussed in this section, including some of their shifted counterparts.

Using the following recurrence relation, a Vieta-Fibonacci polynomial can be generated as [44, 45]

$$VF_n(x) = xVF_{n-1}(x) - VF_{n-2}(x), \ \ n = 2, 3, \cdots \tag{1.29}$$

with conditions

$$VF_0(x) = 0, \quad \text{and} \quad VF_1(x) = 1. \tag{1.30}$$

The power series representation of $VL_n(x)$ is given by the following formula [44]

$$VF_n(x) = \sum_{k=0}^{\lceil \frac{n-1}{2} \rceil} \frac{(-1)^k \Gamma(n-k)}{\Gamma(n-2k)\Gamma(k+1)} x^{n-2k-1}, \;\; n = 2, 3, \cdots, \tag{1.31}$$

where $\lceil \frac{n}{2} \rceil$ represents the Ceiling function.

In addition, one of the nice properties of $VF_n(x)$ is that, it is orthogonal over the interval $[-2, 2]$ with respect to the weight function $w(x)$, i.e.,

$$\Big\langle VF_n(x), VF_m(x) \Big\rangle = \int_{-2}^{2} VF_n(x) VF_m(x) w(x) dx = \begin{cases} 2\pi, & n = m, \\ 0, & n \neq m, \end{cases} \tag{1.32}$$

where $w(x) = \sqrt{4 - x^2}$.

1.7.3 Shifted Vieta-Fibonacci polynomials

In this subsection, the shifted vieta-Fibonacci polynomial is discussed over the interval $[0, 1]$.
The following recurrence relation can be used to generate the shifted Vieta-Fibonacci polynomials as

$$VF_n^*(x) = (4x - 2) VF_{n-1}^*(x) - VF_{n-2}^*(x), \;\; n = 1, 2, \cdots, \tag{1.33}$$

for which

$$VF_0^*(x) = 0, F_1^*(x) = 1! \quad . \tag{1.34}$$

Now, the series form of the shifted Vieta-Lucas polynomial is given by

$$VF_n^*(x) = \sum_{k=0}^{n} (-1)^k \frac{2^{2n-2k-2}\Gamma(2n-2k)}{\Gamma(k+1)\Gamma(1-2k+2n)} x^{n-k-1}, \;\; n = 1, 2, 3, \cdots,$$

or,

$$VF_n^*(x) = \sum_{k=0}^{n} \frac{(-1)^{n-k-1} 2^{2k} \Gamma(n+k+1)}{\Gamma(n-k)\Gamma(2k+2)} x^k. \tag{1.35}$$

Also, $VF_n^*(x)$ has the of orthogonality property corresponding to the weight function $w(x) = \sqrt{x - x^2}$ as

$$\left\langle VF_n^*(x), VF_m^*(x) \right\rangle = \int_0^1 VF_n^*(x) VF_m^*(x) w(x) dx = \begin{cases} \frac{\pi}{8}, & n = m \neq 0, \\ 0, & n \neq m. \end{cases} \tag{1.36}$$

First few shifted Vieta-Fibonacci polynomials are

$$VF_0^*(x) = 0,$$
$$VF_1^*(x) = 1,$$
$$VF_2^*(x) = 4x - 2,$$
$$VF_3^*(x) = 16x^2 - 16x + 3,$$
$$VF_4^*(x) = 64x^3 - 96x^2 + 40x - 4.$$

1.7.4 Kronecker product

Consider two matrices A and B of order $m \times n$ and $p \times q$ respectively. Then their kronecker product $A \otimes B$ is defined by the following block structure of order $mp \times nq$ as

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & \cdots & a_{2n}B \\ \vdots & \vdots & & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & \cdots & a_{mn}B \end{pmatrix},$$

where

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & \cdots & a_{2n} \\ \vdots & \vdots & & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & \cdots & a_{mn} \end{pmatrix}, \quad B = \begin{pmatrix} b_{11} & b_{12} & \cdots & \cdots & b_{1q} \\ b_{21} & b_{22} & \cdots & \cdots & b_{2q} \\ \vdots & \vdots & & \ddots & \vdots \\ b_{p1} & b_{p2} & \cdots & \cdots & b_{pq} \end{pmatrix}.$$

1.8 Challenges and motivation

A key challenge for researchers working with fractional derivatives is understanding their physical significances. Unlike integer-order differential operators, which are local and only depend on the current state, fractional-order differential operators are non-local. This means those take into account not just the present state but the entire history of past states. This feature is especially useful in modeling natural phenomena that exhibit long memory, such as the atmospheric diffusion of pollutants, cellular diffusion processes, network traffic, the behavior of viscoelastic materials, and electronics. These systems involve non-local dynamics that require the broader perspective fractional calculus offers. Furthermore, since fractional derivatives consider the values of a function over an entire interval, those are ideal for modeling systems with long-range interactions across both space and time. This makes fractional differential equations particularly suited for describing complex and anomalous phenomena like transport in porous media, effectively capture the memory and inherent properties of various materials and processes.

Fractional derivatives are challenging because those have a "non-local" property and a "memory effect," making it tough to find the exact solutions analytically. This has led researchers to create various numerical methods to tackle fractional differential equations (FDEs). In the last few years, many researchers are working to find the numerical solutions of fractional order PDEs using various methods viz., finite difference method (FDM), spectral methods, collocation methods, finite element methods, finite volume methods, and the operational matrix method . Operational matrix method is the best method among these, which provides the best approximate solution with less effort. Most of the matrices use in this method have many zero entries, which reduce the computational time.

This ongoing challenge motivates the development of new numerical techniques toward the stable and a good rate of convergence. In this thesis different mathematical models have been explored using fractional derivatives of Caputo type. Some new operational matrix methods have also been explored. Moreover, Operational matrices for Vieta-Fibonacci wavelets of integer order as well as Caputo fractional order derivatives have been developed. These advancements aim to improve the stability and accuracy of numerical solutions for fractional order differential equations.

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