Chapter 1

Introduction

1.1 Fractional Calculus

The introduction of fractional calculus was started with the letters having a message "what might be a derivative of order $\frac{1}{2}$?" After Gottfried Leibnitz, Leonhard Euler started to think about the development and application of fractional calculus. He give the first definition of fractional derivative with arbitrary order by suggesting the integral representation with gamma function. The first application of fractional calculus is developed by Abel for solving an integral equation associated with tautochrone problem. The fractional calculus experiences fast development in 20^{th} century. Many definitions and properties of fractional order differentiation and integration were formulated. There are so many definitions and approaches available at present day. The mathematician Bertizan Ross proposed the following criteria for an operator to be fractional derivative;

1. An analytic function remains analytic after interacting with fractional derivative.

2. The effect of fractional derivative with positive integer order is equal to the value of integer order derivative.

3. In case of negative integer the result of fractional derivative must be equal to the value of that order of the integration.

4. The function remains fixed under zero order fractional derivative or integration.

5. The operator must satisfy the linear property.

6. The operator should follow the semi-group property.

1.1.1 Classical fractional derivative

Let $\beta \in C$ such that $R(\beta) \in (n-1, n], n \in N$ and $R(.)$ represents the real part of complex number. The notation $[\beta]$ denotes the integer part of number and $\{\beta\}$ corresponds to fractional part. The notation $\lfloor \beta \rfloor$ represents the floor function. The followings are the classical fractional operator [1, 2]:

1. Liouville derivative

$$D^{\beta}\zeta(y) = \frac{1}{\Gamma(1-\beta)} \frac{d}{dy} \int_{-\infty}^{y} (y-\eta)^{-\beta} \zeta(\eta) d\eta, \quad -\infty < y < +\infty. \tag{1.1}$$

2. Liouville left-sided derivative

$$D_{0^+}^{\beta}\zeta(y) = \frac{1}{\Gamma(n-\beta)} \frac{d^n}{dy^n} \int_{0}^{y} (y-\eta)^{-\beta+n-1} \zeta(\eta) d\eta, \quad y > 0, \quad n-1 < \beta \leq n. \tag{1.2}$$

3. Liouville right-sided derivative

$$D^{\beta}_{0^-}\zeta(y) = \frac{(-1)^n}{\Gamma(n-\beta)}\frac{d^n}{dy^n}\int_y^{+\infty}(\eta - y)^{-\beta+n-1}\zeta(\eta)d\eta, \quad y < \infty, \quad n-1 < \beta \leq n. \tag{1.3}$$

4. Riemann-Liouville left-sided derivative

$$^{RL}D^{\beta}_{a^+}\zeta(y) = \frac{1}{\Gamma(n-\beta)}\frac{d^n}{dy^n}\int_a^{y}(y - \eta)^{-\beta+n-1}\zeta(\eta)d\eta, \quad y > a, \quad n-1 < \beta \leq n. \tag{1.4}$$

5. Riemann-Liouville right-sided derivative

$$^{RL}D^{\beta}_{b^-}\zeta(y) = \frac{(-1)^n}{\Gamma(n-\beta)}\frac{d^n}{dy^n}\int_y^{b}(\eta - y)^{-\beta+n-1}\zeta(\eta)d\eta, \quad y \leq b, \quad n-1 < \beta \leq n. \tag{1.5}$$

6. Caputo left-sided derivative

$$^{C}D^{\beta}_{a^+}\zeta(y) = \frac{1}{\Gamma(n-\beta)}\int_a^{y}(y - \eta)^{-\beta+n-1}\frac{d^n}{dy^n}\{\zeta(\eta)\}d\eta, \quad y \geq a, \quad n-1 < \beta \leq n. \tag{1.6}$$

7. Caputo right-sided derivative

$$^{C}D^{\beta}_{b^-}\zeta(y) = \frac{(-1)^n}{\Gamma(n-\beta)}\int_y^{b}(\eta - y)^{-\beta+n-1}\frac{d^n}{dy^n}\{\zeta(\eta)\}d\eta, \quad y \leq b, \quad n-1 < \beta \leq n. \tag{1.7}$$

