FRACTIONAL BLOCK BACKWARD DIFFERENTIATION FORMULA FOR SOLVING ORDINARY DIFFERENTIAL EQUATIONS OF FRACTIONAL-ORDER

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UNIVERSITI SAINS MALAYSIA

2025

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by

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**Thesis submitted in fulfilment of the requirements
for the degree of
Doctor of Philosophy**

September 2025

ACKNOWLEDGEMENT

I would like to begin by expressing my utmost appreciation to Ts. Dr. Siti Ainor Mohd Yatim, the head of the supervisory committee, for her priceless counsel, guidance, support, and particularly for her constructive feedback. The successful completion of this thesis was made possible due to the invaluable assistance I obtained from her in numerous facets of the research. I would want to express my gratitude to Dr. Yazariah Mohd Yatim, a member of the supervision committee. I would like to express my sincere gratitude to my esteemed colleagues for their invaluable guidance and support, which has significantly contributed to the successful completion of my thesis. Special recognition is given to Asma Izzati Asnor, who has dedicated significant effort to the discussion and development of the algorithms over the duration of my project. I would like to thank Universiti Utara Malaysia and the Malaysia of Higher Education for providing me with a scholarship and study leave that has allowed me to undertake this research endeavour. I am profoundly grateful for the unwavering support, understanding, and patience exhibited by my spouse, Luqman, as well as my daughters, Sofea and Diana. Additionally, I extend my heartfelt appreciation to my parents, Mohamad Noor and Roszuzana, for their persistent encouragement.

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LIST OF SYMBOLS

α	Fractional order
β, γ, μ	Variables
$\Gamma(\cdot)$	Gamma function
$B(\cdot)$	Beta function
$\mathbb{Z}$	The set of integer number
$\mathbb{C}$	The set of complex number
$E_\alpha(\cdot)$	Mittage-Leffler function
∞	Infinity
${}^{C}D_{t_0}^{\alpha}$	Caputo fractional derivatives
${}^{RL}D_{t_0}^{\alpha}$	Riemann-Liouville fractional derivatives
L	Lipschitz condition
h	Step size
L_i	Linear difference operator
$y_i(t_n)$	The approximate solution
$y_i(t)$	The exact solution
$\pi(x;\bar{h})$	The stability polynomial

LIST OF ABBREVIATIONS

2BBDF	2-point BBDF for solving first order ODEs
2FBBDF(N)	Nth order of 2-point Fractional BBDF for solving FDEs with $\alpha \in (0,1]$
2OBBDF	Fifth order off step 2BBDF
2SBBDF	2-point Superclass BBDF for solving first order ODEs
3BBDF	3-point BBDF for solving first order ODEs
BBDF	Block Backward Differentiation Formula
BBDFO(6)	Sixth order off step 2BBDF
BBDF-VS	Variable step 2BBDF
DI2BBDF	Diagonally implicit 2BBDF
DI2OBBDF	Diagonally implicit 2BBDF with off step points
DIE2OSBBDF	Diagonally implicit extended 2BBDF with off step points
EHPM	Elzaki homotopy perturbation method for solving FDEs
FBBDF2	Variable step variable order 2-point Fractional BBDF for solving FDEs with $\alpha \in (1,2]$
FDEs	Fractional Differential Equations
FDTM	Fractional differential transform method for solving FDEs
FIM-SCP	Finite integration method using shifted Chebyshev polynomial for solving FDEs
FLMM	Fractional linear multistep method
GMBDF	Generalized multistep Adams and BDF
LMM	Linear multistep method
LTE	Local truncation error
MSFDTM	Multistep fractional differential transform method for solving FDEs
MVS-BBDF	Modified variable step BBDF

NBDF	Non-block Backward Differentiation Formula
NODEs	Non-stiff ODEs
NVSBBDF	Novel variable step 2BBDF
ODEs	Ordinary differential equations
SDIBBDF	Singly diagonally implicit BBDF
SDRK	Singly diagonally Runge-Kutta method
VS2FBBDF(N)	Nth order variable step 2-point Fractional BBDF for solving FDEs with $\alpha \in (0,1]$
VSBBDF	Fifth order variable step 2BBDF
VSFBBDF2(N)	Nth order variable step 2-point Fractional BBDF for solving FDEs with $\alpha \in (1,2]$

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FORMULA PEMBEZAAN KE BELAKANG BLOK PECAHAN UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA PERINGKAT PECAHAN

ABSTRAK

Kebanyakan persamaan pembezaan pecahan (PPP) tidak mempunyai penyelesaian analitik yang tepat disebabkan oleh kesan ingatan dalam sistem dunia sebenar. Walaupun pelbagai kaedah berangka telah dibangunkan, kaedah-kaedah ini sering menghadapi kekangan dari segi ketepatan, penumpuan, atau kestabilan, terutamanya apabila digunakan pada masalah yang melibatkan dinamik berubah-ubah. Oleh itu, dalam tesis ini, 2-titik formula pembezaan ke belakang blok pecahan yang baharu (2FPBBP) dirumus bagi menyelesaikan PPP dengan peringkat pecahan, $\alpha \in (0,1]$ dan $\alpha \in (1,2]$. Kaedah pecahan berbilang langkah linear (PBLL) dilaksanakan dengan pengembangan siri Taylor untuk mendapatkan nilai pekali kaedah tersebut. Kaedah 2FPBBP dengan langkah tetap dan berubah dibangunkan dengan peringkat 3, 4, dan 5 untuk menyelesaikan PPP dengan $\alpha \in (0,1]$. Bagi kaedah langkah berubah, strategi memilih nisbah saiz langkah diterangkan untuk mengurangkan lelaran pengiraan. Kaedah ini mempunyai keputusan yang kompetitif berbanding dengan kaedah berangka sedia ada dari segi ketepatan. Kemudian, pelbagai peringkat pecahan, α = 0.7, 0.8, 0.9, dan 1.0, digunakan untuk mengkaji tingkah laku simulasi. Selepas itu, langkah berubah kaedah 2FPBBP dikembangkan kepada kaedah langkah berubah peringkat berubah 2FPBBP untuk menyelesaikan PPP dengan $\alpha \in (1,2]$ secara langsung tanpa mengurangkannya kepada persamaan sistem peringkat pertama. Prosedur yang sama digunakan untuk mendapatkan nilai pekali

