UNIVERSITI PUTRA MALAYSIA

ADAPTIVE STEP SIZE OF DIAGONALLY IMPLICIT BLOCK BACKWARD DIFFERENTIATION FORMULAS FOR SOLVING FIRST AND SECOND ORDER STIFF ORDINARY DIFFERENTIAL EQUATIONS WITH APPLICATIONS

HAZIZAH BINTI MOHD IJAM

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By

HAZIZAH BINTI MOHD IJAM

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

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DEDICATIONS

To:

Allahyarham Mohd Ijam bin Ab Salam
(1946 ~ 2017)

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

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Chairman: Zarina Bibi binti Ibrahim, PhD
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In this thesis, new classes of block methods based on backward differentiation formula (BDF) for solving first and second order stiff ordinary differential equations (ODEs) are developed. These methods are implemented in diagonally implicit structure and generated the solutions of y_{n+1} and y_{n+2} simultaneously in a block. The formulas are constructed by taking a non zero arbitrary, incorporating a free parameter, ρ and hence producing $\rho-$diagonally implicit block backward differentiation formula ($\rho-$DIBBDF) which contain the block backward differentiation formula (BBDF) as a subclass.

Initially, the derivation of $\rho-$DIBBDF in fixed and adaptive step approaches for the solution of first order stiff ODEs have been described. The classes have the advantage of producing a different set of formulas that possess A-stability properties by selecting the ρ value within the interval (-1,1). The order, consistency, zero stability, absolute stability and stability region for the methods have been determined to ensure their applicability in solving the stiff ODEs. The numerical results have marginally better performance for the fixed step formula and competitive achievement for the adaptive step formula when compare to the existing BBDF methods.

To deal with the system of second order stiff ODEs, $\rho-$DIBBDF is formulated suited well with the systems in its original form, without transforms it to the first order ODEs. The convergence and stability properties also have been analyzed. The stability polynomials for the method have been obtained and their stability

regions have been discussed. The methods are implemented in fixed and adaptive step approaches. Comparisons on numerical results to existing BBDF methods demonstrate a comparable performance of both fixed and adaptive step formulas in terms of accuracy.

The $\rho-$DIBBDF algorithms are written in C programming language. All the approximate solutions of the standard problems and application systems of stiff ODEs generated by $\rho-$DIBBDF agrees well with the exact solutions and approximate solutions computed by Matlab stiff solvers. All developed methods with $\rho = -0.75$ have shown to perform the computational work in a lesser time when compared to the existing BBDF methods of the corresponding order.

In conclusion, the proposed methods have shown the suitability and reliability to solve linear and non-linear systems in different level of stiffness with comparison to the existing BBDF methods and Matlab stiff solvers. Thus, the new methods developed can be included as viable alternatives for solving first and second order stiff ODEs.

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

FORMULA BLOK PEMBEZAAN KE BELAKANG PEPENJURU TERSIRAT DENGAN SAIZ LANGKAH BERUBAH BAGI MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA KAKU PERINGKAT PERTAMA DAN KEDUA DENGAN APLIKASI

Oleh

HAZIZAH BINTI MOHD IJAM

Disember 2020

Pengerusi: Zarina Bibi binti Ibrahim, PhD
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Dalam tesis ini, kelas baru bagi kaedah blok berdasarkan formula pembezaan ke belakang (FPB) untuk menyelesaikan persamaan pembezaan biasa (PPB) kaku peringkat pertama dan kedua dibangunkan. Kaedah ini dilaksanakan dalam struktur pepenjuru tersirat dan menghasilkan penyelesaian y_{n+1} dan y_{n+2} secara serentak dalam satu blok. Formula baru ini dibina dengan mengambil nilai pembolehubah bukan sifar dan memasukkan parameter bebas, ρ dan dengan itu menghasilkan formula $\rho-$blok pembezaan ke belakang pepenjuru tersirat ($\rho-$FBPBPT) yang mengandungi formula blok pembezaan ke belakang (FBPB) sebagai subkelas.

