“In his discovery of calculus, Leibniz first introduced the idea of a symbolic method and used the symbol $\frac{d^n y}{dx^n} = D^n y$ for the $n^{th}$ derivative, where $n$ is a non negative integer. L’Hospital asked Leibniz about the possibility of $n$ be a fraction. ‘What if $n = \frac{1}{2}$?’ Leibniz (1695) replied, ‘It will lead to a paradox.’ But he added prophetically, From this paradox, one day useful consequences will be drawn.”

GOTTFRIED LEIBNIZ.
1.1 Literature Review

The concept of fractional calculus is an old and yet new topic. In 1695, L’Hôpital wrote Leibniz about a notation he had used in his publication. He asked what would be the result of taking \( n = \frac{1}{2} \) in the derivative \( \frac{d^n x}{dx^n} \). Leibniz answered: “It will lead to a paradox, from which one day useful consequences will be drawn.” That is the first step of fractional calculus. Since then, many famous mathematicians have worked on this and related questions, creating the field which known today as fractional calculus. As list of mathematicians who have provided important contributions up to the middle of last century, includes Laplace, Fourier, Abel, Liouville, Riemann, Grunwald, Letnikov, Levy, Marchaud, Erdelyi and Riesz. Fractional derivatives describe a non-local approach that models long-range interactions between particles. In some physical processes, it cannot be assumed that particles move according to Brownian motion because particles can show velocities and excursion distances that are likely to have large, even infinite variance and a Gaussian distribution or second-order differential equation are not suited to describe the behavior (see Benson et al.[17]). The probability distribution that can be used is called a Levy \( \alpha \)-stable distribution. The Gaussian function is a special case of this class of distributions. Since from last three centuries, the theory of fractional calculus is developing in the theoretical field of mathematics.
The current state of knowledge in the application of fractional derivatives, the analytical and numerical approaches for solving fractional partial differential equations (FPDE) is explored.

A growing number of works in science and engineering deal with dynamical systems described by fractional order equations that involve derivative and integrals of noninteger order [77, 83, 86, 93]. In particular such models arise in system biology [118], physics [11, 15, 75, 76, 90, 119], chemistry and biochemistry [118], hydrology [17, 64, 65], medicine [48, 49, 58, 94] and finance [47, 74, 87, 112].

These fractional models solved analytically by number of authors. Wyss [95, 111] considered time fractional diffusion equation and Agrawal [7] considered time fractional diffusion-wave equation and obtained its solution in terms of Mittag-Leffler function. Liu et al. [65] obtained the solution of the time-fractional advection-dispersion equation by using integral transform method. Gorenflo et al. [46] derived the fundamental solution for the time fractional diffusion equation. Also Orsingher and Beghin [84] studied the fundamental solution to time-fractional telegraph equation.

Existence and uniqueness of solution of fractional diffusion equations are well studied by Dhaigude [34].

Number of models in the fractional calculus are complex and it is difficult to solve analytically in such cases numerical techniques play very important role. The existing numerical techniques for equations involving fractional differential equations are based on random walk models [45, 46, 67, 73] and it is studied by the finite difference method [21–23, 50, 64, 66, 67, 74, 89, 97, 104], the finite element method [40, 89], numerical quadrature [8, 57], Monte Carlo simulation [41, 72], discrete Adomian decomposition method [18, 122] and the matrix transform method [53, 54, 114].

We mainly concentrate on finite difference methods. Liu et al. [67] developed an explicit finite-difference scheme for the time fractional diffusion equation (TFDE) and its stability as well as convergence is discussed. Yuste and Acedo [116] proposed an explicit finite difference method and new von Neumann type stability analysis for the fractional subdiffusion equation. Zhang et al. [121] investigated a numerical approximation of the Levy-Feller diffusion equation and gave its probabilistic interpretation.

The various researchers have applied finite difference methods and solved space-time FPDEs. Liu et al. [62], Liu et al. [63] and Zhuang et al. [125] developed implicit finite difference scheme for space-time fractional diffusion equation, advection-diffusion equation, Fokker-Planck equation respectively. They also investigated the stability
and convergence of the implicit finite difference scheme. Langlands and Henry [58] investigated the accuracy and stability of an implicit numerical scheme for solving the fractional sub-diffusion equation.