8. Grünwald-Letnikov left-sided derivative

$$^{GL}D^{\beta}_{a^+}\zeta(y) = \lim_{h\to 0}\frac{1}{h^{\beta}}\sum_{l=0}^{\lfloor n\rfloor}\frac{(-1)^l\Gamma(\beta+1)\zeta(y-lh)}{\Gamma(l+1)\Gamma(\beta-l+1)}, \quad nh = y - a. \tag{1.8}$$

9. Grünwald-Letnikov right-sided derivative

$$ {}^{GL}D_{b-}^{\beta}\zeta(y) = \lim_{h\to 0}\frac{1}{h^{\beta}}\sum_{l=0}^{\lfloor n\rfloor}\frac{(-1)^{l}\Gamma(\beta+1)\zeta(y+lh)}{\Gamma(l+1)\Gamma(\beta-l+1)}, \quad nh = b-y. \tag{1.9} $$

10. Riesz derivative

$$ D_{y}^{\beta}\zeta(y) = \frac{-1}{2\cos(\frac{\beta\pi}{2})}\frac{1}{\Gamma(\beta)}\frac{d^{n}}{dy^{n}}\Big[\int_{-infty}^{y}(y-\eta)^{-\beta+n-1}\zeta(\eta)d\eta \tag{1.10} $$

$$ + \int_{y}^{+\infty}(\eta-y)^{-\beta+n-1}\zeta(\eta)d\eta\Big], \quad n-1 < \beta \le n. \tag{1.11} $$

11. Hadamard derivative

$$ {}^{H}D_{+}^{\beta}\zeta(y) = \frac{\beta}{\Gamma(1-\beta)}\int_{0}^{y}\frac{\zeta(y)-\zeta(\eta)}{\{In(\frac{y}{\eta})\}^{1+\beta}}\frac{d\eta}{\eta}, \quad y \le b, \quad n-1 < \beta \le n. \tag{1.12} $$

12. Riemann-Liouville left-sided integral

$$ {}^{RL}I_{a+}^{\beta}\zeta(y) = \frac{1}{\Gamma(\beta)}\int_{a}^{y}(y-\eta)^{\beta-1}\zeta(\eta)d\eta, \quad y \ge a. \tag{1.13} $$

13. Riemann-Liouville right-sided integral

$$ {}^{RL}I_{a+}^{\beta}\zeta(y) = \frac{1}{\Gamma(\beta)}\int_{y}^{b}(\eta-y)^{\beta-1}\zeta(\eta)d\eta, \quad y \le b. \tag{1.14} $$

14. Hadamard integral

$$ {}^{H}I_{+}^{\beta}\zeta(y) = \frac{1}{\Gamma(\beta)}\int_{0}^{y}\frac{\zeta(\eta)}{\{In(\frac{y}{\eta})\}^{1-\beta}}\frac{d\eta}{\eta}, \quad y > 0, \quad \beta > 0. \tag{1.15} $$

1.1.2 Fractional operator with non-singular kernel

Let us consider the function $\zeta(y) \in H^1(a,b), \quad b > a$ and $E_\beta(y) = \sum_{i=0}^{\infty} \frac{y^i}{1+\beta i}$ corresponds to Mittag-Leffler function with one parameter [3]

15. Caputo-Fabrizio derivative

$$^{CF}D_y^{\beta}\zeta(y) = \frac{M(\beta)}{n-\beta}\int_a^y e^{\frac{-\beta}{1-\beta}(y-\eta)}\frac{d^n}{dy^n}\{\zeta(\eta)\}d\eta, \quad y \le b, \quad n-1 < \beta \le n. \tag{1.16}$$

16. Atangana Baleanu Caputo derivative

$$^{ABC}D_y^{\beta}\zeta(y) = \frac{B(\beta)}{n-\beta}\int_a^y E_\beta\{\frac{-\beta}{1-\beta}(y-\eta)^\beta\}\frac{d^n}{dy^n}\{\zeta(\eta)\}d\eta, \quad y \le b, \quad n-1 < \beta \le n. \tag{1.17}$$

17. Atangana Baleanu derivative in Riemann-Liouville type

$$^{ABC}D_y^{\beta}\zeta(y) = \frac{B(\beta)}{n-\beta}\frac{d^n}{dy^n}\int_a^y E_\beta\{\frac{-\beta}{1-\beta}(y-\eta)^\beta\}\{\zeta(\eta)\}d\eta, \quad y > b, \quad n-1 < \beta \le n. \tag{1.18}$$