Pada permulaan, formula $\rho-$FBPBPT dalam pendekatan langkah tetap dan berubah untuk penyelesaian PPB kaku peringkat pertama telah diterbitkan. Kelas ini mempunyai kelebihan untuk menghasilkan satu set formula yang berbeza yang mempunyai sifat kestabilan A dengan menukar nilai ρ dalam selang (-1,1). Urutan, konsistensi, kestabilan sifar, kestabilan mutlak dan rantau kestabilan untuk kaedah ini telah ditentukan untuk memastikan kebolehgunaannya dalam menyelesaikan PPB yang kaku. Hasil berangka menggambarkan prestasi yang sedikit lebih baik untuk formula langkah tetap dan pencapaian kompetitif untuk formula langkah berubah apabila dibandingkan dengan kaedah FBPB sedia ada.

Untuk menangani sistem PPB kaku peringkat kedua, $\rho-$FBPBPT diformulasikan sesuai dengan sistem dalam bentuk asalnya, tanpa mengubahnya menjadi PPB peringkat pertama. Ciri penumpuan dan kestabilan juga telah dianalisis. Polinomial

kestabilan untuk kaedah ini telah diperoleh dan rantau kestabilannya telah dibincangkan. Kaedah ini dilaksanakan dalam pendekatan langkah tetap dan berubah. Perbandingan hasil berangka dengan kaedah FBPB sedia ada menunjukkan prestasi yang setanding untuk kedua-dua formula langkah tetap dan berubah dari segi ketepatan.

Algoritma $\rho-$FBPBPT ditulis dalam bahasa pengaturcaraan C. Semua penyelesaian anggaran bagi masalah standard dan sistem aplikasi PPB yang kaku yang dihasilkan oleh $\rho-$FBPBPT sangat berpadanan dengan penyelesaian sebenar dan penyelesaian anggaran yang dikira oleh penyelesai kaku Matlab. Semua kaedah yang diterbitkan dengan $\rho = -0.75$ menunjukkan ia dapat melakukan kerja pengiraan dalam masa yang lebih rendah jika dibandingkan dengan kelas FBPB sedia ada pada peringkat yang sepadan.

Sebagai kesimpulan, kaedah yang dicadangkan telah menunjukkan kesesuaian dan kebolehpercayaan untuk menyelesaikan sistem linear dan bukan linear dalam tahap kekakuan yang berbeza dibandingkan dengan kaedah FBPB sedia ada dan penyelesai kaku Matlab. Oleh itu, kaedah baru yang dikembangkan ini dapat disertakan sebagai alternatif yang sesuai untuk menyelesaikan PBB kaku peringkat pertama dan kedua.

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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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LIST OF ABBREVIATIONS

ODEs	Ordinary Differential Equations
IVPs	Initial Value Problems
LMM	Linear Multistep Method
BDF	Backward Differentiation Formula
BBDF	Block Backward Differentiation Formula
$\rho-$DIBBDF(m)	$\rho-$Diagonally Implicit Block Backward Differentiation Formula of order m
$\rho-$ASDIBBDF	$\rho-$Adaptive Step Diagonally Implicit Block Backward Differentiation Formula of order 2
$\rho-$2DIBBDF(m)	$\rho-$Diagonally Implicit Block Backward Differentiation Formula of order m for second order ODEs
$\rho-$AS2DIBBDF	$\rho-$Adaptive Step Diagonally Implicit Block Backward Differentiation Formula of order 2 for second order ODEs
BBDF(3)	Block Backward Differentiation Formula of order 3
DIBBDF(3)	Diagonally Implicit Block Backward Differentiation Formula of order 3
NDIBBDF(2)	Diagonally Implicit Block Backward Differentiation Formula of order 2
VSVOBBDF	Variable Step Variable Order Block Backward Differentiation Formula
VSBBDF$-\alpha$	Variable Step Block Backward Differentiation Formula$-\alpha$
BBDF$-\alpha$(3)	Block Backward Differentiation Formula$-\alpha$ of order 3
2DIBBDF(2)	Diagonally Implicit Block Backward Differentiation Formula of order 2 for second order ODEs
BBDF2$-\alpha$(3)	Block Backward Differentiation Formula$-\alpha$ of order 3 for second order ODEs
VS2DIBBDF	Variable Step Diagonally Implicit Block Backward Differentiation Formula for second order ODEs

