UNIVERSITI PUTRA MALAYSIA

FAMILY OF SINGLY DIAGONALLY IMPLICIT BLOCK BACKWARD DIFFERENTIATION FORMULAS FOR SOLVING STIFF ORDINARY DIFFERENTIAL EQUATIONS

SAUFIANIM BINTI JANA AKSAH

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By

SAUFIANIM BINTI JANA AKSAH

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

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DEDICATIONS

To my beloved family
and
Prof. Zarina Bibi Ibrahim

for their endless love and continuous support.

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
Faculty: Science

A new family of singly diagonally implicit block backward differentiation formulas (SDIBBDF) for solving first and second order stiff ordinary differential equations (ODEs) are developed. Motivation in developing the SDIBBDF method arises from the singly diagonally implicit properties that are widely used by researchers in Runge-Kutta (RK) families to improve efficiency of the classical methods. The strategy is to reduce a fully implicit method to lower triangular matrix with equal diagonal elements. In order to achieve a particular order of accuracy, error norm minimization strategy is implemented based on the error constant of the formulas.

Although the derived methods have proven to solve stiff ODEs efficiently, the extended SDIBBDF (ESDIBBDF) methods are introduced by adding extra function evaluation to further improve accuracy. As some of the applied problems available in the literature are modeled as second order ODEs thus, 2ESDIBBDF method is constructed to meet the requirement. Numerical algorithm of the method is designed to solve the second order stiff ODEs directly. Subsequently, the constant step size methods are implemented with the variable step size scheme. The scheme is proposed to optimize the total steps taken by the methods to approximate solutions which later displays a better performance in solving the problems.

Necessary conditions for convergence are studied to ensure that the derived methods are able to approximate solution of a differential equation to any required accuracy. Since absolute stability is a crucial characteristic for a method to be useful therefore, stability graphs of the methods derived are constructed by MAPLE programming.

The stability properties of the methods are discussed to justify their ability for solving stiff problems. Performance of the methods are verified from the numerical results executed via the C++ programming by comparing them with existing methods of the same nature.

Finally, the applications of developed methods in the field of applied sciences, life sciences and engineering are presented. From the numerical experiments conducted, it can be concluded that the proposed methods can serve as an alternative solver for solving stiff ODEs of first and second order directly, and applied problems.

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

KELUARGA BLOK FORMULA PEMBEZAAN KE BELAKANG PEPENJURU TERSIRAT TUNGGAL UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA KAKU

Oleh

SAUFIANIM BINTI JANA AKSAH

Februari 2021

Pengerusi: Zarina Bibi binti Ibrahim, PhD
Fakulti: Sains

Keluarga baru blok formula pembezaan ke belakang pepenjuru tersirat tunggal (BFPBPT) bagi menyelesaikan persamaan pembezaan biasa (PPB) kaku peringkat pertama dan kedua dibangunkan. Galakan bagi membangunkan kaedah BFPBPT ini datang dari ciri-ciri pepenjuru tersirat tunggal yang digunakan secara meluas oleh penyelidik-penyelidik dalam keluarga Runge-Kutta (RK) bagi menambah baik keberkesanan kaedah-kaedah klasikal. Strateginya adalah dengan menurunkan kaedah tersirat penuh ke matriks segi tiga bawah dengan elemen-elemen pepenjuru yang sama. Bagi mencapai peringkat ketepatan khas, strategi peminimuman norma ralat dilaksanakan berdasarkan pemalar ralat formula-formula tersebut.

