UNIVERSITI PUTRA MALAYSIA

DIAGONALLY IMPLICIT BLOCK BACKWARD DIFFERENTIATION FORMULA WITH OFF STEP POINTS FOR SOLVING STIFF ORDINARY DIFFERENTIAL EQUATIONS

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FS 2021 38

DIAGONALLY IMPLICIT BLOCK BACKWARD DIFFERENTIATION FORMULA WITH OFF STEP POINTS FOR SOLVING STIFF ORDINARY DIFFERENTIAL EQUATIONS

By

NORSHAKILA BT ABD RASID

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfillment of the Requirements for the Degree of Doctor Philosophy

May 2021

DEDICATIONS

To my kids, my husband and my parents

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfillment of the requirement for the degree of Doctor Philosophy

DIAGONALLY IMPLICIT BLOCK BACKWARD DIFFERENTIATION FORMULA WITH OFF STEP POINTS FOR SOLVING STIFF ORDINARY DIFFERENTIAL EQUATIONS

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May 2021

Chairman: Zarina Bibi binti Ibrahim, PhD
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This research demonstrates an alternative method for solving stiff ordinary differential equations (ODEs) using a diagonally implicit block backward differentiation formula with off-step points (DOBBDF). The off-step points are the optimal points between two equidistant grid points that help provided stable and high-accuracy solutions. The diagonally implicit form optimized the computational cost since fewer differential coefficients caused reducing the execution times.

The thesis is divided into two significant parts. The first part showed the derivation and implementation of the two-point DOBBDF using constant and variable step-size strategies for solving the first-order stiff ODEs. The methods satisfied the convergence properties and A-stable conditions and yielded the region which contains the whole negative real axis in the complex plane. Numerical results revealed that the derived method excels than the other same kind methods.

The second part described the formulation of DOBBDF for solving second-order ODEs directly. The direct method is the best feature to replace the previously expensive approach. The costly technique involved reducing the higher-order ODEs to first-order ODEs and solve using the first-order method. The new direct methods emphasized approximation at two solution points and two off-step points simultaneously in a block using constant and variable step-size strategies. The methods satisfied the properties of consistency and zero-stable, guaranteed convergent method for directly solving second-order Initial value problems of ODEs.

Last, the DOBBDF is validated with several application models, including cancer, gene regulations, Prothero-Robinson system, and oscillation problems. In conclusion, DOBBDF is a significant alternative solver for the stiff ODEs model in science and engineering.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

FORMULA BLOK PEMBEZAAN KE BELAKANG PEPENJURU TERSIRAT DENGAN TITIK LUAR LANGKAH UNTUK MENYELESAIKAN PERSAMAAN PERBEZAAN BIASA KAKU

Oleh

NORSHAKILA BT ABD RASID

Mei 2021

Pengerusi: Zarina Bibi binti Ibrahim, PhD
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Penyelidikan ini memaparkan kaedah alternatif untuk menyelesaikan persamaan perbezaan biasa kaku (PPBK) dengan menggunakan formula blok pembezaan ke belakang pepenjuru tersirat dengan titik luar langkah (FBPBPTO). Titik luar langkah adalah titik optimum di antara dua titik yang sama jaraknya yang membantu menghasilkan penyelesaian yang lebih stabil dan berkejituan tinggi. Struktur pepenjuru pada formula dapat mengurangkan kos pengiraan kerana pekali pembezaan yang lebih sedikit menyebabkan pengurangan masa pelaksanaan.

Tesis ini terbahagi kepada dua bahagian penting. Bahagian pertama memaparkan penerbitan dan pelaksanaan formula 2 titik FBPBPTO menggunakan strategi saiz langkah tetap dan saiz langkah berubah-ubah untuk menyelesaikan PPBK peringkat pertama. Formula tersebut memenuhi ciri-ciri penumpuan dan kestabilan A justeru menghasilkan graf yang mengandungi keseluruhan bahagian pada paksi negatif didalam ruangan kompleks. Keputusan berangka mendedahkan bahawa formula yang dihasilkan adalah lebih baik daripada formula dari kategori yang sama yang sedia ada.