kaedah. Kaedah Langkah berubah ini terdiri daripada peringkat 2, 3, dan 4, yang digabungkan bersama dalam satu kod untuk mengira penyelesaian. Pembangunan algoritma itu memberi kelebihan kepada proses pengiraan kerana ia mengoptimumkan penyelesaian dan menjimatkan lelaran pengiraan. Keputusan berangka menunjukkan prestasi kaedah lebih baik daripada kaedah perbandingan dari segi ralat mutlak. Sifat penumpuan kaedah yang dibangunkan dikaji dengan menentukan konsistensi dan kestabilan sifarnya. Konsistensi dibuktikan dengan menentukan peringkat kaedah, manakala kestabilan sifar ditentukan dengan menyelesaikan punca-punca bagi polynomial kestabilan, dan syarat yang mesti dipenuhi ialah modulus setiap punca mestilah kurang atau sama dengan 1. Kemudian, rantau kestabilan diplot menggunakan polinomial kestabilan dengan $\alpha = \{0.7, 0.8, 0.9, 1.0\}$ dan $\{1.7, 1.8, 1.9, 2.0\}$ untuk kaedah menyelesaikan PPP dengan $\alpha \in (0,1]$ dan $\alpha \in (1,2]$. Keadaan ini perlu disahkan bagi memastikan bahawa kaedah ini boleh menghasilkan penyelesaian pada sebarang nilai α dan menumpu kepada penyelesaian yang tepat. Kesimpulannya, keaslian tesis ini terletak pada pembangunan kaedah pelbagai peringkat berasaskan blok yang secara langsung menyelesaikan PPP dengan $\alpha \in (0,1]$ dan $\alpha \in (1,2]$, di mana keupayaan itu biasanya tidak dipertimbangkan dalam kaedah yang sedia ada. Hasil daripada kajian ini adalah keupayaannya untuk berfungsi sebagai penyelesaian alternatif untuk menyelesaikan model pecahan dalam bidang kejuruteraan, fizik, dan pelbagai sains gunaan yang lain.

FRACTIONAL BLOCK BACKWARD DIFFERENTIATION FORMULA FOR SOLVING ORDINARY DIFFERENTIAL EQUATIONS OF FRACTIONAL-ORDER

ABSTRACT

Most fractional differential equations (FDEs) lack precise analytical solutions which reflect memory effects in real-world systems. Although various numerical methods have been developed, they often suffer from limitations in accuracy, convergence, or stability, especially when applied to problems involving variable dynamics. Therefore, in this thesis, a new 2-point fractional block backward differentiation formula (2FBBDF) is formulated to solve FDEs with fractional order, $\alpha \in (0,1]$ and $\alpha \in (1,2]$. The fractional linear multistep methods (FLMMs) are implemented with the Taylor series expansion to obtain the coefficient values of the method. The fixed and variable step 2FBBDF methods are developed with orders 3, 4, and 5 to solve FDEs with $\alpha \in (0,1]$. For the variable step method, the strategy of selecting the step size ratio is explained in order to reduce the computational iterations. The method has a competitive result in comparison with the existing numerical methods in terms of accuracy. Then, various fractional orders, α = 0.7, 0.8, 0.9, and 1.0, are considered to study the behaviour of the simulation. Subsequently, the variable step of the 2FBBDF method is extended to the variable step variable order 2FBBDF method to solve FDEs with $\alpha \in (1,2]$ directly without reducing it to first-order systems equations. The similar procedure is applied to obtain the coefficient values of the method. The variable order of the method consists of orders 2, 3, and 4, which are combined together in a single code to compute the solution. The development of algorithms gives an advantage to the computational process because it optimises the solution and saves the computational iterations. Numerical results demonstrate the performance of the method better than the methods of comparison in terms of absolute error. The convergence properties of the proposed methods are studied by determining their consistency and zero stability. The consistency is proved by determining the order of the method, while the zero stability is determined by solving the roots of the stability polynomial, and the condition of the modulus of roots must be less than or equal to 1. Then, the stability region is plotted using the stability polynomial with $\alpha = \{0.7, 0.8, 0.9, 1.0\}$ and $\{1.7, 1.8, 1.9, 2.0\}$ for the method to solve FDEs with $\alpha \in (0,1]$ and $\alpha \in (1,2]$, respectively. These conditions need to be verified to ensure that the methods can produce the solution at any value of α and converge to the exact solution. In conclusion, the originality of this thesis lies in the development of a block-based, variable-order method that directly solves FDEs with $\alpha \in (0,1]$ and $\alpha \in (1,2]$, where that capability not typically considered in existing methods. The consequences of this study are its capacity to serve as alternative solver for resolving fractional models in the field of engineering, physics, and various other applied sciences.

CHAPTER 1

INTRODUCTION

1.1 Introduction

Fractional calculus refers to a theoretical framework that encompasses the concepts of integrals and derivatives of any order. This framework serves to unify and extend the traditional conceptions of differentiation and integration, which are limited to integer orders (Podlubny, 1998). Fractional differential equations (FDEs) have emerged as a generalized form of classical differential equations and have garnered significant attention in recent decades due to its wide-ranging applications in various scientific and engineering disciplines. Numerous empirical observations have indicated that the characteristics of a physical system are influenced not alone by its present state, but also by its past states. Hence, because to the localized nature of the integer order differential operator, classical models are inadequate in providing an optimal depiction of true phenomena. The utilization of differential equations using fractional derivative operators has gained significant traction in the scientific community due to the nonlocal characteristics exhibited by these operators. This approach has proven successful in accurately describing various physical processes, leading to its increasing popularity (Alkresheh, 2017).