Walaupun kaedah-kaedah yang diterbitkan telah terbukti menyelesaikan PPB kaku dengan berkesan, kaedah-kaedah lanjutan BFPBPT (LBFPBPT) diperkenalkan dengan menambah fungsi penilaian tambahan untuk menambah baik lagi ketepatan. Memandangkan sebahagian masalah-masalah gunaan yang terdapat dalam kajian lepas dimodelkan sebagai PPB peringkat kedua, oleh yang demikian kaedah 2LBFPBPT dibina bagi memenuhi permintaan tersebut. Algoritma berangka kaedah tersebut direka untuk menyelesaikan PPB kaku peringkat kedua secara langsung. Seterusnya, kaedah-kaedah saiz langkah malar dilaksanakan dengan skim saiz langkah berubah. Skim ini diusulkan untuk mengoptimumkan jumlah langkah yang diambil oleh kaedah-kaedah tersebut bagi menganggarkan penyelesaian yang seterusnya memaparkan prestasi lebih baik dalam menyelesaikan masalah.

Keadaan-keadaan perlu bagi penumpuan dikaji bagi memastikan bahawa kaedah-

kaedah yang diterbitkan boleh menganggarkan penyelesaian persamaan kepada mana-mana ketetapan yang dinginkan. Memandangkan kestabilan mutlak adalah karakter penting bagi sesuatu kaedah untuk berguna, oleh itu graf kestabilan kaedah-kaedah yang diterbitkan dibina dengan pengaturcaraan MAPLE. Ciri-ciri kestabilan pada kaedah-kaedah dibincangkan untuk menjustifikasi kebolehan kaedah-kaedah tersebut dalam menyelesaikan masalah-masalah kaku. Prestasi kaedah-kaedah disahkan daripada keputusan berangka yang dilaksankan melalui pengaturcaraan C++ dengan membandingkan kaedah-kaedah tersebut dengan kaedah-kaedah sedia ada dari sifat yang sama.

Akhir sekali, aplikasi kaedah-kaedah yang dibangunkan dalam bidang sains gunaan, sains kehidupan dan kejuruteraan dibentangkan. Dari eksperimen berangka yang dijalankan, boleh disimpulkan bahawa kaedah-kaedah yang diusulkan boleh digunakan sebaga penyelesai alternatif untuk PPB kaku peringkat pertama dan kedua langsung, dan masalah-masalah gunaan.

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Zarina Bibi binti Ibrahim, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Zanariah binti Abd Majid, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

Norazak bin Senu, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

ZALILAH MOHD SHARIFF, PhD
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

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LIST OF ABBREVIATIONS

ODE	Ordinary differential equation
IVP	Initial value problem
LMM	Linear multistep method
LTE	Local truncation error
RK	Runge-Kutta
SDIRK	Singly diagonally implicit Runge-Kutta
BDF	Backward differentiation formulas
BBDF	Block backward differentiation formulas
SDIBBDF	Singly diagonally implicit block backward differentiation formulas
ESDIBBDF	Extended singly diagonally implicit block backward differentiation formulas
VSESDIBBDF	Variable step extended singly diagonally implicit block backward differentiation formulas
2ESDIBBDF	Extended singly diagonally implicit block backward differentiation formulas for second order ODEs
VS2ESDIBBDF	Variable step extended singly diagonally implicit block backward differentiation formulas for second order ODEs
MEN	Minimized error norm
ode15s	Variable order method of numerical differentiation formulas
ode23s	Fixed order method of new modified Rosenbrock (2, 3) pair
h	Step size
TIME(s)	Time taken in seconds
AVER	Average error
MAXE	Maximum error

CHAPTER 1

INTRODUCTION

1.1 Introduction

Differential equations (DEs) are the essential mathematical tools to model scientific problems of various fields. Solution for DEs may exists in the form of linear where its derivative occur to the first degree only and nonlinear when second or higher degree derivatives are involved. In addition to that, the equations can be classified as ordinary where the derivatives are taken with respect to a single independent variable or partial when several independent variables are involved.

For this research, we are focusing on the solution of ordinary differential equations (ODEs). In the research involving mathematical modeling of a scientific problems for applied sciences, engineering and life sciences, system of ODEs are usually categorized into stiff and non-stiff. This is due to the decaying components at widely differing rates which exhibit behavior associates with stiffness.