Bahagian kedua membincangkan penerbitan FBPBPTO untuk menyelesaikan secara terus PPBK peringkat kedua. Kaedah penyelesaian secara terus adalah paling baik untuk menggantikan teknik yang sedia ada yang mahal. Teknik yang mahal tersebut melibatkan proses menurunkan PPBK peringkat tinggi kepada PPBK peringkat pertama dan menyelesaikannya menggunakan formula peringkat pertama. Kaedah penyelesaian secara terus ini menekankan penghampiran penyelesaian pada dua titik dan dua titik luar langkah secara serentak di dalam blok menggunakan strategi

saiz langkah tetap dan berubah-ubah. Formula tersebut memenuhi ciri-ciri konsistensi dan kestabilan sifar justeru formula menumpuan dijamin dalam menyelesaikan masalah nilai awal PPBK peringkat kedua secara terus.

Akhir sekali, FBPBPTO diuji dengan beberapa aplikasi model antaranya model kanser, pengaturan gen, sistem Prothero-Robinson dan masalah ayunan. Kesimpulannya, FBPBPTO merupakan kaedah alternatif yang signifikan untuk menyelesaikan model PPBK di dalam bidang sains dan kejuruteraan.

ACKNOWLEDGEMENTS

In the Name of Allah, the Most Beneficent, the Most Merciful.

Alhamdulillah, all praise be to Allah. Peace and blessings be upon him, the Prophet of Allah, Muhammad S.A.W. I am truly grateful to Allah for the excellent health and well-being necessary to complete this thesis finally. I First and foremost, I thanks Allah for His grace, wisdom, and comfort throughout my thesis.

I take this opportunity to express my sincere gratitude to the people who have been instrumental in completing this thesis. I wish to express my deepest gratitude to Professor Dr. Zarina Bibi Ibrahim, chairman of the supervisory committee, for her excellent supervision, valuable guidance, helpful discussion, and continuous encouragement. She has taught me how to find an interesting problem, guide me every step to explore problems independently and provide me with valuable feedback. I am grateful for having the opportunity to work under her supervision. Her valuable assistance and comments in the preparation and completion of this thesis are also highly appreciated. Without her encouragement and guidance, this thesis would not have materialized. I sincerely thank the supervisory committee members, Professor Dr. Zanariah Abdul Majid and Professor Dr. Fudziah Ismail, for their valuable discussion, comments, and helps. I also would like to express my sincere gratitude to all my thesis examination committee members for spending time to read and evaluate my thesis. Special thanks are given to all lecturers at the department of Mathematics UPM and my colleague at Universiti Kuala Lumpur Malaysian Institute of Marine Engineering Technology (UniKL-MIMET) for their excellent guidance academic achievements.

I owe more thanks to the most important people in my life. I would like to thank my loved ones, my dear husband, my dear parents, parents-in-law, my sisters, my brother, and all the family members, who have supported me throughout the entire process, both by keeping me harmonious and helping me putting pieces together. Without their support, it would be impossible for me to get through this hardship. I will be grateful forever for your love.

Finally, I would like to take this opportunity to offer my special thanks to my fellow friends, especially Noraini Zainuddin, Amiratul Ashikin Nasarudin, Saufianim Jana Aksah, Hazizah Mohd Ijam, Iskandar Shah Zawawi, Nor Ain Azeany Nasir for their influences and attention in completing this thesis. My sense of gratitude to everyone, directly and indirectly, has lent their hand in this venture.

This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy. The members of the Supervisory Committee were as follows:

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Declaration by graduate student

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LIST OF ABBREVIATIONS

ODEs	Ordinary Differential Equations
IVPs	Initial Value Problems
BBDF	Block Backward Differentiation Formula
ode15s	MATLAB built-in ODEs solver formulated in numerical differentiation formula (NDFs) and implemented in variable-step, variable order starting from 1 until order 5.
h	The step size
MAXE	Maximum error
TIME	Time taken in microseconds
AVE	Average Error
TOL	User defined tolerance
TS	Total Step
DOBBDF	Diagonal Implicit Block Backward Differentiation Formula with Off-step Points
DOBBDF(2)	DOBBDF of order two for solving first order stiff ODEs
DOBBDF(3)	DOBBDF of order three for solving first order stiff ODEs
VDOBBDF	DOBBDF implemented in variable-step strategy for solving first order stiff ODEs
DOBBDF2	Diagonally Implicit BBDF with off step points for solving second order ODEs directly
VDOBBDF2	DOBBDF2 implemented in variable-step strategy for solving second order ODEs directly

CHAPTER 1

INTRODUCTION

1.1 Introduction

”Differential equation” is a mathematical statement that describes the derivatives of one or more functions. The equation appeared, containing information on the rate of change of the system over time. Differential equations begin by scratching the surface of how to describe real-world change mathematically. Ordinary differential equations (ODEs) and partial differential equations (PDEs) are the two most frequent types of environmental differential equations models. ODEs include ordinary derivatives with one independent variable, whereby PDEs involve partial derivatives with several independent variables.