Multiple definitions exist for the fractional derivative with an order $\alpha > 0$. The two most frequently employed definitions are the Riemann-Liouville and Caputo definitions. These two definitions are often not equivalent. The distinction between these entities lies in the way the evaluation is conducted. Nevertheless, the two definitions are considered comparable when their initial circumstances are homogeneous. In this study, the Caputo fractional derivative is employed because of its ability to incorporate beginning conditions of integer order within the issue formulation.

Typically, the precise analytical solution for FDEs is often unattainable, particularly when dealing with nonlinear issues. Numerical and analytical methods have been employed to derive an approximate solution for these types of problems. While numerical approximation approaches have broad use in practical scenarios, approximate analytical methods offer solutions with great accuracy and profound physical understanding. One of the notable benefits of approximate analytical methods is in their capacity to offer an analytical depiction of the solution, hence enhancing the understanding of the solution across the temporal domain. Conversely, numerical approaches yield solutions in a numerical and discretized format, hence introducing complexity in attaining a continuous representation. The primary objective of this thesis is to investigate and devise analytical techniques for solving initial value problems pertaining to FDEs.

1.2 Problem Statement

Most FDEs lack precise analytical solutions due to their inherent complexity and non-local characteristics. FDEs have become increasingly relevant in modelling real-world phenomena, particularly in systems with memory effects. Consequently, FDEs have been extensively employed as a mathematical framework in numerous practical applications. The adaptability of fractional order derivatives, α, especially for $\alpha \in (0,1]$ and $\alpha \in (1,2]$, facilitates improved alignment with empirical data and increases the predictive precision of the models. There are many approximate methods for solving FDEs, such as the fractional Adams-Moulton method (Scherer et al., 2011), the Grünwald-Letnikov method (Scherer et al., 2011), the multistage Bernstein polynomials (Alshbool & Hashim, 2016), the finite difference time domain method (Alkresheh & Ismail, 2021), the Laplace-residual power series method (Oqielat et al., 2023), the fractional backward differentiation formula method (Huang et al., 2012; Bonab & Javidi, 2020), etc. However, many of these methods have problems with convergence, stability, or accuracy. Moreover, the majority of current methodologies rely on fixed step sizes and tend to be less effective when addressing issues with variable dynamics. Therefore, there is a need to develop adaptable numerical methods such as the Block Backward Differentiation Formulas (BBDF), both in fixed and variable step versions, to efficiently and accurately solve FDEs across different fractional orders, specifically for $\alpha \in (0,1]$ and $\alpha \in (1,2]$.

Even though there are numerous numerical methods have been established for FDEs, the method exhibits limitations related to stability, accuracy, or convergence. A thorough analysis of the stability and convergence properties of the proposed methods is crucial, specifically regarding their zero stability, consistency, and the breadth of their stability region. This analysis is essential to confirm that the methods are dependable and resilient across a diverse array of FDE issues.

The creation of precise and effective fractional numerical methods significantly depends on the processes of derivation and algorithm development. A primary challenge in block-type methods is the implementation of convolution quadrature, especially in calculating the quadrature weights. Therefore, MAPLE software is essential for systematically handling the derivations. However, for practical numerical experimentation and performance validation, the methods must be converted into executable code. Hence, implementing the derived algorithms in C++ programming ensures that the methods can be tested across various problem types and computational setups.

Although various numerical methods exist for solving FDEs, a comparative performance evaluation is essential to determine their computational efficiency and accuracy. Numerous existing methods, although widely used, may not deliver satisfactory results over extended intervals or under high computational costs. A comprehensive comparison between the proposed fractional BBDF methods and established methods is important. This evaluation will ensure the advantages regarding convergence behaviour, error control, and computational efficiency, thereby validating the practical significance of the newly developed methods.

1.3 Research Questions

The research questions for this thesis are listed as follows:

1. How can 2-point Fractional Block Backward Differentiation Formulas (FBBDF) of third to fifth order be derived for solving fractional differential equations (FDEs) with fractional order, $\alpha \in (0,1]$?
2. How can a 2-point Variable Step FBBDF be constructed to effectively solve FDEs with $\alpha \in (0,1]$ and $\alpha \in (1,2]$?
3. What are the stability and convergence properties of the derived methods in terms of their stability region, zero stability, and consistency?
4. How can the proposed method be developed using MAPLE software and subsequently implemented in C++ programming to support numerical experimentation and validation?

5. How does the numerical performance of the derived methods compare to the existing methods in terms of computational efficiency in solving the FDEs problems?

1.4 Objective of the Thesis

The main objective of this thesis is to devise computational techniques for FDEs, specifically referred to as Fractional Block Backward Differentiation Formulas (FBBDF). The objectives of this study are:

1. To derive 2-point FBBDF of third order up to fifth for solving FDEs with fractional order, $\alpha \in (0,1]$.
2. To construct 2-point Variable Step FBBDF for solving FDEs with $\alpha \in (0,1]$ and $\alpha \in (1,2]$.
3. To examine the stability and convergence characteristics of the derived methods through the assessment of their stability region, zero stability, and consistency.
4. To develop efficient algorithms for these methods and implement it in the C++ programming language for facilitating numerical experimentation and validation.
5. To evaluate and compare the numerical performance of the methods against existing methods in terms of computational efficiency for solving FDEs

1.5 Scope of the Thesis

The focus of this thesis pertains to the numerical approximation of FDEs in the form of

$$\left.\begin{aligned} &D^{\alpha} y(t) = f\left(t, y(t)\right), \\ &D^{2\alpha} y(t) = f\left(t, y(t), D^{\alpha} y(t)\right), \\ &\quad y(0) = y_0, \quad D^{\alpha} y(0) = y_0', \quad t \in [a,b], \quad \alpha \in (0,1]. \end{aligned}\right\} \tag{1.1}$$

The results will be obtained by using the developed method. In this thesis, the 2-point fractional BBDF method with fixed and variable step sizes is derived for solving the first-order and second-order FDEs directly. In terms of the computational results, the proposed methods will be evaluated and compared with the existing methods for FDEs. However, the comparison will be limited to some existing methods for second-order FDEs due to a lack of sources and will be compared with the available codes in Matlab. The behaviour of the simulations will be analysed, which is limited to $\alpha = 0.7$, 0.8, 0.9, and 1.0 for first-order FDEs, while $\alpha = 1.7$, 1.8, 1.9, and 2.0 for second-order FDEs. Moreover, the fractional pharmacokinetics model and fractional electric circuit model will be solved using the proposed methods to ensure the competency of the methods in solving the application mathematical model.