Due to the complexity of the problems modeled by DEs up to extend where analytical methods are not adequate to find the accurate solution, numerical methods are the only option. Numerical methods for solving ODEs are commonly categorized as one-step or multistep processes. The difference lies on the number of previous point used to compute solution where one-step uses only one point while multistep method uses several previous points. Family of Runge-Kutta (RK) and backward differentiation formulas (BDF) are among the famous solvers under the one-step and multistep method respectively.

1.2 Ordinary Differential Equations

This research focuses to solve ODEs of various nature; single, system, linear and nonlinear. The work is initially designed to deal with the first order ODEs of the form

$$y'(x) = f(x,y), \quad y(a) = \mu, \quad x \in [a,b], \tag{1.2.1}$$

where $y^T = (y_1(x), y_2(x), \ldots, y_d(x))$, $f^T = (f_1(x), f_2(x), \ldots, f_d(x))$ and $\mu^T = (\mu_1(x), \mu_2(x), \ldots, \mu_d(x))$. Eq. (1.2.1) is said to be linear if $f(x,y) = A(x)y + \Phi(x)$, with $A(x)$ is a constant $d \times d$ matrix and $\Phi(x)$ is a $d-$dimensional vector.

Then, the work is extended to directly solve the second order ODEs with the following form directly.

$$y_i''(x) = f_i(x, y_i, y_i'), \quad y_i(a) = \mu_i, \quad y_i'(a) = \mu_i', \tag{1.2.2}$$

where $i = 1, 2, ..., s$ for $a \leq x \leq b$.

Solution of differential systems is commonly dependent on the exact classification of the equations. On some cases, that respective equation might not possess a real solution. However, when the system has a solution, the concern will be directed to whether that solution is the only one possible or not. By that, we present the following definition.

Definition 1.1 *A function $f : R \times R^d \to R^d$ is said to satisfy Lipschitz condition in its second variable if there exist a constant L such that for any $x \in [a, b]$ and $y_1, y_2 \in R^d$,*

$$|f(x, y_1) - f(x, y_2)| \leq L|y_1 - y_2|, \tag{1.2.3}$$

where L is called Lipschitz constant.

The Lipschitz condition is a necessary condition for the existence of unique solution to Eq. (1.2.1). Therefore, the following theorem should be considered.

Theorem 1.1 *Let $f(x, y(x))$ be defined and continuous $\forall$ points $\big(x, y(x)\big)$ in a domain D defined by $a \leq x \leq b, y \in (-\infty, \infty)$, a and b are finite, and that $f(x, y(x))$ satisfies Lipschitz condition. Then for any given number μ, there exists a unique solution $y(x)$ of Eq. (1.2.1), where $\forall \; \big(x, y(x)\big) \in D$, $y(x)$ is continuous and differentiable.*

Detailed proof on the theorem can be found in Henrici (1962).

1.3 Stiffness

Throughout years, there have been numbers of definition for stiffness proposed by researchers from various field based on the perspective of their research background. Therefore, there is no consensus on the definition of stiffness as agreed by Shampine and Thompson (2007) which stated that no universally accepted definition of stiffness exists. For instance, in the field of numerical analysis, Curtis and Hirschfelder (1952) has mentioned that stiff equations are equations where implicit methods perform better, usually tremendously better, than explicit one. While according to Dahlquist (1974), stiffness is systems containing very fast components as well as very slow components.

In addition to that, a system is said to be stiff in a particular interval when a numerical method with a finite region of absolute stability, applied to a system with initial condition, is forced to use a certain interval of integration of step length which is excessively small in relation to the smoothness of the exact solution in that interval, Lambert (1991). By referring to the argument raised by Brugnano et al. (2011), the most successful definitions seems to be the one based on particular effects of the phenomenon (stiff) rather than on the phenomenon itself.

Therefore, for this research, we interpreted the behavior of stiffness based on the definition by Lambert (1973).