18. Caputo-Fabrizio with Gaussian kernel

$$^{CF}D_y^{\beta}\zeta(y) = \frac{1+\beta^2}{\sqrt{(\pi^\beta(1-\beta))}}\int_a^y e^{\frac{-\beta}{1-\beta}(y-\eta)^2}\{\zeta(\eta)\}d\eta, \quad y > a, \zeta(a) = 0. \tag{1.19}$$

1.1.3 Variable order fractional derivative and integration [4]

The variable order fractional derivative are non-local operator. These operators are useful in characterizing the memory property of a system. The hereditary property and self-similarity of a system can be derived by variable order differential equations. Variable order fractional derivatives are useful in determining the memory effect in two ways. First one is memory change with spatial and time coordinates. Second one is connected with the memory of orders. This can be effective by the previous values of orders of derivatives.

1. **Type 1 (V1) derivative**

   The type 1 variable order derivative of order $n-1<\beta(x,t)\leq n$ is defined as follows.

$$ {}_0D_t^{\beta(x,t)}\zeta(x,t)=\frac{1}{\Gamma(n-\beta(x,t))}\int_0^t (t-\eta)^{-\beta(x,t)+n-1}\frac{\partial^n}{\partial\eta^n}\{\zeta(x,\eta)\}d\eta, \quad n-1<\beta(x,t)\leq n. \tag{1.20}$$

   This is equivalent to the well-known definition of Caputo's definition of fractional order derivative if we consider $\beta(x,t)$ as a constant.

2. **Type 2 (V2)** derivative

   The type 2 variable order fractional derivative ia defined as follows.

$$ {}_0D_t^{\beta(x,t)}\zeta(x,t)=\int_0^t \frac{1}{\Gamma(n-\beta(x,\eta))}(t-\eta)^{-\beta(x,\eta)+n-1}\frac{\partial^n}{\partial\eta^n}\{\zeta(x,\eta)\}d\eta, \quad n-1<\beta(x,t)\leq n. \tag{1.21}$$

   If we consider the order $\beta(x,t)$ as constant, this $V2$ type derivative reduces to the Riemann-Liouville definition.

1.2 Diffusion Phenomena

Diffusion is the process in which any matter or material atoms or molecules is transported or moved from one system to another with random molecular motions [5]. This process is not due to any action of force, it is a result of random moments of atoms with resulting in the uniform distribution of that matter or material atoms. It occurs in all types of materials having temperature above absolute zero. It occurs from the region of higher concentration to lower concentration even in the absence of driving force or concentration gradient. The diffusion process is related with the Markov process. The Markov process has three properties: drift, a random process and jump process. Thus a diffusion process is a Markov process that has continuous sample paths.

1.2.1 Derivation of diffusion equation [6]

The diffusion and conduction processes have a analogy. The diffusion is transport of molecules or material atoms with in effect of a random motion. Conduction is transport of electrons and heat by random motion. These mechanisms perform by Brownian motion in gases and liquids by vacancy or interstitial diffusion in solids. The cause or driving force for this diffusion phenomena is concentration gradient. The diffusion phenomenon is co-related to the mass transfer process. Mass transfer is happened when a mixture of substance travels from one point to another point in a medium. The process diffusion or convection is occurred by the mass transfer. So, it is said that the diffusion process is mass transfer in a fluid or stationary solid under the influence of concentration gradient. While convection is mass transfer between a boundary surface and a moving fluid. The difference between diffusion and convection can be understood by the example in which we dip a sugar piece into water. Then sugar is slowly and gradually dissolved in water. Thus is called diffusion. But if we stir it with a spoon and create forces to dissolve it, then this is called convection. Thus diffusion is slower and convection is faster.