1.6 Outline of the Thesis

The thesis is structured into a total of eight chapters. Chapter 1 offers a concise overview and fundamental understanding of fractional calculus. This chapter further explores the problem statement, research questions, research objectives, and scope of the study.

Chapter 2 provides some of the terminology that is relevant to the investigation of fractional calculus. Subsequently, a comprehensive examination is conducted on prior investigations pertaining to FDEs that have been successfully resolved through the application of diverse numerical techniques. Additionally, a review of the literature pertaining to the Block Backward Differentiation Formula (BBDF) method is conducted in relation to the present study.

In Chapter 3, the derivation of the *N*-th order 2-point Fractional Block Backward Differentiation Formula (2FBBDF(*N*)) is presented for solving FDEs with $\alpha \in (0,1]$. The values of *N* considered in this derivation are 3, 4, and 5, which represent the order of the method. Furthermore, this thesis provides a description of the process involved in developing prediction formulas for each order of the method. The computational data is presented in this chapter to validate the efficacy of the 2FBBDF(*N*) method against the existing numerical methods.

In order to improve the efficiency of the method, the 2FBBDF(*N*) method is extended into a variable step method. Thus, the construction of the *N*-th order Variable Step 2-point Fractional Block Backward Differentiation Formula (VS2FBBDF(*N*)), *N* = 3,4,5, is discussed in Chapter 4. This chapter discusses the derivation of the predictor formula, the strategy of selecting the step size, and numerical findings that will be compared with the methods developed in Chapter 3. Besides, the applied problem of the fractional three-compartment pharmacokinetics model will be solved to demonstrate the applicability of the proposed methods.

In Chapter 5, the convergence and stability properties of the derived methods are examined. The determination of the order and error constant are included in this chapter. Theoretical results will be supported by providing numerical evidence.

Chapter 6 presents an improved derivation of the VS2FBBDF(*N*) that is utilised for the numerical solution of FDEs with $\alpha \in (1,2]$. Hence, the variable order VS2FBBDF (VSFBBDF2(*N*)), $N = 2,3,4$, is developed. The predictors of the derived methods are presented, and the implementation of the method to be variable step variable order, FBBDF2, in a single code will be constructed. The details of the strategy for choosing step size and order of the method will be discussed. Using the designed algorithms, the problems are solved directly without reducing it to FDEs with $\alpha \in (0,1]$. Numerical results of the developed method are compared with several existing methods available in the literature to measure its performance. In addition, the application problem of the fractional electric circuit models will be solved using the proposed method.

Furthermore, the convergence and stability properties of the FBBDF2 method are analysed in Chapter 7. The analysis includes determination of order, error constant, zero stability, and stability region of the method. In order to confirm the theoretical findings, some calculations will be provided. Finally, the findings of the research will be concluded in Chapter 8 along with the recommendations for future research.

CHAPTER 2

BACKGROUND THEORY AND LITERATURE REVIEW

2.1 Introduction

In this chapter, some basic concepts and definitions which play an important role in the theory of fractional calculus, and in the development of the proposed method are introduced. Furthermore, this chapter also reviewed the research manuscripts that have inspired and contributed to the development of the proposed method.

2.2 Fractional Calculus

Fractional calculus is a fascinating branch of mathematics that extends the classical concepts of integration and differentiation beyond integer orders. While classical calculus deals with derivatives of whole numbers (like first derivative, second derivative), fractional calculus introduces the idea of derivatives and integrals with non-integer (fractional) powers.

This seemingly abstract concept has surprisingly practical applications. Fractional calculus can provide more accurate models for real-world phenomena that exhibit memory effects or complex dynamics. These phenomena are often poorly described by classical integer-order derivatives. The concept first emerged in the correspondence between the great mathematician Gottfried Wilhelm Leibniz and Marquis de L'Hôpital in 1695. Leibniz pondered the meaning of a "$\frac{d^n y}{dx^n}$ if $n = \frac{1}{2}$". This seemingly odd question sparked curiosity in other mathematicians like Euler (Dalir & Bashour, 2010).

In recent decades, fractional calculus has experienced a resurgence. This is partly due to the development of more robust mathematical tools and computational techniques. But more importantly, scientists and engineers have begun to recognize the power of fractional calculus to model complex real-world phenomena. These phenomena often exhibit memory effects or non-local behaviour, which can be challenging to capture with classical integer-order calculus.

Today, fractional calculus finds applications in diverse fields like signal processing (Gonzalez & Petráš, 2015), control theory (Buedo-Fernández & Nieto, 2020), electrochemistry (Oldham, 2010), viscoelastic material (Paola et al., 2011), and even finance (Kumar & Singh, 2021). As research continues, we can expect fractional calculus to play an increasingly important role in our understanding of the natural world and in the development of new technologies. Therefore, the information related to the fractional calculus will be introduced in this chapter.

2.2.1 Special Functions

Three prominent special functions in fractional calculus are introduced in this subsection: Gamma function, the beta function, and the Mittag-Leffler function. These functions possess properties that make them particularly useful for fractional analysis.

