EXTENDED TWO-POINT AND THREE-POINT BLOCK BACKWARD DIFFERENTIATION FORMULAS FOR SOLVING FIRST ORDER STIFF ORDINARY DIFFERENTIAL EQUATIONS

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By

NURSYAZWANI BINTI MOHAMAD NOOR

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

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DEDICATIONS

To my family, husband, lecturers and all the related peoples which involved in this research for their support and patience.

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

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This thesis focuses on solving first order stiff Ordinary Differential Equations (ODEs) using 2-point and 3-point block methods. The 2-point block method will compute the solutions y_{n+1} and y_{n+2} at points x_{n+1} and x_{n+2} simultaneously in a block at each step. Thus, the derivations of 2-point block methods of third and fifth order are presented. Order and error constant of the methods are determined. Newton's Method is used to implement in the 2-point block methods. The numerical results for each method are presented and compared with the existing methods.

Furthermore, the stability properties of all 2-point block methods are analysed to ensure that the methods are $A(\alpha)$-stable. Hence, its suitable for solving stiff problems. Convergence characteristics of the methods are also investigated.

The 2-point block method with fifth order is then extended to 3-point block method with same order. Advantage of the 3-point block method is the solutions will be approximated at three points concurrently which are x_{n+1}, x_{n+2} and x_{n+3}. Thus, the derivation of 3-point block method using Taylor's series expansion is presented. Order and error constant of the method are verified. Stability and convergence properties of the method are investigated by determining the zero-stable, stability region, $A(\alpha)$-stable and consistency. The 3-point block method is implemented by using Newton's iteration to measure its efficiency. Numerical results of the method are presented and performance of the method are compared with the existing methods.

An application problem of SIR model is solved by using the proposed methods. The numerical results are presented in tables for s, i and r groups for each method. Based on the analysis, the proposed methods can be an alternative solver for solving the application problem.

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

PERLANJUTAN DUA-TITIK DAN TIGA-TITIK BLOK RUMUS BEZA KE BELAKANG BAGI MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA KAKU PERINGKAT PERTAMA

Oleh

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Tesis ini memfokuskan kepada penyelesaian Persamaan Pembezaan Biasa (ODEs) kaku peringkat pertama dengan menggunakan kaedah 2-titik dan 3-titik blok. Kaedah 2-titik blok akan menghitung penyelesaian y_{n+1} dan y_{n+2} pada titik x_{n+1} dan x_{n+2} secara serentak dalam satu blok pada setiap langkah. Oleh itu, penerbitan kaedah 2-titik blok bagi peringkat ketiga dan kelima dibentangkan. Peringkat dan ralat pemalar bagi setiap kaedah ditentukan. Kaedah Newton digunakan untuk diimplementasikan kepada kaedah 2-titik blok. Keputusan berangka bagi setiap kaedah dibentangkan dan dibandingkan dengan kaedah yang sedia ada.

Tambahan pula, sifat kestabilan untuk kesemua kaedah 2-titik blok dianalisis bagi memastikan bahawa kaedah tersebut adalah kestabilan $A(\alpha)$. Oleh itu, ia sesuai untuk menyelesaikan masalah kaku. Ciri-ciri penumpuan kaedah juga dikaji.

Kaedah 2-titik blok dengan peringkat kelima kemudiannya dilanjutkan kepada kaedah 3-titik blok dengan peringkat yang sama. Kelebihan kaedah 3-titik blok ini adalah penyelesaiannya diberikan serentak pada tiga titik iaitu x_{n+1}, x_{n+2} dan x_{n+3}. Oleh itu, terbitan kaedah blok 3-titik menggunakan pengembangan siri Taylor dibentangkan. Peringkat dan ralat pemalar kaedah tersebut disahkan. Kestabilan dan sifat penumpuan juga dikaji secara terperinci dengan menentukan kestabilan sifar, rantau kestabilan, kestabilan $A(\alpha)$ dan konsitensi. Kaedah 3-titik blok diimplementasikan dengan menggunakan Newton iterasi untuk mengukur kecekapannya. Keputusan berangka kaedah tersebut dibentangkan dan prestasi kaedah dibandingkan dengan kaedah-kaedah yang sedia ada.

Masalah aplikasi model SIR diselesaikan dengan menggunakan kaedah yang dicadangkan. Keputusan berangka dibentangkan dalam jadual bagi kumpulan s, i dan r untuk setiap kaedah. Berdasarkan analisis, kaedah yang dicadangkan boleh menjadi penyelesaian alternatif untuk menyelesaikan masalah aplikasi tersebut.