Concentration gradient :

Let there are two media having concentration η_1 and η_2, respectively. If these are bring together then the molecules in a concentrated region will move or disperse into rest of the medium. The difference in concentration is the concentration gradient

$$\frac{-\Delta\eta_1}{\Delta x} = \frac{\eta_1 - \eta_2}{\Delta x} \tag{1.22}$$

Fick's law:

In the year 1855, Adolf Fick was the first who found the analogy between convection and diffusion. Let F is the rate of transfer per unit area of section, η is the concentration of diffusing substance and x is spatial co-ordinates which is measured normal to the section then according to this law

$$F \propto \frac{\partial \eta}{\partial x}, \tag{1.23}$$

$$\Rightarrow F = -D\frac{\partial \eta}{\partial x}, \tag{1.24}$$

where D is called diffusion coefficient . The negative sign in this equation corresponds the occurrences in the direction opposite to that of increasing concentration. This equation is valid for isotropic medium. The derivation of diffusion equation is performed with the help of Fick's law. Let us consider a volume of rectangular parallelepiped having sides parallel to the axes and length of $2dx$, $2dy$ and $2dz$ (see

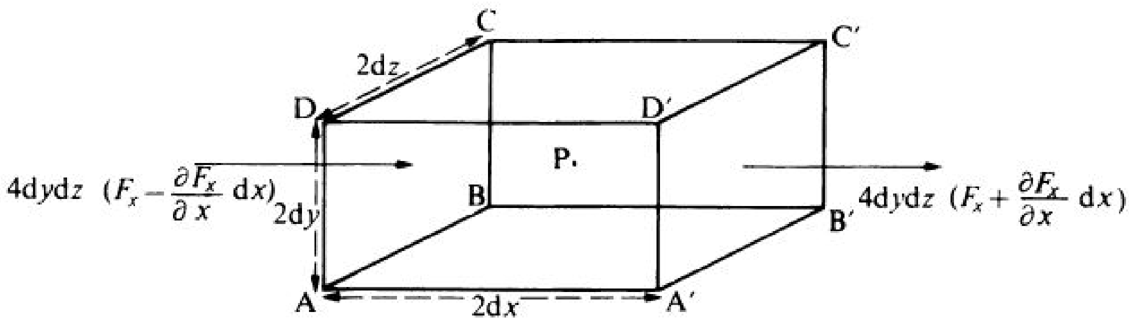

FIGURE 1.1: Geometry of considered rectangular volume

Fig.1.1). The concentration at center $P(x, y, z)$ of parallelepiped is η. The entering rate of diffusing substance through $ABCD$ is given by

$$4dxdydz(F_x - \frac{\partial F_x}{\partial x}dx),$$

with F_x is known as rate of transfer in one unit area. Similarly, diffusing matter pass with a rate of

$$4dxdydz(F_x - \frac{\partial F_x}{\partial x}dx),$$

The net contribution in the X direction

$$4dxdydz(F_x - \frac{\partial F_x}{\partial x}dx) - 4dxdydz(F_x - \frac{\partial F_x}{\partial x}dx) = -8dxdydz\frac{\partial F_x}{\partial x}.$$

Thus in the similar way, the net contribution in Y and Z directions is obtained as

$$-8dxdydz\frac{\partial F_y}{\partial y}, -8dxdydz\frac{\partial F_z}{\partial z},$$

respectively. The substance which is diffusing increases with a rate of

$$8dxdydz\frac{\partial \eta}{\partial t}.$$

Hence we have the following relation

$$8dxdydz\frac{\partial \eta}{\partial t} = -8dxdydz\frac{\partial F_y}{\partial y} - 8dxdydz\frac{\partial F_z}{\partial z} - 8dxdydz\frac{\partial F_x}{\partial x}. \tag{1.25}$$

$$\Rightarrow \frac{\partial \eta}{\partial t} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} + \frac{\partial F_x}{\partial x} = 0. \tag{1.26}$$

Considering diffusion coefficient as constants and using Fick's law, we have

$$\begin{aligned} \frac{\partial \eta}{\partial t} &= D\Big(\frac{\partial^2 \eta}{\partial y^2} + \frac{\partial^2 \eta}{\partial^2 z^2} + \frac{\partial^2 \eta}{\partial x^2}\Big), \\ \frac{\partial \eta}{\partial t} &= D\nabla^2 \eta. \end{aligned} \tag{1.27}$$