2.2.1(a) Gamma function

Defintion 2.1: (Podlubny, 1998) The gamma function is expressed using a Euler integral of the second kind. This integral formulation, denoted by Γ(z),

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt, \quad \mathrm{Re}(z) > 0, \tag{2.1}$$

where $t^{z-1} = e^{(z-1)\log(t)}$.

The following properties hold for the Euler gamma function (Alkresheh, 2017).

1. The gamma function exhibits analyticity across $z \in \mathbb{C}$ and excluding non-positive integers.

2. $\Gamma(z) = \dfrac{\Gamma(z+1)}{z}, \quad z \in \mathbb{Z}_0^- = \{0,-1,-2,\ldots\},$

3. Reduction formula: $\Gamma(z+1) = z\Gamma(z) = n!, \quad \mathrm{Re}(z) > 0,$

4. $\Gamma(z)\Gamma(1-z) = \dfrac{\pi}{\sin(\pi z)}, \quad z \notin \mathbb{Z}_0, \quad \mathrm{Re}(z) \in (0,1),$

5. $\Gamma\left(\dfrac{1}{2}\right) = \sqrt{\pi}$, and

6. The Legendre duplicate formula: $\Gamma(2z) = \dfrac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z)\Gamma\left(z+\dfrac{1}{2}\right), \quad z \in \mathbb{C}.$

2.2.1(b) Beta function

Definition 2.2: (Podlubny, 1998) The Beta function has a mathematical definition expressed as an Euler integral of the first kind

$$B(z,w) = \int_0^1 t^{z-1}(1-t)^{w-1}dt, \quad \mathrm{Re}(z) > 0, \quad \mathrm{Re}(w) > 0. \tag{2.2}$$

The behavior of this function depends on the Gamma function according to the relationship

$$B(z,w) = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}, \quad z,w \notin \mathbb{Z}_0^- = \{0,-1,-2,\ldots\}. \tag{2.3}$$

2.2.1(c) Mittag-Leffler

Definition 2.3: (Podlubny, 1998) The Mittag-Leffler function of order α denoted by $E_{\alpha}(z)$. The order $\alpha > 0$ is defined by its power series, that converges in the entire complex plane

$$E_{\alpha}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}, \quad \mathrm{Re}(\alpha) > 0. \tag{2.4}$$

The Mittag-Leffler function gives a simple generalization of the exponential function to which it reduces for $\alpha = 1$.

Definition 2.4: (Podlubny, 1998) Let $\alpha, \beta > 0$, then the Mittag-Leffler function of two parameters $E_{\alpha,\beta}(z)$ is defined as

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad z, \beta \in \mathbb{C}, \quad \mathrm{Re}(\alpha) > 0. \tag{2.5}$$

2.2.2 Riemann-Liouville Fractional Derivatives

One of the most prevalent kinds of fractional derivatives is the Riemann-Liouville derivative. In the middle of the 19th century, Joseph Liouville and Bernhard Riemann independently defined them. The idea of fractional integrals, or integrals of a function where the order of integration is not an integer, forms the basis for these derivatives. Thus, the following definition is for the Riemann-Liouville fractional derivatives.

Definition 2.5: (Demirci & Ozalp, 2012) The Riemann-Liouville fractional derivative of order $\alpha > 0$ of a function $y:(0,\infty) \to \mathrm{Re}$ is defined by

$$ {}^{RL}D_{t_0}^{\alpha} y(t) = \frac{1}{\Gamma(n-\alpha)} \left(\frac{d}{dt}\right)^{n} \int_{t_0}^{t} (t-\tau)^{n-\alpha-1} y(\tau) d\tau, \tag{2.6} $$

where $n = [\alpha]+1$ and $[\alpha]$ is the integer part of α.

2.2.3 Caputo Fractional Derivatives

The definition of Caputo fractional derivatives builds upon the foundation of Riemann-Liouville fractional derivatives. According to Zabidi et al. (2020), ${}^{C}D_{t_0}^{\alpha} y(t) = {}^{RL}D_{t_0}^{\alpha} \left(y(t) - y(t_0)\right)$ where ${}^{C}D_{t_0}^{\alpha} y(t)$ refers to the following definition.

Definition 2.6: (Podlubny, 1998) The Caputo fractional derivatives is defined as

$$ {}^{C}D_{t_0}^{\alpha} y(t) = \frac{1}{\Gamma(n-\alpha)} \int_{t_0}^{t} \frac{y'(\tau)}{(t-\tau)^{\alpha}} d\tau, \tag{2.7} $$

where $n = [\alpha]+1$ and $[\alpha]$ is the integer part of α.

The Caputo derivative offers a distinct benefit in that it adheres to classical initial conditions, unlike some other fractional derivatives. This characteristic, evident in the fact that the derivative of a constant is zero, makes it well-suited for modeling the rate of change (Demirci & Ozalp, 2012).

2.2.4 Fractional Differential Equations

Ordinary differential equations (ODEs) are widely used in science and engineering to describe the dynamics of systems, emphasizing the rates at which things change. However, what if the rate of change is not solely instantaneous, such as velocity, but rather relies on the complete history of the system? Ordinary differential equations of fractional order (FDEs) are used in this context.

FDEs are an extension of classical ODEs. Instead of utilizing derivatives of integer order (1st, 2nd, etc.), they integrate fractional derivatives. These derivatives exhibit a "memory effect," in which the current state is influenced not only by the recent past but by the complete history of the system. The definition of the multi-order FDEs is written in Daftardar-Gejji & Jafari (2007) as

$$D_*^{\alpha} y(t) = f\left(t, y(t), D_*^{\beta_1} y(t), \ldots, D_*^{\beta_n} y(t)\right), \quad y_0^{(k)} = c_k, \quad k = 0, \ldots, m, \tag{2.8}$$

where $m < \alpha \le m+1$, $0 < \beta_1 < \beta_2 < \ldots < \beta_n < \alpha$ and D_*^{α} denotes Caputo fractional derivative of order α into a system of FDEs. Let us assume that the function $f\left(t, y(t)\right)$ fulfills the Lipschitz conditions required for the existence and uniqueness of the solution of equation (2.8).