The oscillation of mass-spring, drug dissipation, Malthusian population, decaying radioactive, predator-prey phenomena are real-world applications modeled mathematically using ODEs. Consider the general form of a simple, single ODEs as follows:

$$y'(t) = \alpha y, \quad y(a) = y_0, \quad t \in [a,b]. \tag{1.1.1}$$

α is a constant. If $\alpha > 0$, the exponential function in t that growing as t increases is termed exponential growth. If $\alpha < 0$, on the other hand, it becomes exponential decay, with the values of y gradually approaching zero over time, (1.1.1) has a solution of $y(t) = y_0 e^{\alpha t}$, which gives information about how quantities change and, in turn, provides indirect insight into how and why the change occurs see Figures 1.1 and 1.2. As time passed, different complex models arose and were designated without theoretical solutions. The solution techniques grow more challenging as the model becomes sophisticated. Thus, over the five decades or more, there has been an increase in numerical methods to surmount the shortcomings. However, the solvers are still grounded to the classical explicit, and implicit methods since these two techniques are widely adopted to solve various scientific and applied engineering domains. Besides that, the criteria based on the complexity, behavior of outcome, the execution time of code, and the accuracy of the results decided the most suitable approaches when solving problems.

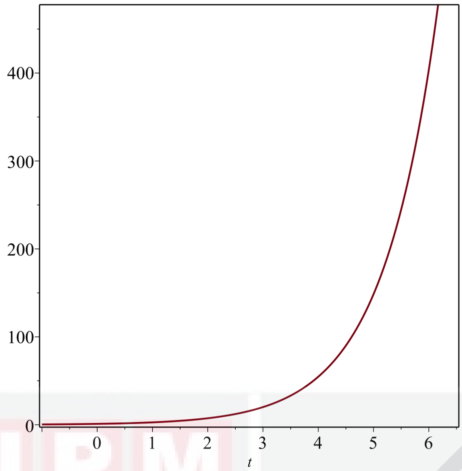

Figure 1.1: Graph of exponential growth $\alpha > 0$

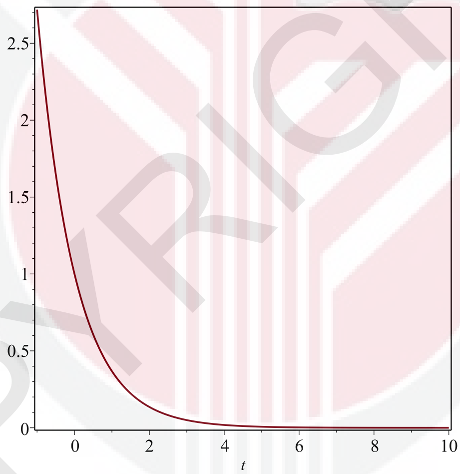

Figure 1.2: Graph of exponential decay $\alpha < 0$

1.2 Problem statement

ODEs have a wide range of applications and can forecast the environment and the outcome of the process. As we mentioned in the previous section, it assists in forecasting exponential growth and decay as well the expansion of population and species. Throughout this thesis, we will solve ODEs with a starting condition that defines the unknown function's value at a certain point in the domain or called the initial value problem (IVPs) of ODEs. The IVPs involves first and second order ODEs that revolve around four kinds of ODEs viz. homogenous, non-homogenous, linear, and non-linear problems.

The general form of first order ODEs can mathematically define as

$$y' = f(x,y), \quad y(a) = y_0, \quad a \leq x \leq b. \tag{1.2.1}$$

The Second order ODEs is in the form of:

$$y'' = f(x,y,y'), \quad y(a) = y_0, \quad y'(a) = y'_0 \quad a \leq x \leq b. \tag{1.2.2}$$

(1.2.2) can be transformed into a system of ODEs of the first order explicit form by introducing new dependent variables. The system of first order ODEs is in the form of:

$$\hat{y}' = f(x,\hat{y}) = A\hat{y} + \psi(x), \quad \hat{y}(a) = \omega, \quad a \leq x \leq b. \tag{1.2.3}$$

where $\hat{y} = (y_i)^T$, $\omega = (\omega_i)^T$, where $i = 1,2,3,...,n$ and A is a $n \times n$ matrix with the eigenvalues λ_i, $i = 1,2,3,...,n$.

