



UNIVERSITI PUTRA MALAYSIA

***BLOCK BACKWARD DIFFERENTIATION FORMULA WITH OFF-STEP
POINTS FOR SOLVING FIRST ORDER STIFF ORDINARY
DIFFERENTIAL EQUATIONS***

AMIRATUL ASHIKIN BINTI MOHD NASARUDIN

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DIFFERENTIAL EQUATIONS**

By

AMIRATUL ASHIKIN BINTI MOHD NASARUDIN

**Thesis Submitted to the School of Graduate Studies, Universiti Putra
Malaysia, in Fulfillment of the Requirements for the Master of Science**

June 2020

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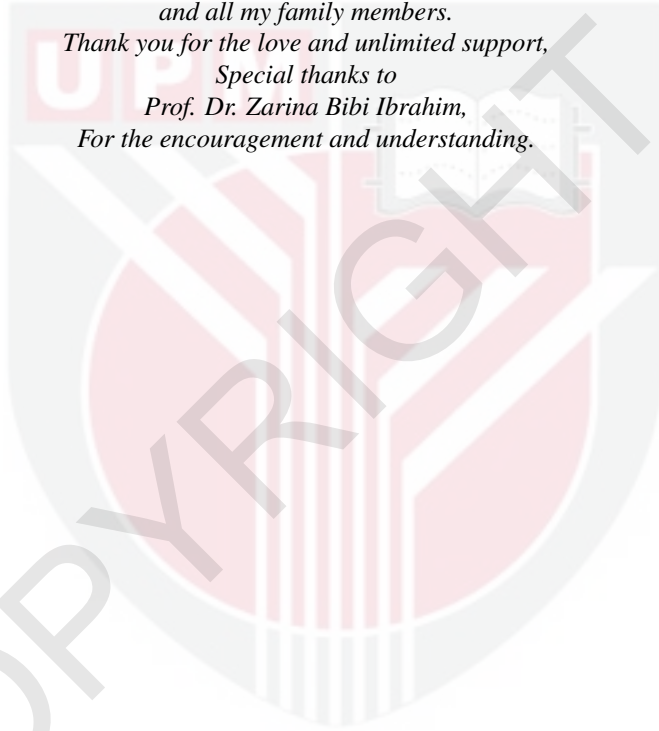


DEDICATIONS

To:

*My mother, Salmiah Hassan
My father, Mohd Nasarudin Ismail
and all my family members.*

*Thank you for the love and unlimited support,
Special thanks to
Prof. Dr. Zarina Bibi Ibrahim,
For the encouragement and understanding.*



Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Master of Science

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By

AMIRATUL ASHIKIN BINTI MOHD NASARUDIN

June 2020

Chairman: Zarina Bibi Binti Ibrahim, PhD
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This thesis compiles four new numerical methods that are successfully derived and presented based on Block Backward Differentiation Formulas (BBDFs) for the numerical solution of stiff Ordinary Differential Equations (ODEs). The first method is a one-point block order three BDF with one off-step point. The second method is developed by increasing the order of one-point block BDF with one off-step point to order four in order to increase the accuracy of the approximate solution. The third and fourth method are extension of the one-point block to two-point block BDFs method with off-step points.

The order and error constant of the methods are determined. Conditions for convergence and stability properties for all newly developed methods are discussed and verified so that the derived methods are suitable for solving stiff ODEs. Comparisons of stability regions are also investigated with the existing methods. Newton's iteration method is implemented in all developed methods. Numerical results are presented to verify the accuracy of the block BDF with off-step points for solving stiff ODEs and compared to the existing related methods of similar properties.