Theorem 2.1: Existence (Diethelm & Ford, 2002) Assume that $\mathcal{D} := \left[0, \chi^*\right] \times \left[y_0^{(0)} - \alpha, y_0^{(0)} + \alpha\right]$ with some $\chi^* > 0$ and some $\alpha > 0$, and let the function $f : \mathcal{D} \to \mathbb{R}$ be continuous. Furthermore, define

$$\chi := \min\left\{\chi^*, \left(\frac{\beta\Gamma(\alpha+1)}{\|f\|_{\infty}}\right)^{\frac{1}{\alpha}}\right\}. \tag{2.9}$$

Then, there exists a function $y : [0, \chi] \to \mathbb{R}$ solving the initial value problem (2.8).

Theorem 2.2: Uniqueness (Diethelm & Ford, 2002) Assume that $\mathcal{D} := \left[0, \chi^*\right] \times \left[y_0^{(0)} - \alpha, y_0^{(0)} + \alpha\right]$ with some $\chi^* > 0$ and some $\alpha > 0$. Furthermore, let the function $f : \mathcal{D} \to \mathbb{R}$ be bounded on $\mathcal{D}$ and fulfill a Lipschitz condition with respect to the second variable; i.e.,

$$\left|f(t,y) - f(t,z)\right| \le L\left|y - z\right|, \tag{2.10}$$

with some constant $L > 0$ independent of t, y, and z. Then, denoting χ as in Theorem 2.1, there exists at most one function $y : [0, \chi] \to \mathbb{R}$ solving the initial value problem (2.8). Refer to (Diethelm & Ford, 2002) for the details.

2.3 Linear Multistep Method

A linear multistep method (LMM) is known as the computational approximation of y_{n+k} by a linear relationship between y_{n+j} and f_{n+j}, $j = 0,1,\ldots,k$. The LMM for ODEs is briefly explained by Lambert (1973) in the following definition.

Definition 2.7: (Lambert, 1973) The general LMM for first and second order ODEs are as follows.

1. First order,

$$\sum_{j=0}^{k} \gamma_j y_{n+j} = h \sum_{j=0}^{k} \beta_j y'_{n+j}, \tag{2.11}$$

2. Second Order,

$$\sum_{j=0}^{k} \gamma_j y_{n+j} = h \sum_{j=0}^{k} \beta_j y'_{n+j} + h^2 \sum_{j=0}^{k} \mu_j y''_{n+j}, \tag{2.12}$$

where γ_j, β_j, and μ_j are constants by assuming that γ_0, β_0, and μ_0 are not zero, with $\gamma_k \neq 0$. k is the order of the method and h is the step size.

In this research, we consider the following general formula of fractional LMM (FLMM).

Definition 2.8: (Galeone & Garrappa, 2006) The general FLMM for FDEs is as follows.

1. For $0 < \alpha < 1$:

$$\sum_{j=0}^{k} \gamma_j y_{n+j} = h^{\alpha} \sum_{j=0}^{k} \beta_j \, {}^{C}D^{\alpha} y_{n+j}, \tag{2.13}$$

2. For $1 < \alpha < 2$:

$$\sum_{j=0}^{k} \gamma_j y_{n+j} = h^{\alpha} \sum_{j=0}^{k} \beta_j \, {}^{C}D^{\alpha} y_{n+j} + h^{2\alpha} \sum_{j=0}^{k} \mu_j \, {}^{C}D^{2\alpha} y_{n+j}, \tag{2.14}$$

where α is the fractional-order.

Definition 2.9: (Galeone & Garrappa, 2006; Zainuddin, 2016) The linear difference operator, L_h, associated with the FLMMs (2.13) and (2.14) are defined as:

1. For $0 < \alpha < 1$:

$$L\left[y(t_n);t;\alpha\right] = \sum_{j=0}^{k} \gamma_j y_{n+j} - h^{\alpha} \sum_{j=0}^{k} \beta_j \, {}^{C}D_{t_0}^{\alpha} y_{n+j}, \tag{2.15}$$

2. For $1 < \alpha < 2$:

$$L\left[y(t_n);t;\alpha\right] = \sum_{j=0}^{k} \gamma_j y_{n+j} - h^{\alpha} \sum_{j=0}^{k} \beta_j \, {}^{C}D_{t_0}^{\alpha} y_{n+j} - h^{2\alpha} \sum_{j=0}^{k} \mu_j \, {}^{C}D_{t_0}^{2\alpha} y_{n+j}, \tag{2.16}$$

where $y(t_n)$ is the arbitrary function, continuously differentiable on $[a,b]$. The function $y(t_n)$ may have higher derivatives.

By utilising the Taylor series expansion of the functions y_{n+j}, ${}^{C}D_{t_0}^{\alpha} y_{n+j}$, and ${}^{C}D_{t_0}^{2\alpha} y_{n+j}$ around the point t_n, and then gathering the derivatives *y*, we obtain

$$L\left[y\left(t_n\right);t;\alpha\right] = C_0\left(n,\alpha\right)y\left(t_n\right) + \sum_{k=1}^{m} h^k C_k\left(n,\alpha\right)y^{(k)}\left(t_n\right) + h^{m+1}R_{m+1}, \tag{2.17}$$

where R_{m+1} is the remainder originates from the Taylor's expansion, and

$$\left.\begin{aligned} C_0\left(n,\alpha\right) &= \sum_{j=0}^{n} \gamma_j, \\ C_k\left(n,\alpha\right) &= \sum_{j=0}^{n} \frac{\left(j\right)^k}{k!}\gamma_j - \sum_{j=0}^{n} \frac{\left(j\right)^{k-\alpha}}{\Gamma\left(k+1-\alpha\right)}\beta_j, \quad k = 1,2,3,\cdots. \end{aligned}\right\} \tag{2.18}$$