Liu et al. [65] developed the numerical technique for fractional diffusion equation with nonlinear source term. Also Zhang and Liu [121] consider Riesz space fractional diffusion equation with nonlinear source term and Yang et al. [118] provided the numerical solution of fractional Fokker Plank equation with nonlinear source term and proved its stability as well as convergence.
1.2 Finite Difference Method

The finite difference method is a universal and efficient numerical method for solving differential equations. It’s intensive development, began at the end of 1940’s and the beginning of 1950’s and stimulated by the need to cope with a number of complex problems of science and technology. Powerful computers provided an impetus of paramount importance for the development and application of the finite difference method which in itself is simple in utilization. A large number of complicated multidimensional problems in electrodynamics, elasticity theory, fluid mechanics, gas dynamics, theory of particle and radiation transfer, atmosphere and ocean dynamics and plasma physics are solved employing the finite difference techniques.

The finite difference method for partial differential equations has a relatively short history. After the fundamental theoretical paper by Cournt, Friedrichs and Lewy (1928) on the solution of the problems of mathematical physics by means of finite differences. Now a day finite difference methods are extended to obtain the solution of fractional differential equations.

1.2.1 Finite Difference Formulae of Partial Derivatives

The finite difference approximations to partial derivatives can be obtained from Taylor’s series expansions. Let \( u(x, t) \) be a function of two variables \( x \) and \( t \). Let the subscripts \( j \) represents \( x \) and
subscript $n$ represents time $t$. Let mesh spacing in $x$ and $t$ directions are denoted by $\Delta x$ and $\Delta t$. Thus $u(x, t)$ can be represented by $u(j \Delta x, n \Delta t) = u^n_j$. The Taylor’s series expansion of $u^n_j$ about the grid point $(j, n)$ gives

$$u^n_{j+1} = u^n_j + \left[ (\Delta x) \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} + \ldots \right]_j^n \quad (1.2.1)$$

$$u^n_{j-1} = u^n_j - \left[ (\Delta x) \frac{\partial u}{\partial x} - \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} + \ldots \right]_j^n \quad (1.2.2)$$

Solving for $\frac{\partial u}{\partial x}$, equation (1.2.1) gives

$$\left( \frac{\partial u}{\partial x} \right)_j^n = \frac{u^n_{j+1} - u^n_j}{\Delta x} + O(\Delta x) \quad (forward) \quad (1.2.3)$$

while equation (1.2.2) gives

$$\left( \frac{\partial u}{\partial x} \right)_j^n = \frac{u^n_j - u^n_{j-1}}{\Delta x} + O(\Delta x) \quad (backward) \quad (1.2.4)$$

The above forward and backward finite difference approximations are first order accurate.

Subtracting equation (1.2.2) from equation (1.2.1), we obtain

$$\left( \frac{\partial u}{\partial x} \right)_j^n = \frac{u^n_{j+1} - u^n_{j-1}}{2\Delta x} + O(\Delta x)^2 \quad (1.2.5)$$

This is a central difference approximation to the derivative $\frac{\partial u}{\partial x}$, and is second order accurate, in the sense that it has a truncation error of order $O(\Delta x)^2$. The central difference approximation to the second order partial derivative $\frac{\partial^2 u}{\partial x^2}$ can be similarly obtained by adding
equations (1.2.1) and (1.2.2),

\[
\left( \frac{\partial^2 u}{\partial x^2} \right)_j^n = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} + O(\Delta x)^2
\]

(1.2.6)

which is second order accurate.

**Errors Involved in Numerical Solutions**

In the study of the numerical solution of differential equations with finite differences, a variety of schemes are available for the discretization of the problem. In many situations, questions arise regarding the round-off and truncation errors involved in the numerical computations, as well as the stability and the convergence of the finite difference scheme. Here we present a brief description of physical significance of these terminologies.

**Round-off Errors**

Computations are rarely made in exact arithmetic. This means that real numbers are represented in ”floating point” form and as a result, errors are caused due to the rounding-off of real numbers. Even though modern computers represent numbers to twelve or more places of decimals, in extreme case such errors, called round-off errors, accumulate and become a main source of error.

**Truncation Error**

In finite difference representation of derivatives with Taylor’s series expansion, the higher order terms are neglected by truncating the series and the error caused due to such truncation is called the truncation error. For example, in forward difference of the first derivative
to the order $\Delta x$ as follows

$$O(\Delta x) = -\frac{1}{2}(\Delta x)f''(x_0) - \frac{1}{6}(\Delta x)^2 f'''(x_0) + ...$$  \hspace{1cm} (1.2.7)

represents the truncation error and the lowest order term on the right hand side that is $\Delta x$ gives the order of the method.