The final part of the thesis is by applying the formulated methods in solving the global warming problem and home heating problem as the example that the derived method can be applied to solve a real life application. In conclusion, by adding off-step point, the accuracy is improved. Therefore, it can be an alternative solver for solving first order stiff ODEs.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Master Sains

**FORMULASI BLOK PEMBEZAAN KE BELAKANG DENGAN
TITIK-TITIK LUAR LANGKAH UNTUK MENYELESAIKAN
PERSAMAAN PEMBEZAAN BIASA KAKU PERINGKAT PERTAMA**

Oleh

AMIRATUL ASHIKIN BINTI MOHD NASARUDIN

Jun 2020

Pengerusi: Zarina Bibi Binti Ibrahim, PhD
Fakulti: Sains

Tesis ini merangkumi empat kaedah berangka yang baru berjaya diterbitkan berasaskan Rumus Beza ke Belakang secara Blok (BFBB) sebagai penyelesaian berangka untuk persamaan pembezaan biasa (PPB) kaku yang telah berjaya diterbitkan. Kaedah pertama adalah satu-titik blok peringkat tiga FBB dengan satu titik luar langkah. Kaedah kedua diterbitkan dengan meningkatkan peringkat kaedah satu-titik blok FBB dengan satu titik luar langkah kepada peringkat empat untuk meningkatkan ketepatan anggaran penyelesaian. Kaedah ketiga dan keempat merupakan lanjutan daripada satu-titik blok ke dua-titik BFBB dengan titik-titik luar langkah.

Peringkat dan ralat pemalar bagi setiap kaedah ditentukan. Syarat-syarat untuk penumpuan dan ciri-ciri kestabilan bagi kesemua kaedah yang baru diterbitkan telah dibincangkan dan disahkan bahawa kaedah-kaedah tersebut sesuai untuk menyelesaikan PPB kaku. Perbandingan rantau kestabilan dengan kaedah-kaedah sedia ada juga diselidik. Kaedah lalaran Newton diimplementasikan kepada kesemua kaedah-kaedah yang telah diterbitkan. Keputusan berangka dibentangkan untuk mengesahkan ketepatan blok FBB dengan titik-titik luar langkah dalam menyelesaikan PPB kaku dan membandigkannya dengan kaedah-kaedah berkaitan sedia ada yang mempunyai ciri-ciri yang sama.

Bahagian akhir tesis adalah dengan mengaplikasi kaedah-kaedah yang telah diterbitkan dalam menyelesaikan masalah kepanasan global dan masalah pemanasan rumah sebagai contoh bahawa kaedah yang diterbitkan boleh diaplikasikan dalam aplikasi kehidupan sebenar. Kesimpulannya, dengan menambah titik luar langkah, ketepatan boleh ditingkatkan. Oleh itu, ianya boleh menjadi salah satu alat penyele-

saian alternatif untuk menyelesaikan PPB kaku.



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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 Master of Science. 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
BBDFO(3)	1-point Block Backward Differentiation Formula with Off-Step Point of Order Three
BBDFO(4)	1-point Block Backward Differentiation Formula with Off-Step Point of Order Four
BDF(3)	Classical Backward Differentiation Formula of Order Three
BDF(4)	Classical Backward Differentiation Formula of Order Four
BBDFO(5)	2-point Block Backward Differentiation Formula with Off-Step Points of Order Five
BBDFO(6)	2-point Block Backward Differentiation Formula with Off-Step Point of Order Six
BBDF(5)	Fifth Order Block Backward Differentiation Formulas
BBDF(6)	Sixth Order Block Backward Differentiation Formulas
h	Step size
MAXE	Maximum Global Error
AVE	Average Maximum Global Error
CO_2	Carbon Dioxide gas
t	Time
ode15s	Variable Order Numerical Differentiation Formulas

CHAPTER 1

INTRODUCTION

1.1 Ordinary Differential Equations

Ordinary differential equations (ODEs) are known to play an important role in real-life problems involving mathematical modelling such as in physics, medical area, engineering and economics. ODEs are equations which relate a function, f with one independent variable and its derivatives. The general form of first-order ODE is given below:

$$\frac{dy}{dx} = y' = f(x,y), \quad (1.1)$$

with initial condition

$$y(a) = \eta$$

at certain interval of x where $x \in [a, b]$.