Definition 2.10: (Galeone & Garrappa, 2006) The Taylor's series expansion of y_{n+j}, ${}^{C}D_{t_0}^{\alpha} y_{n+j}$, and ${}^{C}D_{t_0}^{2\alpha} y_{n+j}$ about t_n are defined as follows.

$$\left.\begin{aligned} y_{n+j} &= y_n + jhy_n' + \frac{\left(jh\right)^2}{2!}y_n'' + \frac{\left(jh\right)^3}{3!}y_n''' + \cdots, \\ {}^{C}D_{t_0}^{\alpha} y_{n+j} &= \frac{\left(jh\right)^{1-\alpha}}{\Gamma\left(2-\alpha\right)}y_n' + \frac{\left(jh\right)^{2-\alpha}}{\Gamma\left(3-\alpha\right)}y_n'' + \frac{\left(jh\right)^{3-\alpha}}{\Gamma\left(4-\alpha\right)}y_n''' + \cdots, \\ {}^{C}D_{t_0}^{2\alpha} y_{n+j} &= \frac{\left(jh\right)^{1-\alpha}}{\Gamma\left(2-\alpha\right)}y_n'' + \frac{\left(jh\right)^{2-\alpha}}{\Gamma\left(3-\alpha\right)}y_n''' + \frac{\left(jh\right)^{3-\alpha}}{\Gamma\left(4-\alpha\right)}y_n^{(4)} + \cdots. \end{aligned}\right\} \tag{2.19}$$

To determine the order of FLMMs, we will be referring to the following definitions respectively.

Definition 2.11: (Galeone & Garrappa, 2006; Henrici, 1962) The FLMM (2.15) for $\alpha \in \left(0,1\right]$ is considered to have an order of *p* if $C_0 = C_1 = \cdots = C_p = 0,\ C_{p+1} \neq 0$ where C_{p+1} is the error constant for the method.

Definition 2.12: (Lambert, 1973) The FLMM (2.16) for $\alpha \in (1,2]$ is said to be of order p if $C_0 = C_1 = \cdots = C_p = C_{p+1} = 0$, $C_{p+2} \neq 0$ where C_{p+2} is the error constant.

The FLMM is analyzed by considering the following theorem and definitions.

Theorem 2.3: (Lambert, 1973) The FLMM is convergent if and only if it satisfies both consistency and zero stability.

Definition 2.13: (Lambert, 1973) The FLMM is considered consistent if its order is greater than or equal to p, where $p \geq 1$.

Definition 2.14: The FLMM is considered to be zero stable when all roots of the initial characteristics of the polynomial have moduli equal to or less than one, and each root with a modulus of one is a simple root.

Definition 2.15: The FLMM is deemed to be absolutely stable in a region, R for a given $\bar{h}$ if each of the roots, x_s of the stability polynomial, $\pi(x;\bar{h}) = 0$, satisfies the condition $|x_s| \leq 1$, where $s = 1, 2, \ldots, k$.

Definition 2.16: The FLMM is said to be A-stable if the region of absolute stability encompasses the complete left-hand half-plane $R(\bar{h}) < 0$.

2.4 Literature Review

This section reviewed significant contributions that have influenced and made valuable contributions to the formulation of the suggested methodologies. The FDEs problems addressed in this thesis will be resolved through the implementation of block backwards differentiation formula (BBDF) techniques. Therefore, this section will provide a summary of the pertinent research concerning on numerical methods of FDEs and BBDF methods.

2.4.1 Numerical Methods for Fractional Differential Equations

Over the past two decades, a considerable number of scholars have conducted research on FDEs. As a result, several effective approximation analytical and numerical techniques have been introduced to address the challenges associated with solving such problems. This subsection provides a comprehensive assessment of current studies pertaining to the identification of approximate analytical and numerical solutions for fractional order initial value problems, as well as systems of initial value problems involving FDEs.

Diethelm & Ford (2002) focused on investigating the presence, singularity, and structural resilience of solutions to nonlinear FDEs. The differential operator is applied using the Riemann-Liouville definition, and the beginning conditions are stated following Caputo's recommendation, so enabling a physically significant interpretation. Diethelm et al. (2004) further expand upon previous research by introducing a one-step fractional Adams-Bashforth-Moulton scheme as a solution method for FDEs. The numerical data acquired using the derived method are analysed for various fractional orders, α. It is seen that the simulation is converging towards 1 exhibits a decreased approximation error.

Galeone & Garrappa (2006) examined the numerical algorithms associated with the k-step Adams-Moulton Multistep Method for solving FDEs. The investigation of the stability aspects of the method is conducted in order to ascertain its validity as a numerical approach for solving FDEs. Rehman & Khan (2011) developed a Legendre wavelet operational matrix of fractional order integration and utilized it for the purpose of solving FDEs. The proposed method aims to minimize the storage demand of FIVPs within a system. In conclusion, the outcomes obtained from the used approaches exhibit a high degree of similarity to those given by the Haar wavelet method. Nevertheless, this methodology has a drawback in the form of high computing complexity when dealing with nonlinear situations.

Rida & Arafa (2011) have proposed an application of the Mittag-Leffler Function Method for linear FDEs. The solution is formulated using a power series. The findings indicate that the approach is highly efficient and practical in addressing linear FDEs. Subsequently, the linear multistep method (LMM) attracted some researchers to develop a numerical algorithm suitable for solving FDEs. Biala & Jator (2015) have introduced a set of implicit Adams methods (IAMs) that incorporate derivatives of the Caputo type. Heris & Javidi (2018) focused on exploring the fractional backward differential formulas for FDEs with time delay (FDDEs), specifically in the Caputo sense. The numerical experiments are presented in order to demonstrate the potential and constraints of the various methodologies being examined.