VSBBDF2$-\alpha$	Variable Step Block Backward Differentiation Formula$-\alpha$ for second order ODEs
ode15s	Variable order solver in numerical differentiation formula
ode23s	Modifies implicit Rosenbrock formula in Matlab
h	Step size
TOL	Tolerance limit
MTD	Method
SS	Total success steps
FS	Total failure steps
TS	Total steps taken
TIME	Time taken in seconds
AVER	Average error
MAXE	Maximum error
EXACT	Exact solutions
LTE	Local Truncation Error
SF	Safety Factor
EC	Error Constant

CHAPTER 1

INTRODUCTION

1.1 Introduction

Since beginning of this century, modern theory of the numerical solution of ordinary differential equations (ODEs) has been established, starting with Adams, Runge and Kutta. The theory is currently well understood and software development is available for a wide variety of problems. The ODEs are used to formulate mathematically and thus aid to solve physical and other problems including functions of certain variables, such as problem of determining the charge or current in an electrical circuit, problem of determining the vibrations of a wire or membrane and chemical kinetic reactions.

Initial value problems (IVPs) with stiff ODEs are ubiquitous in applications of science and engineering, particularly in the studies of nuclear reactors, electrical circuits, vibrations, chemical reactions, astrochemical kinetics, electrical networks, dynamics and control theory. Stiff ODEs also occur in many non-industrial areas like weather prediction, mathematical biology and pharmacokinetics.

1.2 Problem to be Solved

Throughout this thesis, without loss of generality, we shall be concerned with $d-$th order $s-$dimensional systems of ODEs of the form:

$$\widetilde{y}_i^{(d)} = f_i(x,\widetilde{y}), \quad \widetilde{y}(a) = \widetilde{\eta}, \quad x \in [a,b] \tag{1.1}$$

where $i = 1,2,\ldots,s,$ $d = 1,2,$ $\widetilde{y}(x) = (y_1, y_1', \ldots, y_s^{(d-1)})^T,$ $\widetilde{\eta} = (\eta_1, \eta_1', \ldots, \eta_s^{(d-1)})^T$. With regard to Eq. (1.1), we shall assume that the following theorem in Lambert (1991) are satisfied.

Theorem 1.1 *Let $f(x,\widetilde{y})$ be defined and continuous for all $(x,\widetilde{y})$ in the region D defined by $a \le x \le b$, $-\infty < \widetilde{y} < \infty$, where a and b are finite and let there exist a constant L such that*

$$|f(x,\widetilde{y}) - f(x,\widetilde{y}^*)| \le L|\widetilde{y} - \widetilde{y}^*|, \tag{1.2}$$

holds for every x, $\widetilde{y}$, $\widetilde{y}^*$ such that $(x,\widetilde{y})$ and $(x,\widetilde{y}^*)$ are both in D. Then, if $\widetilde{\eta}$ is any given number, there exists a unique solution $\widetilde{y}(x)$ of problem in Eq. (1.1), where $\widetilde{y}(x)$ is continuous and differentiable for all $(x,\widetilde{y}) \in D$.

Proof: See Henrici (1962)

The requirement in Eq. (1.2) is known as Lipschitz condition and the constant L as Lipschitz constant. Throughout this work, we shall assume that Theorem 1.1 is satisfied and established the existence of the unique solution of Eq. (1.1).

1.3 Stiff System of Ordinary Differential Equations

The literature lacks a precise description of stiffness. Nevertheless, recently Söderlind et al. (2015) presented a critical analysis of the classical stiffness theories and the statements on the stiff nature are summarised below:

(i) Stiff equations are equations where certain implicit methods work better, typically tremendously better than explicit ones, especially backward differentiation formula (BDF) (Curtiss and Hirschfelder (1952)).