The function $f(x,y)$ guaranteeing the existence of a unique solution of the IVPs in (1.2.1) by the following theorem Lambert (1973)

Theorem 1.1 *Let $f(x,y)$ be defined and continuous fo all points (x,y) in the region D defined by $a \leq x \leq b$, $-\infty < y < \infty$, a and b finite, and let there exist a constant L such that, for every x, y, y^* such that (x,y) and (x,y^*) are both in D:*

$$|f(x,y) - f(x,y^*)| \leq L|y - y^*|. \tag{1.2.4}$$

Then, if y_0 is any given number, there exists a unique solution $y(x)$ of the IVPs of (1.2.1)*, where $y(x)$ is continuous and differentiable for all (x,y) in D.*

The proof of theorem can be found in Henrici (1962).

Frequent dynamic ODEs models are governed by the unique behavior identified as stiffness. Due to the stiffness, only a few applicable methods are suitable in all spatial regions since the solution would not have reached zero in a limited period, and the approximate will be unstable. Roughly, a stiff system can be seen as one in which components have very widely varying time-scale evaluations. Figure 1.2 depicts the geometrical significance of stiffness.

Stiffness is an efficiency issue that is concerned about how much time computation takes. One of the most challenging aspects of studying stiff differential systems is the lack of a solid mathematical description of the idea of stiffness. The earlier discovery of the issue by Crank and Nicolson (1996) and Fox and Goodwin (1949) noticed the stiffness difficulty while working on problems involving nonlinear heat equations in the form of ODEs. Curtiss and Hirschfelder (1952) established the worldwide fact that the implicit technique performs significantly better than the explicit method for stiff problems. The measuring tools to determine the stiffness level ranging from mildly to highly stiff through the eigenvalue of the ODEs. The system's eigenvalues can theoretically provide measured stiffness by demonstrating that the larger λ_i magnitude when $\lambda_i < 0$, the quicker the system responds. Furthermore, the degree of stiffness can also be identified using the stiffness ratio, where the calculation involves the absolute value of the greatest eigenvalue divided by the lowest eigenvalue. Lambert (1973) provides a more specific mathematic definition of stiffness, which is as follows:

Definition 1.2.1 *The linear system* (1.2.3) *is said to be stiff if*

i. $Re\lambda_i < 0, i = 1,2,\ldots,n,$ *and*

ii. $max_{i=1,2,\ldots,n}|Re\lambda_i| \leq min_{i=1,2,\ldots,n}|Re\lambda_i|$, *where* $\lambda_i, i = 1,2,\ldots,n$ *are the eigenvalues of A. The ratio*

$$\frac{max_{i=1,2,\ldots,n}|Re\lambda_i|}{min_{i=1,2,\ldots,n}|Re\lambda_i|}$$

is called stiffness ratio.

To effectively handle the stiff issue, it is necessary to understand what stiff ODEs are and where they occur. Besides that, the purpose of designing a more accurate solver is to provide efficient and stable alternatives methods in solving stiff. A short description of the linear multistep method (LMM) will be presented in the next section, along with some fundamental terminology relevant to the study.

1.3 Linear Multistep Method

Lambert (1973) presented the first and second order linear multistep method (LMM) as follows:

Definition 1.3.1

$$\sum_{j=0}^{k} \alpha_j y_{n+j} - h \sum_{j=0}^{k} \beta_j f_{n+j} = 0, \tag{1.3.1}$$

$$\sum_{j=0}^{k}\alpha_j y_{n+j} - h\sum_{j=0}^{k}\beta_j f_{n+j} - h^2\sum_{j=0}^{k}\gamma_j f_{n+j} = 0, \tag{1.3.2}$$

α_j, β_j and γ_j are constant coefficients and not all coefficients α_0, β_0 and γ_0 equal to zero. h is known as distance size between points in the formula and k symbolized as order of the method.

The linear k-step method is based on evaluations of both y_{n+j} and f_{n+j} where $j = 0, 1, \ldots, k$, to approximate the solutions of y_n.