Recently, there has been a growing emphasis on solving stiff FDEs in the field of academic research. The increased interest can be ascribed to the prevalence of challenging problems in this domain. Zhou & Zhang (2019) focused on addressing the challenges associated with solving stiff problems. Therefore, they suggested a technique that expanded upon the one-leg method by incorporating γ-order Caputo derivatives. An analysis of the method's stability demonstrates that it is capable of solving stiff FDEs while maintaining the stability. Alkresheh & Ismail (2021) investigate the application of the Multistep fractional differential transform method (MSFDTM) for the estimation of stiff FDEs. The stiff systems of FDEs were solved using the MSFDTM and the Fractional Differential Transform Method (FDTM). The solutions obtained were then compared with the exact solution. Based on the results, it has been determined that the MSFDTM outperforms the FDTM.

In 2021, Malo et al. introduced a hybrid method known as the Elzaki homotopy perturbation method (EHPM). The approach involves utilizing both the Elzaki transform and the homotopy perturbation method. Subsequently, the researchers successfully addressed the challenges associated with fractional stiff systems by employing the suggested approach. The outcomes clearly demonstrate that the EHPM is a highly efficient method for resolving these issues. Furthermore, Duangpan et al. (2021) propose a novel approach to address the challenge of solving stiff fractional problems. The Finite Integration Method using Shifted Chebyshev Polynomial (FIM-SCP) is devised to approximate stiff fractional problems expressed as integro-differential equations.

Zabidi et al. (2022) present a novel Adams-type multistep approach for the numerical solution of FDEs. The method is formulated through the utilization of Lagrange interpolation while also including the principles of the Adams-Moulton approach in scenarios involving fractional values. The Caputo derivative operator was utilized in this study to compute the fractional derivative. The examination of the suggested approach is presented in terms of the method's order, order of accuracy, and convergence analysis, with the method being proven to converge. Basim et al. (2023) introduced a method with the fractional and variable order Jacobi operational matrix (JOM) to solve FDEs. The results show that the approximation of the solution converges slower towards the exact solution even when the fractional order, α, used is nearer to the integer order.

Sayed et al. (2024) proposed an alleviated shifted Gegenbauer spectral method using operational matrices and spectral techniques to solve both integer and fractional-order equations. While it demonstrated strong accuracy, it becomes computationally expensive for complex boundary conditions. Meanwhile, Rahimkhani & Heydari (2025) developed a hybrid method combining fractional-Genocchi wavelets and neural networks to solve Ψ-fractional equations, showing flexibility and convergence. However, the method's performance is sensitive to neural network parameters and carries higher computational costs.

Throughout the reviewing of the literature, we concluded that the existing numerical methods are able to solve FDEs in their own technique. However, the difficulties to obtain the results are quite challenging when they need to deal with the higher computational cost and slower rate to converge towards the exact solution for various α at the end point of the interval. Hence, the numerical method of the Block Backward Differentiation Formula (BBDF) will be introduced to solve FDEs because this method is able to approximate the solution at multiple points concurrently.

2.4.2 Block Backward Differentiation Formula (BBDF)

In general, the block method can be divided into two types which are the one-step method and the multistep method. For the one-step method, the value of y_{n+1} can be determined if and only if y_n is known, no knowledge of any preceding values of y_{n+1}, y_{n+2}, $\cdots$, is required (Henrici, 1962). The one-step method was then improved to the multistep method. Multistep methods are consisting of Adam's method and classical Backward Differentiation Formula (BDF) or it's known as Gear's method. Chu & Hamilton (1987) proposed a multi-block method described as the k-block r-point method in order to minimize the computational time.

Omar (1999) developed the multistep method's codes for explicit methods. The methods proposed are $r = 2$ and $r = 3$ points block methods. The methods were used to solve non-stiff ODEs (NODEs). Majid (2004) furthered the study on the r-point Implicit Block Method to solve NODEs. In the study, $r = 2$, 3, and 4 were used to develop the constant step size r-point block methods. Then, Ibrahim et al. (2005) implement the block method in the Generalised Multistep Adams and BDF (GMBDF) to solve first ODEs. The improvement of the method is compared with the non-block GMBDF, and it shows that the block method gives the smallest error as compared to the non-block method.

2.4.2(a) BBDF method for first-order ODEs

In 2007, Ibrahim et al. build upon prior research and propose an extension of Gear's method for solving first-order stiff ODEs. They provide a block method termed the fully implicit r-point BBDF method, with r values of 2 and 3, as an improved numerical approximation technique. The investigation revealed that the 2-point BBDF (2BBDF) and 3-point BBDF (3BBDF) methods decreased the total number of steps by approximately 50% and 66.67%, respectively. Furthermore, both methods also demonstrate a higher execution speed compared to the non-block method (NBDF). In their 2012 study, Nasir et al. introduced the fifth-order Backward Differentiation calculation (BBDF(5)) by augmenting the number of backvalues used in the calculation. When comparing the approach with the BDF method, it was observed that the BBDF(5) performed better than the BDF in terms of computational time, total number of steps executed, and average error. Suleiman et al. (2014) enhance the BBDF approach by refining it into a superior version called superclass BBDF (2SBBDF). The proposed method is formulated by considering the additional future point and the independent parameter, ρ. The selection of ρ is determined by the stability criterion.

In 2012, Zawawi et al. developed the diagonally implicit 2-point BBDF method (DI2BBDF) by including the diagonally implicit multistep method (Majid and Suleiman, 2006) into the BBDF method. The method is referred to as "diagonally implicit" due to the fact that the coefficients of the elements in the higher triangular matrix are zero. Aksah et al. (2019) expand on the concept by introducing the singly diagonally implicit BBDF method (SDIBBDF). The approach is altered by incorporating the singly diagonally Runge-Kutta method (SDRK) (Al-Rabeh, 1987) and transforming the fully implicit BBDF into a lower triangular matrix with equally diagonal elements. In 2019, Ibrahim & Zawawi introduced a modification to the BBDF technique, resulting in the BBDF(α) method of order 4. This modification included the addition of an independent parameter α. The stability qualities of α determines its values.