Reaction-diffusion phenomenon comprises the reaction process with diffusion process. In this common phenomenon, the concentration of the chemical substances change with change in space and time. And another local chemical reactions occur with transformation of substances into each other. This process is denoted by diffusion equation with adding of a reaction term $R(\eta)$ as

$$\frac{\partial \eta}{\partial t} = D\nabla^2 \eta + R(\eta). \tag{1.28}$$

Complex system along with anomalous diffusion:

In physics, the basic rule and theory based structure correspond the investigation of complex system structural and dynamical properties. The study of complex system plays a crucial role in many fields like as bio-polymers, polymers, liquid crystals, and life science. The pattern in complex system is different from the classical exponential Debye pattern [21]

$$\psi(\eta) = \psi_0\, e^{\frac{-\eta}{\tau}} \tag{1.29}$$

and with the help of Kohlravsh-Williams-Watts stretched exponential law [22], we obtain the following expression

$$\psi(\eta) = \psi_0 e^{(\frac{-\eta}{\tau})^\beta}, \quad 0 < \beta < 1. \tag{1.30}$$

Using the asymptotic power law, the following relation is derived as

$$\psi(\eta) = \psi_0 \Big(1 + \frac{\eta}{\tau}\Big)^{-n}, \quad n > 0 \tag{1.31}$$

In the same way, diffusion process does not follow the Gaussian statistics occurring in many complex systems and so Fick's law fails in describing this transport behavior. In the non-complex system, the linear time dependence of mean square displacement is observed which is consistent with Brownian motion. With the help of central limit theorem and Markovian nature

$$< x^2(t) >\sim K_1(t). \tag{1.32}$$

But in complex system, we found the non-linear behavior of mean square displacement as

$$< x^2(t) >\sim K_\beta t^\beta, \tag{1.33}$$

where the coefficient K_β denotes the generalized diffusion coefficient. We have picked up here the power law pattern, many other patterns also exist in nature like as logarithmic and time dependence. The above equation is in consistent with central limit theorem. This non-Gaussian behavior of complex system is due to waiting time distributions and broad spatial jump. Standard diffusion process is although in ubiquity but not every diffusion phenomenon occurring in universe is standard.

TABLE 1.1: Different type of fractional diffusion

Diffusion type	Scale	Medium
Richardson diffusion	$< x^2(t) >\sim t^3$	atmosphere turbulence
Super-diffusion	$< x^2(t) >\sim t^\gamma$, $1 < \gamma < 2$	transport in polymers turbulent plasmas Levy fights
Standard diffusion	$< x^2(t) >\sim t$	homogeneous media
Sub-diffusion	$< x^2(t) >\sim t^\gamma$ $0 < \gamma < 1$	porous media fractal media disordered media
Ultra slow diffusion	$< x^2(t) >\sim t(\ln t)^\gamma$ $1 < \gamma < 4$	Deterministic diffusion Sinai diffusion

Many phenomenon with experimental measurements show the validity of fractional diffusion equation. The summary table for fractional diffusion occurring in different fields is given in Table 1.1. The mathematical form of diffusion equation is represented as

$$\frac{\partial^\gamma u(x,t)}{\partial t^\gamma} = D\frac{\partial^2 u(x,t)}{\partial x^2}. \tag{1.34}$$

Memory concept of fractional derivatives

The main concerned problem for the researchers is to find out the physical meaning of fractional derivative. Memory concept of models is usually associated with fractional derivative. The meaning of memory of a system shows that "how much information this system contains/carries from its previous stage?" The integer order system carries the information only from its previous one stage. But the fractional derivative carries information from many past stages. The reason behind this is that fractional derivatives are non-local and integro-differential operators. In this work, the author has studied the Scott-Blair's model for showing the utility of fractional order derivative in memory concepts. In observations of this model, it is found that there are two stages of memory: the first one fresh memory and second one working memory. The fresh stage has short time-period with permanent retention. The fractional model of system depicts the working stage of memory. It is derived that the order of fractional derivative is equal to the index of memory.

1.3 Application of diffusion equation

The diffusion equation is a partial differential equation. Its application can be seen in many fields like medical science, earth science, chemical science and mechanical engineering.

1.3.1 Medical Science [7]

(i) The diffusion equation can be used in modeling of many diseases. In tumor or cancer treatment, this equation plays a crucial role because the diffusion of cancerous cells into normal cells can be depicted by diffusion equation system.