Numerous numerical methods are able to solve equation (1.1) but may not necessarily work well. This is because ODEs are divided into two types which are stiff and non-stiff. Usually, the non-stiff ODEs are advisable to be solved using the explicit method. Meanwhile, the stiff ODEs often solved by the implicit method. Many problems in sciences carried "stiff" behavior. Curtiss and Hirschfelder (1952) are the first to use the term stiff in numerical field. Therefore, stiff ODEs are the type of ODE tested in this thesis. There are several definitions of stiffness collected from previous researchers:

- (i) Stiff problems are characterized by the fact that the numerical solution of slow smooth movements is considerably perturbed by nearby rapid solutions, (Hairer and Wanner, 1999).
- (ii) Stiff equations are equations where certain implicit methods, in particular BDF, perform better, usually tremendously better than explicit ones, (Curtiss and Hirschfelder, 1952).
- (iii) An ordinary differential equation problem is stiff if the solution being sought varies slowly, but there are nearby solutions that vary rapidly, so the numerical method must take small steps to obtain satisfactory results, (Moler, 2003).
- (iv) An initial value problem is stiff if the absolute stability properties dictate a much smaller step size than is needed to satisfy approximation requirement alone, (Petzold, 1983).

As a conclusion, the definition of stiffness consider in this research is the one defined by Lambert (1973).

Definition 1.1.1 *Lambert (1973)*

The system of (1.1) is said to be stiff if

- (i) $Re(\lambda_i) < 0, \quad i= 1, \dots, s$
- (ii) $\max_i |Re(\lambda_i)| \gg \min_i |Re(\lambda_i)|$ where λ_i are the eigenvalues of the Jacobian matrix $J = \frac{\partial f}{\partial y}$.

However, in solving stiff ODEs, any numerical method must satisfy some conditions. This is because not any randomly numerical method can solve stiff problems especially explicit method. To determine the methods are suitable to solve stiff ODE, following definitions are stated,

Definition 1.1.2 *Dahlquist (1963)*

If the numerical method possesses A-stable condition, therefore the method is suitable to solve for stiff ODEs.

Definition 1.1.3 *Lambert (1973)*

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

The involvement of off-step point in solving ODEs is not a new issue. Off-step point is believed to improve the approximation of the solution for ODEs. In the next section, a brief explanation on the definition of off-step point will be presented.

1.2 Off-Step Point

There is no general accepted definition for off-step point given but usually off-step point indicates any point located between two points, x_{n+i} and x_{n+i+1} where $i = \mathbb{Z}$. In this project, we let the off-step point be defined as in Lee and Ismail (2014):

$$x_{n+\frac{d}{2}} = x_n + \frac{d}{2}h \quad \text{for} \quad d = 1, 3 \tag{1.2}$$

The off-step points used in this project are $x_{n+\frac{1}{2}}$ and $x_{n+\frac{3}{2}}$. Based on Enright and Higham (1991) strategy, they have tested several points for choosing the points as

the off-step point. The off-step point is chosen as half of the step size, $\frac{1}{2}h$ because it is believed can obtain the optimized point and a zero stable formula.

In the following section, the review on linear multistep method (LMM) is given and some definitions related to the study are provided.

1.3 Linear Multistep Method

The implementation of implicit LMM is more relevant to solve stiff problems. The idea of LMM proposed by Dahlquist (1959) which capture the attention of Henrici (1962) to explore the method. Hence, one of the famous definition of LMM is formed by Lambert (1973),

Definition 1.3.1 Lambert (1973)

The general form of linear k -step method for first order ODEs are given as follows:

$$\sum_{j=1}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f_{n+j} \quad (1.3)$$

where α_j and β_j are constants where we assume that $\alpha_k \neq 0$ and that not both α_0 and β_0 are zero. k is defined as the order of the method and h is the step size.