(ii) The essence of stiffness is that the solution to be computed is slowly varying but that perturbations exist which are rapidly damped (Dekker and Verwer (1984)).

(iii) Stiff equations are problems for which explicit methods do not work (Hairer and Wanner (1996)).

Prior to that, Brugnano et al. (2011) also compiled some intuitive definitions relating to stiffness, which have repeating quotes cited from Söderlind et al. (2015), except:

(i) Systems containing very fast components as well as very slow components (Dahlquist (1973)).

(ii) A stiff system is one for which λ_{max} is enormous so that either the stability or the error bound or both can only be assured by unreasonable restrictions on the step size... Enormous means enormous relative to the scale which here is $\bar{x}$ (the integration interval)... (Miranker (1975)).

(iii) If a numerical method with a finite region of absolute stability, applied to a system with any initial condition, is forced to use in a certain interval of integration a step length which is excessively small in relation to the smoothness of the exact solution in that interval, then the system is said to be stiff in that interval (Lambert (1991)).

It is important to note that this thesis follows the comprehensive definition of stiffness in Lambert (1973) given as follows:

Definition 1.1 *Consider the system of*

$$y' = Ay + \Phi(x), \tag{1.3}$$

where A is a constant $s \times s$ matrix with distinct eigenvalues, λ_i and corresponding eigenvectors, c_i, $i = 1, 2, \ldots, s$. The general solution of the system takes the form

$$y(x) = \sum_{i=0}^{s} \kappa_i e^{\lambda_i x} c_i + \Psi(x),$$

where κ_i are arbitrary constants and $\Psi(x)$ is a particular integral.

The system in Eq. (1.3) is said to be stiff if:

(i) $Re(\lambda_i) < 0$, *and*

(ii) $\max_i |Re(\lambda_i)| >> \min_i |Re(\lambda_i)|$ *where the ratio,* $S = \dfrac{\max_i |Re(\lambda_i)|}{\min_i |Re(\lambda_i)|}$ *is called the stiffness ratio or stiffness index.*

and λ_i are the eigenvalues of the Jacobian matrix, $J = \dfrac{\partial f}{\partial \widetilde{y}}$ evaluated at $(x, \widetilde{y})$. Following this definition, the stiff system has S greater than 1.

1.4 Linear Multistep Method

A numerical method involves a number of consecutive approximations of $y_{n+j}, j = 0, 1, \ldots, k$, from which it will compute y_n, $n = 0, 1, \ldots, N$ sequentially and also involve the function of f in Eq. (1.1). The integer k is called the step number of the method. If $k = 1$, then the method is called as a one-step method. While if $k > 1$, the method is called as a multistep or $k-$step method. This subsection presents some definitions of linear multistep method (LMM) established by Lambert (1973) as below.

Definition 1.2 *The general form of linear $k-$step methods are written as:*
In the case of first order ODEs,

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j y'_{n+j}, \tag{1.4}$$

In the case of second order ODEs,

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j y'_{n+j} + h^2 \sum_{j=0}^{k} \gamma_j y''_{n+j}, \tag{1.5}$$

where h is the step size. α_j, β_j *and* γ_j *need to be constant and* α_0, β_0 *and* γ_0 *are not all zero. It can be simplified by assuming* $\alpha_k = 1$ *as* $\alpha_k \neq 0$*. The equation in (1.4) is explicit if* $\beta_k = 0$ *and implicit otherwise.*

Definition 1.3 *The Taylor's series expansion of* $y(x_n + h)$ *about* x_n *is defined by:*

$$y(x_n + h) = y(x_n) + hy' + \frac{h^2}{2!} y''(x_n) + \cdots + \frac{h^q}{q!} y^{(q)}(x_n), \tag{1.6}$$

where $q = 3, 4, \ldots$.