(ii) Diffusion equation is used in interactive medical image segmentation. The nonlinear isotropic and anisotropic diffusion methods are used in the treatment of sinus disease.

(iii) The diffusion based models represent better results in biomedical imaging like X-Ray.

1.3.2 Geological Science [8]

The earth is made up of lithospheric plate or tectonic plate. According to the famous plate tectonic theory, the crust of earth is combination of oceanic and continental plates. The movements of these plates are either convergent or divergent. When two plates converge the cooling effect between these plates are depicted by the diffusion equation. Some other applications can also be seen in the erosion of faults which are created due to divergence or convergence of tectonic plates.

1.3.3 Chemical Science [9]

The reaction between two substances causes by the mass transfer which is carried by the diffusion process. Diffusion equation has a key role in performing chemical reactions and mass transfer. The transport of penetrant molecules through polymeric membrane is done by the diffusion phenomena.

1.3.4 Physical Science [10]

The theories of current flow in semi-conductors are based upon the diffusion phenomena. In a region with mobile carrier electrons and electric field has low intensity, the current flow occurs due to diffusion phenomena. The diffusion of quantum waves in quantum physics is studied with the help of diffusion equation. The core design of pressurized water reactor in nuclear physics is based upon the diffusion theory. The nuclear fission is started with the bombarding of neutron on Uranium atom. The distribution of neutron flux in spatial direction in any diffusive medium is determined with the help of diffusion equation.

1.3.5 Ground water contamination problem [11]

Nowadays groundwater contamination is a concerning issue of many countries. The availability of drinking water on the earth is less than 1% of whole water available on earth. The main source of drinking water is ground water. But due to increasing pollution, this water is contaminating day by day. The diffusion equation plays a crucial role in studying this contamination diffusing in groundwater.

1.3.6 Economics [12]

The application of reaction-diffusion equation can be seen in lag-lead structure of competing economic entities. The complex interdependence between the economy of two countries which is a macro-economic variable is modeled by inter temporal diffusion.

1.4 Numerical methods

Derivation of the solution of differential equation is a tough task from the earlier time. The analytical methods have their own limitations as those are unable to find out the solution of complex non-linear differential equation specially the fractional one. This problem can be tackled by the numerical methods. These methods are easy to apply and give better results even for complex fractional differential equation. Many numerical methods have been developed till now. Some of those are as follows:

(i) **Finite difference method** [23, 24]

This is one of the oldest methods to find the numerical solutions of differential equations. After discretization of computation domain, the derivatives involve in differential equation are replaced by difference formulas. This gives the recursive algorithm and solution can be obtained by applying any of forward Euler scheme, backward Euler scheme and Crank-Nicolson scheme.

(ii) **Finite element method** [25]

In this method, firstly the domain is divided into sub-domains referred as elements. The interpolation functions are selected to approximate the unknown function. The Ritz variational or Galerkin method is used to formulate a system of equations. After solving such system, the solution can be obtained.

(iii) **Operational matrix method based upon polynomials** [26, 27]

A matrix of differentiation or integration is derived by using any polynomial. The approximation of all derivatives and unknown functions in terms of matrix are placed in given differential equation. In the end, the solution is obtained by collocating previous equation at nodes of that polynomial.

(iv) **Operational matrix method based upon wavelets** [28, 29]

This method is same as previous one. Here operational matrix is derived by using wavelet function.

(v) **Reproducing kernel method** [30]

A reproducing kernel space is defined in this method which depends upon the differential equation. In this space every member function satisfies the boundary condition. The unknown function is approximated with the help of functions belonging to that reproducing kernel space. The solution can be found out after determining the value of unknowns with the help of inner product.

(vi) **Homotopy perturbation method** [31]

An auxiliary operator L and initial approximation are chosen according to the given problem and a homotopy equation is determined. With the help of this homotopy equation, a series of successive solution is derived.

(vii) **Neural network method** [32]

In this method, feedforward networks are used for finding numerical solution. It uses the fact that these networks with linear output having no bias can be used in approximation of arbitrary functions and its applications.

(viii) **B-spline method** [33]

B-spline or basis spline functions are used for curve-fitting or fitting of numerical data. In B-spline method, unknown functions and its derivatives are approximated with help of these functions in collocation step.

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