Formula of LMM (1.3) can be derived using interpolating polynomial, generating function or Taylor's series expansion. To construct the linear difference operator L , we use Taylor's series expansion for clearer picture,

$$y(x + jh) = y(x) + \frac{(jh)^1}{1!} y'(x) + \frac{(jh)^2}{2!} y''(x) + \frac{(jh)^3}{3!} y^{(3)}(x) + \dots, \quad (1.4)$$

Definition 1.3.2 Lambert (1973)

The associated linear difference operator L for equation (1.3) simplified as following equation,

$$L[y(x); h] = \sum_{j=0}^k [\alpha_j y(x + jh) - h\beta_j y'(x + jh)] \quad (1.5)$$

where $y(x)$ is an arbitrary function, continuously differentiable on $[a, b]$.

Corresponding to the strategy of the research, we are adapting the linear difference operator L associated with the developed methods where we consider the step size as $\frac{h}{2}$ given by Abasi et al. (2014)

Definition 1.3.3 Abasi et al. (2014)

Following linear difference operator L formed when the step size is taken at half of the step size:

$$L[y(x), h] = \sum_{j=0}^k [\alpha_j y(x + j\frac{h}{2}) - h\beta_j y'(x + j\frac{h}{2})]. \quad (1.6)$$

Operator L in equation (1.6) is introduced to help in determining the order of proposed methods. The functions $y(x + j\frac{h}{2})$ and $y'(x + j\frac{h}{2})$ can be expanded using Taylor series at x such below

$$\begin{aligned} y(x + j\frac{h}{2}) &= y(x) + \frac{(j\frac{h}{2})^1}{1!} y'(x) + \frac{(j\frac{h}{2})^2}{2!} y''(x) + \frac{(j\frac{h}{2})^3}{3!} y^{(3)}(x) + \dots, \\ y'(x + j\frac{h}{2}) &= y'(x) + \frac{(j\frac{h}{2})^1}{1!} y''(x) + \frac{(j\frac{h}{2})^2}{2!} y^{(3)}(x) + \frac{(j\frac{h}{2})^3}{3!} y^{(4)}(x) + \dots. \end{aligned} \quad (1.7)$$

The coefficients of $y(x)$ and derivatives of $y(x)$ in (1.6) are collected after the expansion give the following equation

$$L[y(x); h] = C_0 y(x) + C_1 h y'(x) + \dots + C_p h^p y^{(p)}(x) + \dots \quad (1.8)$$

where Abasi et al. (2014) gives C_p as

$$\begin{aligned} C_0 &= \sum_{j=0}^k \alpha_j, \\ C_1 &= \sum_{j=0}^k (j\alpha_j) - 2 \sum_{j=0}^k \beta_j, \\ &\vdots \\ C_p &= \frac{1}{p!} \sum_{j=0}^k j^p \alpha_j - \frac{2}{(p-1)!} \sum_{j=0}^k j^{(p-1)} \beta_j. \end{aligned} \quad (1.9)$$

From equation (1.5), Henrici (1962) stated the definition to determine the order of LMM. In this research, definition below are used to determine the order of the proposed methods associated with the LMM formed by the new proposed method.

Definition 1.3.4 Henrici (1962)

The LMM (1.3) is said to be of order p if $C_0 = C_1 = \dots = C_p = 0$, $C_{p+1} \neq 0$ where C_{p+1} is error constant.

The most important analysis for any formulated numerical method is to check the

convergence of the method. In LMM case, Henrici (1962) already stated the necessary condition for any LMM to be convergent.

Definition 1.3.5 *Henrici (1962)*

The necessary and sufficient conditions for a method to be convergent are that it be consistence and zero-stable.

The justification of this statement is because the magnitude of the local truncation error controlled by consistency while the zero stability controlled the error that propagated at each step of calculation which described by Abasi et al. (2014).

Lambert (1973) gives the condition for any LMM (1.9) to be consistent and zero-stable as below,

Definition 1.3.6 *Lambert (1973)*

The LMM (1.3) is said to be consistent if it has order $p \geq 1$.

Definition 1.3.7 *Lambert (1973)*

Method (1.3) is said to be zero-stable if it satisfied root condition where the condition states that if all the roots of first characteristics polynomial have modulus less than or equal to unity and those of modulus unity are simple.