Definition 1.4 *The linear difference operator L associated with Eq. (1.5) is:*

$$L[y(x) : h] = \sum_{j=0}^{k} \Big[\alpha_j y(x + jh) - h\beta_j y'(x + jh) - h^2 \gamma_j y''(x + jh) \Big], \tag{1.7}$$

where $y(x)$ *is an arbitrary function and continuously differentiable on* $[a, b]$*. Expanding* $y(x + jh), y'(x + jh)$ *and* $y''(x + jh)$ *as Taylor's series in Eq. (1.6) and collecting the common terms gives:*

$$L[y(x) : h] = C_0 y(x) + C_1 h y'(x) + \cdots + C_q h^q y^q(x). \tag{1.8}$$

The constants C_q are defined as:

$$\begin{aligned}
C_0 &= \sum_{j=0}^{k} \alpha_j, \\
C_1 &= \sum_{j=0}^{k} \left[j\alpha_j - \beta_j \right], \\
&\vdots \\
C_q &= \sum_{j=0}^{k} \left[\frac{j^q \alpha_j}{q!} - \frac{j^{q-1} \beta_j}{(q-1)!} - \frac{j^{q-2} \gamma_j}{(q-2)!} \right], q = 2, 3, \ldots.
\end{aligned} \tag{1.9}$$

Following that, the order of the method can be determined by using the following definitions provided by Henrici (1962).

Definition 1.5 *The first order LMM in Eq. (1.4) is of order p if* $C_0 = C_1 = \cdots = C_p = 0, C_{p+1} \neq 0$*, where* C_{p+1} *being the error constant.*

Definition 1.6 *The second order LMM in Eq. (1.5) is of order p if* $C_0 = C_1 = \cdots = C_{p+1} = 0, C_{p+2} \neq 0$*, where* C_{p+2} *being the error constant.*

A key feature of an acceptable LMM is that the solution generated by the method converges to an exact solution as the step size approaches zero. Hall and Watt (1976) stated that an LMM in Eq. (1.4) is convergent if and only if it is consistent and zero stable. The proof for the theorem can be found in Hall and Watt (1976). The following consistency conditions given by Lambert (1973) must be fulfilled for this theorem to be satisfied.

Definition 1.7 *The LMM is said to be consistent if it has order $p \geq 1$. The method is consistent if and only if the following conditions are satisfied:*

$$\begin{aligned} \sum_{j=0}^{k} \alpha_j &= 0, \\ \sum_{j=0}^{k} j\alpha_j &= \sum_{j=0}^{k} \beta_j. \end{aligned} \tag{1.10}$$

The first and second characteristic polynomials of the LMM are defines as

$$\begin{aligned} \rho(\xi) &= \sum_{j=0}^{k} \alpha_j \xi^j, \\ \sigma(\xi) &= \sum_{j=0}^{k} \beta_j \xi^j. \end{aligned} \tag{1.11}$$

The LMM is consistent if and only if $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$. ξ_1 is called the principal root and the following roots $\xi_s, s = 2, 3, \ldots, k$, are called spurious roots. The characteristic polynomial of the method may be written as follows

$$\pi(r, H) = \rho(r) - H\sigma(r) = 0, \tag{1.12}$$

where $H = h\lambda$ and $\lambda = \dfrac{\partial f}{\partial y}$ is a complex parameter.

Definition 1.8 *The LMM is said to have zero stability if no root of its characteristic polynomial has a modulus higher than one and if any root with a modulus of one is simple.*

The following definitions provided by Dahlquist (1963) pertinent to absolute stability, $A-$stability as described below.

Definition 1.9 *The LMM is said to be absolutely stable in a region $\Re_A$, if all the roots of the stability polynomial satisfy $|r_s| < 1, s = 1, 2, \ldots, k$.*

Definition 1.10 *A numerical method is said to be $A-$stable if $\Re_A \supseteq \{H \mid Re(H) < 0\}$. This means that the stability region covers the whole left-hand of the $H-$plane as shown in Figure 1.1.*