**Stability**

In numerical solution of differential equations with finite differences, errors are introduced at almost every stage of the calculations. The solution scheme is said to be stable if the error involved in numerical computations are not amplified without bounds.

**Convergence**

The numerical solution is said to be convergent if the numerical solution approaches the exact solution of the problem as the time and space steps tend to zero. We note that the conditions of stability and convergence are related to each other. The total error involved in finite difference calculations consists of the discretization error plus the round-off error. The discretization error increases with increasing mesh size while the round-off error decreases with increasing mesh size. Therefore, the total error is expected to exhibit a minimum as the mesh size is decreased.
1.3 Difference Scheme

The problem of finite difference scheme for the numerical solution of the initial boundary value problem is considered by many researchers see [81, 88, 100]. In case of an analytical solution of a partial differential equation, its solution is found in a region of continuous change of the variables \(x\) and \(t\), but in the case of approximate solution of partial differential equation by method of finite-difference is determined only at some discrete points of \((x, t)\) plane. Consider the set of points

\[
a = x_0 < x_1 < ... < x_N = b
\]  

(1.3.1)

It is called the computing mesh in the interval \([a, b]\) or the computational grid or spatial grid. The points \(x_j\) from the set (1.3.1) are called nodes of the spatial grid. Similarly to the set (1.3.1), we define a mesh on the \(t\) axis as follows:

\[
0 = t_0 < t_1 < ... < t_N = T
\]  

(1.3.2)

The meshes (1.3.1) and (1.3.2) are called uniform, if the following conditions are satisfied

\[
x_j = a + jh; \quad j = 1, 2, ..., M
\]

\[
t_n = n\tau; \quad n = 0, 1, ..., N
\]
The quantity $h = \frac{(b-a)}{M}$ is called the step of the spatial mesh and $
abla = \frac{T}{N}$ is called the time step. Now to introduce the uniform mesh $G_h$ in the $(x, t)$ plane as finite set of points of intersection of straight lines

$$x_j = a + jh; \ j = 1, 2, \ldots, M$$
$$t_n = n\tau; \ n = 0, 1, \ldots, N$$

*Fig. 1.1: The uniform mesh $G_h$ in the $(x, t) – plane.$*

The function $u_j^n = u(x_j, t_n)$ is determined at the nodes of the grid $G_h$ is called a grid function.

### 1.3.1 Finite Difference Schemes

There are three important finite difference schemes. They are

(i) Explicit finite difference scheme
(ii) Implicit finite difference scheme
(iii) Crank-Nicolson finite difference scheme.

Now, we see one by one.

**Explicit finite difference scheme**

We consider a diffusion equation in a finite region $0 \leq x \leq L$ in the form

$$\frac{\partial u(x, t)}{\partial t} = \nu \frac{\partial^2 u(x, t)}{\partial x^2}, \quad 0 < x < L, \ t > 0 \quad (1.3.3)$$

To construct the uniform mesh $G_h$ in the $(x, t)$ - plane as in fig. 1.1, the region $0 \leq x \leq L$ is divided into $M$ equal parts of mesh size $\Delta x = \frac{L}{M}$. The diffusion equation (1.3.3) is discretized by using the forward difference for time derivative and central difference for space derivative. We get

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \nu \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{(\Delta x)^2} \quad (1.3.4)$$

where

$$u(x, t) = u(j \Delta x, n \Delta t) \equiv u^n_j$$

Equation (1.3.4) is rearranged as

$$u_j^{n+1} = ru_j^{n} + (1 - 2r)u_j^n + ru_{j+1}^n \quad (1.3.5)$$

where

$$r = \frac{\nu \Delta t}{(\Delta x)^2}, \quad j = 1, 2, ..., M - 1, \ n = 0, 1, 2, ...$$
with the truncation error of order $O[(\Delta t), (\Delta x)^2]$. The equation (1.3.5) is called the explicit form of finite-difference approximation of the diffusion equation (1.3.3), because it involves only one unknown $u_j^{n+1}$ for the time level $n + 1$, which can be directly calculated from equation (1.3.5) when the potentials $u_{j-1}^n$, $u_j^n$ and $u_{j+1}^n$ at the previous time level $n$ are known.

The finite difference molecules for the explicit scheme.