Definition 1.2 *The linear system in Eq. (1.2.1) is said to be stiff if*

1. $Re(\lambda_i) < 0$, $i = 1, 2, \ldots, d$
2. $\max_i |Re(\lambda_i)| >> \min_i |Re(\lambda_i)|$, *where* λ_i *are the eigenvalues of A and*
3. *the ratio* $S = \dfrac{\max_i |Re(\lambda_i)|}{\min_i |Re(\lambda_i)|}$ *is called the stiffness ratio.*

1.4 Linear Multistep Method

This section provides the crucial elements for the analysis of a linear multistep method (LMM) which is the order, convergence and stability of the method. A brief review on LMM by Lambert (1991) will be given first.

Definition 1.3 *The general LMM for first and second order ODEs are as follows.*
First order:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j y'_{n+j} \tag{1.4.1}$$

Second order:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j y'_{n+j} + h^2 c_j y''_{n+j} \tag{1.4.2}$$

where α_j, β_j *and* θ_j *are constants by assuming that not both* α_0, β_0 *and* θ_0 *are zero, with* $\alpha_k \neq 0$. *k is the order of the method and h is the step size.*

To determine order of LMM for first and second order ODEs, we will be referring to the following definitions respectively by Henrici (1962).

Definition 1.4 *The LMM in Eq. (1.4.1) is said to be of order p if*

$$C_0 = C_1 = \ldots = C_p = 0, \quad C_{p+1} \neq 0 \tag{1.4.3}$$

where C_{p+1} *is error constant.*

Definition 1.5 *The LMM in Eq. (1.4.2) is said to be of order p if*

$$C_0 = C_1 = ... = C_p = C_{p+1} = 0, \quad C_{p+2} \neq 0 \tag{1.4.4}$$

where C_{p+2} is error constant.

Convergence analysis of LMM is based on the following definition.

Definition 1.6 *The LMM is said to be convergent if for all initial value problems (IVPs) satisfying the conditions stated in Theorem 1.1, the following holds for all $x \in [a,b]$, and for all solutions y_n of the difference equation satisfying the starting conditions $y_\mu = \eta_\mu(h)$ for which $\lim_{h\to 0} \eta_\mu(h) = \eta$, $\mu = 0, 1, ..., k-1$,*

$$\lim_{h\to 0, n\to\infty} y_n = y(x_n).$$

Moreover, the following theorem stated the necessary conditions for convergence as elaborated by Buchanan and Turner (1992).

Theorem 1.2 *The LMM is convergent if and only if it is zero stable and consistent.*

The following definitions on consistency, zero stability, absolute stability and $A-$stability of the LMM are as reviewed in Lambert (1973) adn Lambert (1991). For consistency of LMM, the following two definitions will be applied.

Definition 1.7 *The LMM is said to be consistent if it has order $p \geq 1$.*

Definition 1.8 *A block method is consistent if and only if*

$$\begin{aligned} &(i) \sum_{j=0}^{k} A_j = 0, \\ &(ii) \sum_{j=0}^{k} jA_j = \sum_{j=0}^{k} B_j, \end{aligned} \tag{1.4.5}$$

where A_j, B_j are $r \times r$ matrices and the linear difference operator of the method is

$$L[y(x);h] = \sum_{j=0}^{k} A_j y(x+jh) - \sum_{j=0}^{k} hB_j y'(x+jh) \tag{1.4.6}$$

Meanwhile, zero stable LMM is expected to have specific property of roots for its characteristic polynomial.

Definition 1.9 *An LMM is said to be zero stable if no root of the first stability polynomial, $p(\zeta)$, has modulus greater than one, and if every root with modulus one is simple.*

Where the characteristic polynomial is in the respective form.

Definition 1.10 *The characteristic polynomial of LMM in Eq. (1.2.1) assumes*

$$\pi(r,h\lambda) = \rho(r) - h\lambda\phi(r) = 0,$$

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

Many applied problems generally comprise systems of equations with solutions containing elements whose rates of change differ distinctly. In most cases, the property of stability governs the numerical process. Thus, a method is considered useful when it has a region of absolute stability.