The first order LMM in (1.3.1) is identified as implicit method if $\beta_k \neq 0$ whilts it called explicit method if $\beta_k = 0$. The implementation of LMM need advanced calculation of starting points of $y_0, y_1, \ldots, y_{k-1}$ and it can be realized through predictor corrector methods.

1.4 Theoretical analysis of the method

Each new approach develope must be validated theoretically for ensuring efficient approximations. The following definitions stated in Lambert (1973) defined the principles criteria for LMM comprising order of the method, convergence and zero stability.

1.4.1 Order of method

The order of LMM can be determined by referring to the definition stated by Lambert (1973) as follow

Definition 1.4.1 *The linear difference operator, L associated with* (1.3.1) *is:*

$$L[y(x):h] = \sum_{j=0}^{k}\left[\alpha_j y(x+jh) - h\beta_j y'(x+jh)\right]. \tag{1.4.1}$$

expanding $y(x+jh)$ and $y'(x+jh)$ as Taylor series about x_n:

$$y(x_n+h) = y(x_n) + hy'(x_n) + \frac{h^2}{2!}y''(x_n) + \frac{h^3}{3!}y^{(3)}(x_n) + \frac{h^4}{4!}y^{(4)}(x_n) + \ldots, \tag{1.4.2}$$

$$y'(x_n+h) = y'(x_n) + hy''(x_n) + \frac{h^2}{2!}y^{(3)}(x_n) + \frac{h^3}{3!}y^{(4)}(x_n) + \frac{h^4}{4!}y^{(5)}(x_n) + \ldots, \quad (1.4.3)$$

substituting the equations (1.4.2) *and* (1.4.3) *to the* (1.3.1) *and collecting the derivative gives:*

$$L[y(x):h] = C_0 y(x) + C_1 hy'(x) + C_2 hy''(x) + C_3 hy'''(x) + \cdots + C_q h^q y^q(x). \quad (1.4.4)$$

The expansion will be truncated depending on the order of the method.

Definition 1.4.2 *Linear multistep method* (1.3.1) *is said to be of order q if, $C_0 = C_1 = C_2 = C_3 = \cdots = C_q = 0$ and $C_{q+1} \neq 0$ is called as an error constant where $q = 2, 3, \ldots$.*

$$\begin{aligned} C_0 &= \sum_{j=0}^{k} \alpha_j \\ C_1 &= \sum_{j=0}^{k} (j\alpha_j - \beta_j) \\ C_2 &= \sum_{j=0}^{k} (\frac{(j)^2}{2!}\alpha_j - j\beta_j) \\ &\vdots \\ C_q &= \sum_{j=0}^{k} [\frac{j^q \alpha_j}{q!} - \frac{j^{q-1}\beta_j}{(q-1)!}]. \end{aligned} \quad (1.4.5)$$

1.4.2 Convergence and zero stability

Definition 1.4.3 *Linear multistep method* (1.3.1) *is said to be convergent if for all initial value problems subject to the hypotheses of Theorem 1.1:*

$$\lim_{h \to 0} y_n = y(x_n), \quad (1.4.6)$$

holds for all $x \in [a,b]$, and for all solutions $\{y_n\}$.

Definition 1.4.4 *The necessary and sufficient conditions for the linear multistep method (LMM) of* (1.3.1) *to be convergent are that it must be consistent and zero stable.*

Definition 1.4.5 *Linear multistep method* (1.3.1) *is said to be consistent if it has order* $q \geq 1$ *and the method is also consistent if and only if:*

$$(i) \quad \sum_{j=0}^{k} \alpha_j = 0,$$

$$(ii) \quad \sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_j. \tag{1.4.7}$$

Definition 1.4.6 *Linear multistep method* (1.3.1) *is said to be zero-stable if no root of the first characteristic polynomial has modulus greater than one:*

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j = 0. \tag{1.4.8}$$

Definition 1.4.7 *A method is said to be A-stable if* $R_A \subseteq h|Re(h) < 0$

Definition 1.4.8 *Linear multistep method* (1.3.1) *is said to be absolutely stable if all the roots of the stability polynomial satisfy* $|r_s| < 1, s = 1, 2, \ldots, k$

1.5 Objective of Study

The main objectives of this research are:

1. To develop fixed coefficients of diagonally implicit BBDF with off-step points of order two (2) and order three (3) for solving first and second order linear and nonlinear stiff ODEs.
2. To construct variable time-step diagonally implicit BBDF with off-step points method for solving first and second order stiff ODEs.
3. To investigate the convergence properties and stability of the derived methods.
4. To develop the algorithm in C++ environment for the implementations of the method in fixed step followed by variable step strategy.