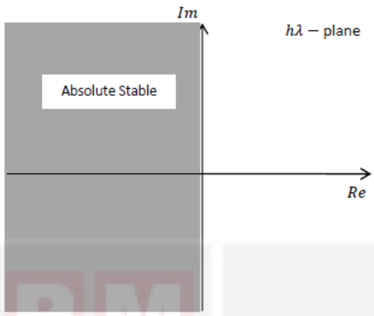

Figure 1.1: Absolute stability region for an $A-$stable method

Nonetheless, the requirement of $A-$stability imposes severe constraints on selecting suitable LMMs. This constraint is known as the second barrier of Dahlquist, which states that the order for an $A-$stable LMM must be less than or equal to 2 (see Dahlquist (1963)). This demanding criterion motivates the concept of stiff stability and $A(\alpha)-$stability by Widlund (1967) and redefined by Butcher (2009) as illustrated in Figure 1.2 and presented in definitions given below.

Definition 1.11 *A numerical method is stiffly stable with stiffness abscissa, D if all complex numbers H are included in the stability region, so that $Re(H) \leq -D$.*

Definition 1.12 *A numerical method is said to be $A(\alpha)-$stable, $\alpha \in \left(0, \pi/2\right)$ if $\Re_A \supseteq \{H \mid -\alpha < \pi - arg(H) < \alpha\}$.*

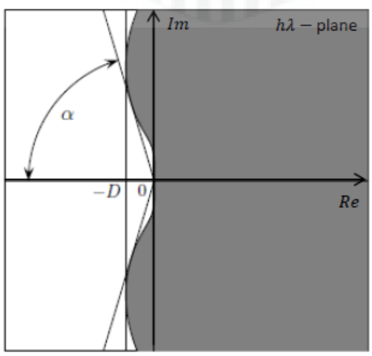

Figure 1.2: $A(\alpha)-$stability and stiff stability as featured in Butcher (2009)

1.5 Problem Statement

Stiff problems generally occur when different parts of the ODEs systems have differing time dependencies. As stiff ODEs arise in many branches, it is required to be solved efficiently. Unfortunately, because of the solution with both slowly and rapidly varying components within a narrow interval, the analytical solutions for most of these realistic stiff systems have been far from trivial; therefore a numerical method is advocated.

One common technique used to solve second order ODEs is to transform them into equivalent first order systems. Nevertheless, these approaches will require more computational time and hence affect the efficiency of the developed methods. To gain some advantage in computational work, we will treat the system of second order ODEs directly.

BDF is the most common class of implicit LMM, which is well-suited to dealing with stiffness. The block method's employment with a diagonally implicit structure in BDF is expected to accelerate the integration process. This advantage has motivated us to formulate a new diagonally implicit class of block backward differentiation formula (BBDF) and thus enhance the performance of existing BBDF methods for solving the standard stiff systems and some application problems arising in the literature.

1.6 Objectives of the Thesis

The main objectives of this research are:

(i) To derive diagonally implicit classes of BBDF in fixed step size by taking a non zero arbitrary, $\beta_{k-1,k}$ and introducing a free parameter, ρ for solving first and second order stiff ODEs.

(ii) To derive diagonally implicit classes of BBDF with non zero $\beta_{k-1,k}$ in adaptive step size for solving first and second order stiff ODEs.

(iii) To analyze the stability and convergence properties of the derived methods.

(iv) To illustrate the performance of the derived methods in terms of the maximum error and computational time.

(v) To provide the numerical solutions of the derived methods for some stiff mathematical models and application system in medical science, chemical engineering and physical fields.

1.7 Scope and Limitation of the Thesis

This research concentrates on solving first and second order stiff ODEs with different level of stiffness ranging from the mildly to highly stiff systems. Therefore, this study required to explicate the purpose of fixed and adaptive step size approaches in the execution of the new classes of BBDF for solving the standard and application stiff problems. By implementing such a strategy, we can increase and exploit the potential of the existing BBDF methods successfully.

In terms of the numerical results, our developed methods will be compared with the existing classes of BBDF in the literature and the established stiff solvers in Matlab, i.e. ode15s and ode23s. However, the execution time presented is limited to some numerical results due to unavailable codes and different environment and equipment.