The main idea to solve for ODEs in this thesis is using block LMM method. In the next section, the definition of block method is described.

1.4 Block Methods

A block method is recognized as a method that computes concurrently solution values at different points along x -axis, see Ibrahim (2006). Mehrkanoon et al. (2009) detailed the advantages of block method by stating that at each application of a block method, the solution will be approximated at more than one point. The number of points depending on the structure of the block method. Thus, Chu and Hamilton (1987) represents b -block r -point method as,

Definition 1.4.1 *Chu and Hamilton (1987)*

Let Y_m and F_m be vectors defined by

$$\begin{aligned} Y_m &= [y_{n+1}, y_{n+1}, y_{n+2}, \dots, y_{n+r-1}]^t, \\ F_m &= [f_{n+1}, f_{n+1}, f_{n+2}, \dots, f_{n+r-1}]^t, \end{aligned} \quad (1.10)$$

A general k -block, r -point method can be written as

$$Y_m = \sum_{i=1}^k A_i Y_{m-i} + h \sum_{i=0}^k B_i F_{m-i} \quad (1.11)$$

where A_i 's and B_i 's are $r \times r$ coefficients matrix and $m = 0, 1, 2, \dots$ represent the block number, $n = mr$ is the first step number in the m^{th} block and r is the proposed block size.

1.5 Problem Statement

We consider the solution of first order ODEs with off-step points where we propose

$$y' = f(x, y),$$

with the given initial point

$$y_0 = y(x_0),$$

in the interval

$$a \leq x \leq b$$

and solved using 1-point and 2-point Block BDF method with off-step points.

1.6 Objectives of the thesis

This study concerns on the development of efficient codes that are based on BBDF methods for the numerical solution of stiff ODEs. The main objectives are summarized as follows:

- (i) to derive 1-point and 2-point block BDF methods with off-step points of order three, four, five and six that are suitable for solving stiff ODEs,
- (ii) to analyse the stability and convergence of the derived methods,
- (iii) to implement methods as in (i) with fixed step sizes using Newton's Iteration,
- (iv) to improve the stability region and the accuracy of the methods in (i),

- (v) to apply methods 2-point block BDF methods with off-step points using global warming problem and home heating problem.

1.7 Scope and motivation of the study

This research focused on the development of 1-point and 2-point block BDF with off-step point methods. Methods formed are verified using the first order stiff ODEs and the implementation of Newton's Iteration only tested for constant step size. From the literature, many researchers stated that the off-step point included in the derivation can improve the stability region and the accuracy of the methods. Therefore, these hypotheses motivate us to conduct the research.

1.8 Outline of the thesis

This thesis consists of six chapters including this chapter as follows:

Chapter 1 of the thesis consists of introduction of ODEs and some basic theory which include the definitions of stiff problems and properties of stability and convergence.

In chapters 2 present the review of previous research related in solving first order ODEs using BDF method and block method with off-step points are presented.

Chapter 3 gives the details on the derivation of 1-point block BDF with off-step point of order three and order four for solving first order stiff ODEs. The convergence and A -stable analysis of the methods are explained. The numerical results are compared with the existing methods.

In Chapter 4, the derivation of fifth and sixth order 2-point BBDF with off-step points and the stabilities of the methods are discussed. Numerical results are compared with related existing methods.

Chapter 5 is the application part of the thesis. In this chapter, the formulated methods are tested on global warming problem and home heating problem.

The last chapter, Chapter 6 concludes the study and summarized the entire thesis. This chapter includes some suggestion for future research.

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LIST OF PUBLICATION

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

Amiratul Ashikin Nasarudin, Zarina Bibi Ibrahim and Nor Ain Azeany Mohd Nasir., (2019). Numerical Solution for Application Problems by Third Order 1-point Block Backward Differentiation Formula with Off-Step Point. *Journal of Advance Research in Dynamical & Control Systems, Special Issue for SCIMATHIC2019*, Vol 11(12): 24–32. (SCOPUS)

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