**Implicit finite difference scheme**

We replace the time derivative by forward difference and space derivative by central difference at time level $n + 1$ in the equation (1.3.3), we have

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \nu \frac{u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{(\Delta x)^2} \quad (1.3.6)$$

Equation (1.3.6) is rearranged as

$$-ru_j^{n+1} + (1 + 2r)u_j^{n+1} - ru_{j+1}^{n+1} = u_j^n$$
Crank-Nicolson finite difference scheme

In 1947, Crank and Nicolson proposed a method in which \( \frac{\partial^2 u}{\partial x^2} \) is replaced by the average of its finite-difference approximations on the \( n^{th} \) and \( (n + 1)^{th} \) time level. The diffusion equation (1.3.3) is discretized as follows:

\[
\frac{u_{j+1}^{n+1} - u_j^n}{\Delta t} = \nu \frac{1}{2} \left\{ \frac{u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{(\Delta x)^2} + \frac{u_j^n - 2u_j^n + u_{j+1}^n}{(\Delta x)^2} \right\}
\]

(1.3.7)

Equation (1.3.7) is rearranged as

\[-ru_{j-1}^{n+1} + (2 + 2r)u_j^{n+1} - ru_{j+1}^{n+1} = ru_{j-1}^n + (2 - 2r)u_j^n + ru_{j+1}^n\]

The finite difference molecules for the Crank-Nicolson scheme.
1.4 Definitions and Basic Results

In this section, we set up notations, basic definitions and main properties of Riemann-Liouville integral as well as relation between Riemann-Liouville integral as well as Caputo fractional derivative from fractional calculus.

**Gerschgorin’s Circle Theorem or Brauer’s Theorem**[100]

It is stated as follows:

**Theorem 1.4.1.** Let $P_s$ be the sum of the moduli of the elements along the $s^{th}$ row excluding the diagonal element $a_{ss}$. Then the each eigenvalue of matrix $A$ lies inside or on the boundary of at least one of the circles $|\lambda - a_{ss}| = P_s$.

Now, we define useful definitions

**Definition 1.4.1.** [44] Let $||X||$ be a vector norm. Then the corresponding natural matrix norm is denoted by $||A||$ and is defined as

$$||A|| = \max_{||X||=1} \left\{ \frac{||AX||}{||X||} \right\}$$

Also the row norm $||A||_\infty$ and column norm $||A||_1$ are defined as follows:

$$||A||_\infty = \max_{1 \leq i \leq n} \left\{ \sum_{j=1}^{n} |a_{ij}| \right\}$$

$$||A||_1 = \max_{1 \leq j \leq n} \left\{ \sum_{i=1}^{n} |a_{ij}| \right\}$$
**Definition 1.4.2.** [56] A real function $f(x), x > 0$ is said to be in space $C_\alpha, \alpha \in \mathbb{R}$ if there exists a real number $p > \alpha$ such that $f(x) = x^p f_1(x)$ where $f_1(x) \in C[0, \infty)$.

**Definition 1.4.3.** [56] A function $f(x), x > 0$ is said to be in space $C^m_\alpha, m \in \mathbb{N} \cup \{0\}$ if $f^m \in C_\alpha$.

The Mittag-Leffler function is very useful in the study of fractional differential equations. We define Mittag-Leffler functions of one and two parameters as follows

**Definition 1.4.4.** [86] Mittag-Leffler function of one parameter is denoted by $E_\alpha(z)$ and is defined as

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}.$$ 

Here $\alpha > 0$ is a parameter.

**Definition 1.4.5.** [86] Mittag-Leffler function of two parameter is denoted as $E_{\alpha,\beta}(z)$ and is defined as

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}.$$ 

Here $\alpha > 0, \beta > 0$ are the parameters.

**Definition 1.4.6.** [86] Let $f \in C_\alpha$ and $\alpha \geq -1$, then Riemann-Liouville fractional integral of $f(x,t)$ with respect to $t$ of order $\alpha$ is denoted by $J^\alpha f(x,t)$ and is defined as

$$J^\alpha f(x,t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} f(x,\tau) d\tau, t > 0, \alpha > 0$$
The well known property \([86]\) of the Riemann-Liouville operator \(J^\alpha\) is
\[
J^\alpha t^\gamma = \frac{\Gamma(\gamma + 1)t^{\gamma + \alpha}}{\Gamma(\gamma + \alpha + 1)}
\]