Definition 1.11 *The LMM in Eq. (1.2.1) is said to be absolutely stable in a region R for a given H if and only if for that H, all the roots, $r_s = r_s(H)$ of the stability polynomial of the linear $k-$step method, $\pi(r,H) = \rho(r) - H\phi(r)$, satisfy $|r_s| < 1$, $s = 1,2,\ldots,k$ where $H = h\lambda$ and $\rho(r)$ and $\phi(r)$ are the first and second characteristic polynomials respectively. Otherwise the method is said to be absolutely unstable.*

Figure 1.1 shows the illustration of the absolute stability region for LMM on plane H by Ibrahim et al. (2019).

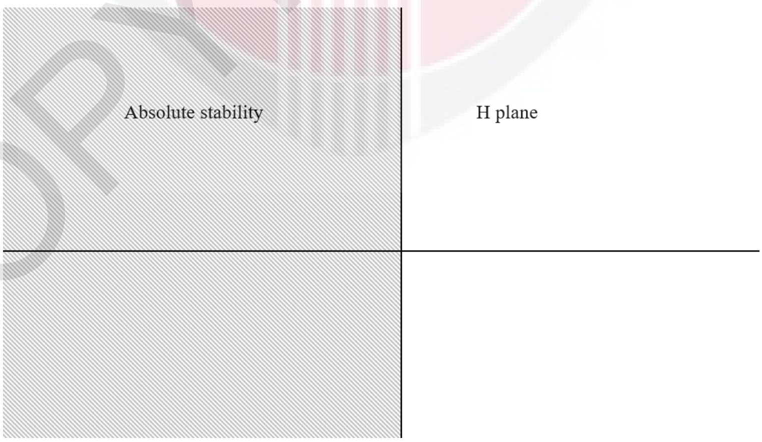

Figure 1.1: The region of absolute stability for LMM

For a method to be capable for solving stiff ODEs, it must possessed an $A-$stability which an essential property for stiffness solver.

Definition 1.12 *A numerical method is said to be A−stable if its region of absolute stability contains the whole left-hand half-plane,* $Re(h\lambda) < 0$.

However, the following statement by Dahlquist (1963) revealed that

Definition 1.13 *(i) An explicit LMM cannot be A−stable.*
(ii) The order of an A−stable implicit LMM cannot exceeded two.
(iii) The second order A−stable implicit LMM with smallest error constant is the Trapezoidal rule.

In view of this, we present here the two less demanding stability properties which are acceptable for the solutions of many stiff problems as reviewed in Butcher (2009).

Definition 1.14 *A method is stiffly stable with stiffness abscissa D if the stability region includes all complex numbers z such that* $Re(z) \leq -D$.

Definition 1.15 *A numerical algorithm is said to be* $A(\alpha)-$*stable for some* $\alpha \in \left[0, \frac{\pi}{2}\right]$ *if the region of absolute stability includes the infinite wedge*

$$S_\alpha = \{H : |Arg(-H)| < \alpha, H \neq 0\}. \tag{1.4.7}$$

Besides, the local truncation error (LTE) that will be elaborated throughout this research has the following definition.

Definition 1.16 *The LTE at* x_{n+k} *of Eq. (1.2.3) is defined as Eq. (1.4.6) when* $y(x)$ *is the theoretical solution of the IVPs in Eq. (1.2.1).*

1.5 Problem Statement

Phenomenon of stiffness in ODEs occurs in a wide range of scientific fields, such as in the studies of electrical circuits, vibrations, chemical reactions and infectious disease. In addition to that, some of these applied problems are often modeled in the form of second order ODEs.

Based on the common practice, the second order ODEs is solved by reducing the problems into a system of first order ODEs. Then, a suitable method is used to solve the system. However, due to the higher computational cost yields from this practice, the direct numerical approaches are come in handy due to their efficiency in accuracy and execution time when computing the solutions.