5. To measure the accuracy of proposed methods with proven solvers regarding the accuracy and computational time.

6. To test the efficiency of the proposed methods in solving first and second-order ODEs with applications.

1.6 Scope of Study

Our scope is pertaining to the derivation and theoretical analysis for solving ODEs up to the first and second order only. We approximate directly without reducing to first order when solving second order stiff ODEs. Two solutions and two-off step points will be calculated simultaneously within the same compartment at a single iteration with the imposed of fixed coefficients or step-changing strategy. The methods are tested with well-known, scientific real-life cases of linear and nonlinear stiff IVPs and show the processor time and accuracy performance metrics. The output establishes and the conclusion is confined to the test problems presented in this thesis, which comprises cancer problems, gene regulations, prothero robinson, mass spring system, and the duffing oscillatory equation.

1.7 Outline of Study

There are eight chapters in this thesis. A short overview of stiff ODE systems and specific terminology relevant to the research are presented in Chapter 1. The study objectives, problem statements, and scope of the study are outlined in this chapter. Chapter 2 shows the background studies of numerical methods used for solving stiff

ODEs Chapter 3 discusses the fixed step diagonally implicit BBDF with off-step

points methods. The theoretical analysis comprises convergence and A-stability, which are conduct to the proposed methods. The methods are applied to the linear and nonlinear stiff problems, and the results show the relationship between stiffness and computational method accuracy. Chapter 4 presents the extended form of the

method in Chapter 3 by imposing the variable step strategy. The step-size ratios are restricted to be equal $r = 1, r = 2$, and $r = 5/8$. The method is satisfied to be convergent and A-stable method. The test problems comprise highly stiff problems and are taken from the literature to measure the stiffness effect on computational accuracy and CPU times. Chapter 5 laid out the framework for the derivation of the direct

solver fixed step diagonally implicit BBDF with off-step points to solve second order ODEs directly. Theoretical analysis has been conducted to prove it as a convergent method. The numerical results are compared with the other proven direct solver and first order methods, consists of solver derived in Chapter 4 and ode15s to corroborate the results. Chapter 6 shows the formulation of the variable step implementation of the method in Chapter 5 for solving second order directly. The same step ratios in Chapter 4 are applied. The implementation and the summary of the algorithm are shown. The method is verified with singles and systems of mildly and highly stiff second order ODEs. The numerical accuracy is compared with proven solvers and the fixed step direct method in Chapter 5 to support the method's efficiency. All

the methods in Chapters 3-6 are tested with real-life scientific cases of linear and nonlinear stiff IVP. Chapter 7 discusses pertinent observations from the results obtained and decided which methods are the best fit as an alternative solver for stiff first and second order ODEs. Lastly, the summary of this research which includes the conclusion and planning of improvement are shown in Chapter 8.

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BIODATA OF STUDENT

Norshakila binti Abd Rasid was born in Hospital Changkat Melintang, Perak on 18th January 1989. She received her earlier education in Sekolah Kebangsaan Bota Kanan and her secondary education in Sekolah Menengah Kebangsaan Raja Permaisuri Bainun, Ipoh, Perak from year 2002 until 2006. In 2007, she continued her foundation study in Malacca Matriculation College, taking the Sciences Biology. She then continued her tertiary education in 2008 at Universiti Putra Malaysia (UPM) and graduated with a Bachelor of Science (Honors) major in Mathematics in 2011. Within the same year and same university, she pursued a Master's degree and graduated with a Master of Science by 2014, majoring in Differential Game Theory. Later, in September 2015, she registered as a Doctor of Philosophy (Ph.D.) candidate in Universiti Putra Malaysia, taking Computational model. Currently, she is a part-time candidate for the Ph.D. and works as a full-time lecturer at Universiti Kuala Lumpur campus Malaysian Institute of Marine Engineering Technology (UniKL-MIMET) located at Lumut, Perak.

PUBLICATION

The following are the list of publications that arise from this study.

Norshakila Abd Rasid, **Zarina Bibi Ibrahim Zanariah Abdul Majid** and **Fudziah Ismail** (2021). Formulation of a New Implicit Method for Group Implicit BBDF in Solving Related Stiff Ordinary Differential Equations. *Mathematics and Statistics,*, Vol 8(8): 3310 - 3322.