**Definition 1.4.7.** [56] For \(m\) to be the smallest integer that exceeds \(\alpha > 0\), the Caputo fractional derivative of \(u(x, t)\) with respect to \(t\) of order \(\alpha > 0\) is denoted by \(D^\alpha_t u(x, t)\) and is defined as
\[
D^\alpha_t u(x, t) = \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \left\{ \begin{array}{ll}
\frac{1}{\Gamma(m+\alpha)} \int_0^t (t - \tau)^{m-\alpha-1} \frac{\partial^m u(x, t)}{\partial t^m} d\tau \\
\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x, y, \xi)}{\partial \xi} \frac{d\xi}{(t - \xi)^\alpha}, & 0 < \alpha < 1; \\
\frac{1}{\Gamma(2-\beta)} \int_0^t \frac{\partial^2 u(x, y, \xi)}{\partial x^2} \frac{d\eta}{(t - \eta)^{\beta - 1}}, & 1 < \beta < 2;
\end{array} \right.
\]

Note that the relation between Riemann-Liouville operator and Caputo fractional differential operator is given as follows
\[
J^\alpha(D^\alpha f(x, t)) = (J^{m-\alpha} f^{(m)})(t) = f(x, t) - \sum_{k=0}^{m-1} \frac{f^{(k)}(x, 0)}{k!} t^k,
\]

The Riemann-Liouville fractional derivative of order \(\beta(1 < \beta \leq 2)\) is denoted by \(R D^\beta_x u(x, t)\) and is defined as
\[
R D^\beta_x u(x, t) = \left\{ \begin{array}{ll}
\frac{1}{\Gamma(2-\beta)} \int_0^t \frac{\partial^2 u(x, y, \xi)}{\partial x^2} \frac{d\eta}{(t - \eta)^{\beta - 1}}, & 1 < \beta < 2; \\
\frac{\partial u(x, y, t)}{\partial t}, & \beta = 2.
\end{array} \right.
\]

where as the Caputo fractional derivative of \(u(x, y, t)\) of order \(\alpha(0 < \alpha \leq 1)\) is defined [56] as
\[
\frac{\partial^\alpha u(x, y, t)}{\partial t^\alpha} = \left\{ \begin{array}{ll}
\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x, y, \xi)}{\partial \xi} \frac{d\xi}{(t - \xi)^\alpha}, & 0 < \alpha < 1; \\
\frac{\partial u(x, y, t)}{\partial t}, & \alpha = 1.
\end{array} \right.
\]
and the Riemann-Liouville fractional derivatives $D^\beta_x u(x, y, t)$ and $D^\gamma_y u(x, y, t)$ is defined as

$$D^\beta_x u(x, y, t) = \begin{cases} \frac{1}{\Gamma(2-\beta)} \frac{\partial^2}{\partial x^2} \int_0^t \frac{u(\eta, y, t) d\eta}{(x-\eta)^\beta}, & 1 < \beta < 2; \\ \frac{\partial^2 u}{\partial x^2}, & \beta = 2. \end{cases}$$

$$D^\gamma_y u(x, y, t) = \begin{cases} \frac{1}{\Gamma(2-\Gamma)} \frac{\partial^2}{\partial y^2} \int_0^t \frac{u(x, \zeta, t) d\zeta}{(y-\zeta)^\Gamma}, & 1 < \gamma < 2; \\ \frac{\partial^2 u}{\partial y^2}, & \gamma = 2. \end{cases}$$

### 1.5 Plan of the Thesis

Chapter-2 is developed for the discrete Adomian decomposition method and the solution of fractional diffusion equation, fractional Schrodinger equation, fractional Burger’s equation as well as system of fractional Burger’s equations respectively are obtained. The method is illustrated by suitable examples for all types of equations. The graphical representation of solution is also given using MATLAB software. Chapter-3 is devoted for a implicit finite difference scheme for time fractional, space-time fractional and two dimensional space-time fractional semilinear partial differential equations respectively. It is proved that the implicit finite difference scheme is stable as well it is convergent in each case. Numerical solution of the test problem is obtained and it is simulated by using MATLAB software. In Chapter-4 the variable order semilinear fractional diffusion equation is studied. The stability and convergence is proved by using Fourier
method. Finally test problems are discussed using MATLAB. In Chapter-5 the study of the more general weighted average finite difference scheme is taken up. Using Greschgorin’s circle theorem it is shown that the weighted average finite difference scheme is conditionally stable. Numerical solution of the test problem is obtained and it is simulated by using MATLAB software.