In this research, a series of singly diagonally implicit block backward differentiation formulas (SDIBBDF) are derived for solving the first order stiff ODEs and to solve directly the second order stiff ODEs. Throughout this research, the proposed formulas will be having various modifications to improve its performances in solving the problems. As for the foundation of the formula itself, the idea is to implement strategies from two different families of numerical methods namely the RK and the block BDF methods.

1.6 Objectives of the Study

This study concerns on the derivation of new block multistep formulas with the implementation of singly diagonally implicit approaches that are established and widely known among the researchers of RK fields. The proposed formulas are expected to solve the first and second order stiff ODEs efficiently for both constant and variable step size mode. Our aim here is to achieve the following objectives:

1. To derive the constant step size SDIBBDF for solving first order stiff ODEs.
2. To construct the constant and variable step size extended SDIBBDF (ESDIBBDF) methods with additional function evaluation for first and second order stiff ODEs.
3. To justify convergence and stability properties of the derived methods.
4. To evaluate performances of the derived methods with comparison of existing methods.
5. To verify efficiency of the proposed methods to solve for applied problem of various fields.

1.7 Scope of Study

This research focuses on the derivation of SDIBBDF and ESDIBBDF methods for solving the first and second order stiff ODEs, where the second order stiff ODEs will be solved directly without reducing it to first order. The ESDIBBDF methods derived will undergo numbers of modification in order to improve its efficiency in approximating numerical solutions. They are designed in a constant manner which later extended to a variable step size form. Some of the numerical experiment conducted are limited to the results available in scientific literatures only.

1.8 Outline of Thesis

In the first chapter, theorems and definitions related with the first and second order stiff ODEs are stated. Basic properties of the LMM as the foundation in developing the proposed formula are introduced. Objectives, scope and limitation, and outline of the thesis are also presented in this chapter.

Next chapter presents the scientific literature and theories behind the earlier numerical methods with singly diagonally implicit properties, error norm minimization and implementation of block strategy to LMM. It is followed by the review on variable step size scheme and direct solver method for second order ODEs.

Chapter 3 provides the preliminary research on two point SDIBBDF method of constant step size for solving first order stiff ODEs. Implementation of error norm minimization to the derived method is also presented in this chapter. Order of the method is verified here along with the analysis of convergence and stability to ensure its capability in solving the stiff ODEs. Efficiency of the methods is justified through numerical experiment by comparing the results with existing methods available in the literature.

To improve performance of the methods derived earlier for solving first order stiff ODEs, family of extended SDIBBDF (ESDIBBDF) methods with extra function evaluation is introduced in Chapter 4. Each method possessed a different dimension of solution point and order. Order and convergence of the new extended methods are justified, and stability graphs of each methods are constructed and analyzed. Results for all methods in the family of ESDIBBDF are compared with existing methods in terms of accuracy and computational time.

In Chapter 5, ESDIBBDF method is designed for the variable step size scheme to solve the first order stiff ODEs. Strategy for step size selection is discussed in details. Order, convergence and stability region of the method are analysed. Performance of the variable step size ESDIBBDF method in solving the proposed test problems is proven through the numerical experiment conducted.

The ESDIBBDF method to solve directly the second order stiff ODEs is presented in Chapter 6. Details on the derivation and order of the method are described. Necessary conditions for convergence are investigated and stability region of the method is constructed. Numerical results of the developed method are compared with several existing methods available in the scientific literature.

Chapter 7 discussed on the development of variable step size ESDIBBDF method for second order stiff ODEs. The strategy applied to maintain or varying the step size ratio is elaborated. Algorithm that shows flow of the computational process is available in this chapter. Comparison between numerical results of the method with existing solvers will justify the role of ESDIBBDF method as an alternative solver.

In Chapter 8, selected methods introduced in Chapter 3 to Chapter 7 are adapted to solve real-life scientific problems under the field of applied science, engineering and life sciences. Numerical experiments are conducted to justify performance of the methods in comparison with existing methods and well-known mathematical solver for solving the applied problems.

Lastly, the entire thesis is summarized and the overall conclusion of the works are presented in Chapter 9. Future studies for continuation of the research are also given in the chapter.

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