This thesis comprises the formulation of new diagonally implicit classes of BBDF methods in fixed step size of order two and three only. Observed from the analysis of stability properties and numerical experiments conducted, as we increase the order of the methods, it becomes less stable and less accurate. This set of circumstances put a limitation on our research to not extend for higher order, such as order four and five.

In addition, the pharmacokinetics models, chemicals reactions and physical systems which exhibit stiffness are solved to ensure the capability of the developed methods in solving real-world problems.

1.8 Outline of the Thesis

This thesis is divided into eight chapters. In Chapter 1, the introduction is presented briefly encompassing the mathematical concepts of stiff ODEs, objectives, scopes and outline of this thesis. In Chapter 2, related literature on the block methods, BBDF, the diagonally implicit structure of the formula, adaptive step approach and direct methods are reviewed.

Chapter 3 provided detailed derivation and implementation of $\rho-$Diagonally Implicit Block Backward Differentiation Formula ($\rho-$DIBBDF) of order 2 and 3 in fixed step size. The subject in Chapter 4 will be the extension of the idea in Chapter 3, where the $\rho-$DIBBDF of order 2 in adaptive step size is to be derived. The order, convergence, stability regions and restrictive requirement on the step size of the methods are investigated. Implementation of the methods using Newton's iteration is also presented. The numerical results for some standard stiff and application problems are illustrated for both fixed and adaptive step formula and compared with several existing BBDF classes and Matlab's solvers.

The formulation of the $\rho-$DIBBDF for solving second order stiff ODEs in fixed and adaptive step approaches have been presented in Chapter 5 and Chapter 6, respectively. The analysis of the methods, including the order, consistency, zero stability and stability region, are explained. Implementation of the methods using Newton's iteration is also discussed. Numerical results and the comparisons of their performance with existing BBDF classes, ode15s and ode23s were given in the last section of the chapter.

In Chapter 7, the numerical solutions for some biological, physical and chemical dynamic systems approximated by the fixed step and adaptive step size formulae developed in this thesis are provided. To demonstrate the capability of our methods, the solution curves for all application systems of real-world problems examined are plotted. Finally, the conclusion of this thesis which includes the summary and recommendation for future work are presented in Chapter 8.

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BIODATA OF STUDENT

The student, HAZIZAH BINTI MOHD IJAM, was born in 6 November 1983. She obtained her Bachelor of Science with education majoring in Mathematics from Universiti Putra Malaysia in 2006. Several years later, she furthered her studies in a Master of Sciences, from the Institute for Mathematical Research (INSPEM), Universiti Putra Malaysia and completed in 2014. She is currently enrolled in the area of Computational Mathematics from INSPEM. Her research interest involves numerical analysis where the derivation and stability properties of new block backward differentiation methods are studied in solving stiff ordinary differential equations in real-life phenomena.

LIST OF PUBLICATIONS

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

Journal articles:

Hazizah Mohd Ijam, Zarina Bibi Ibrahim, Zanariah Abdul Majid and Norazak Senu (2020). Stability Analysis of a Diagonally Implicit Scheme of Block Backward Differentiation Formula for Stiff Pharmacokinetics Models. *Advances in Difference Equations*, Vol 2020: 400. doi:10.1186/s13662-020-02846-z

Hazizah Mohd Ijam and Zarina Bibi Ibrahim (2019). Diagonally Implicit Block Backward Differentiation Formula with Optimal Stability Properties for Stiff Ordinary Differential Equations. *Symmetry*, Vol 11: 1342. doi:10.3390/sym11111342

Hazizah Mohd Ijam, Zarina Bibi Ibrahim, Zanariah Abdul Majid, Norazak Senu and Khairil Iskandar Othman (2019). $\rho-$Diagonally Implicit Block Backward Differentiation Formula for Solving Stiff Ordinary Differential Equations. *Journal of Advance Research in Dynamical & Control Systems: SCIEMATHIC 2019*, Vol 11, Special Issue-12.

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Researchers: Prof. Dr. Zarina Bibi Ibrahim, Assoc. Prof. Dr. Khairil Iskandar Othman and **Hazizah Mohd Ijam**