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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
RLC	Resistor, Inductor and Capacitor
BDF	Backward Differentiation Formula
LMM	Linear Multistep Method
DAEs	Delay Algebraic Equations
BVPs	Boundary Value Problems
FDEs	Fuzzy Differential Equations
L_i	Linear Difference Operator
BBDF	Block Backward Differentiation Formula
2BBDF(3)I	2-point Block Backward Differentiation Formula of Third Order with $\rho = \frac{7}{8}$
2BBDF(3)II	2-point Block Backward Differentiation Formula of Third Order with $\rho = -\frac{7}{8}$
E2BBDF(5)	Extended 2-point Block Backward Differentiation Formula of Fifth Order
E3BBDF(5)	Extended 3-point Block Backward Differentiation Formula of Fifth Order
SIR	Susceptible, Infected, Recovery

CHAPTER 1

INTRODUCTION

1.1 Introduction

Ordinary differential equation (ODEs) are an equation containing the function, its derivative, the independent and dependent variables. The general formula of n-th order ODEs are defined as follows.

$$F\left(x, y, \frac{dy}{dx}, \cdots, \frac{d^n y}{dx^n}\right) = 0 \tag{1.1}$$

where F is the function, x is the independent variable and y is the dependent variable. In real life, there are various application problems often leads to an ODEs. For example in physical sciences, the physicians used an ODEs in the Newton's second law which states that the mass of an object times its acceleration same as the total force acting on it and this problem are applied to the free falling object. Other than physical sciences, the ODEs also arise in the fields of economics, medicine, psychology, operations research and etc. Usually the function in an applications represents the physical quantities, the derivatives represent their rates of change, and the equation define as a relationship between the function and the rate of change.

Equation (1.1) can be solved using various of numerical method likes the Euler, Runge-Kutta, Adams-Bashforth, Adams-Moulton, Backward Differentiation Formula (BDF) methods and many more. Among the mentioned numerical methods, there are two types of methods that can be distinguished which are single-step method and multistep method. The single-step method is used to approximate the solution using a previous point. Meanwhile, the multistep method is used to evaluate the solution using more than one previous points. Not all the numerical methods works well to solve equation (1.1) because the ODEs comprised of the non-stiff and stiff ODEs. The non-stiff ODEs are normally solved using the explicit methods while the stiff ODEs are usually solved using the implicit methods.

1.2 Stiff System of Ordinary Differential Equations

There is no precise definition of stiffness, thus Brugnano et al. (2011) compiled the following various definitions which studied by other researchers.

1. Stiff equations are equations where certain implicit methods perform better, usually tremendously better than explicit ones (Curtiss and Hirschfelder, 1952).

2. They represent coupled physical systems having components varying with

very different times scale: that is they are systems having some components varying much more rapidly than the others (Liniger, 1972).

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

4. 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 restriction on step size, h... Enormous means enormous relative to the scale which here is $\bar{x}$ (the integration interval)... (Miranker, 1975).

5. If a numerical method with a finite region of absolute stability, applied to a system with any initial condition, is forced to use 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).

6. The stiff problems are characterized by the fact that the numerical solution of slow smooth movements is considerably perturbed by nearby rapid solutions (Ernst and Gerhard, 1999).

In this research, the system of first order ODEs is considered in the form of

$$\tilde{y}' = \tilde{f}(x,\tilde{y}) = A\tilde{y} + \tilde{\phi}(x), \qquad \tilde{y}(a) = \tilde{\eta}, \qquad a \le x \le b \tag{1.2}$$

where $\tilde{y}^T = (y_1, y_2, \cdots, y_m)$, $\tilde{\eta}^T = (\eta_1, \eta_2, \cdots, \eta_m)$ and A is a $m \times m$ matrix with the eigenvalues λ_t, $t = 1, 2, \cdots, m$. To verify the system (1.2) is stiff, we preferred the definition of stiffness which is widely used among the researchers given by Lambert (1973) as follows.

Definition 1.1 *The linear system (1.2) is said to be stiff if*

1. $Re(\lambda_t) < 0$, $t = 1, 2, \cdots, m$, *and*

2. $\max_{t=1,2,\cdots,m} |Re(\lambda_t)| >> \min_{t=1,2,\cdots,m} |Re(\lambda_t)|$, *where* λ_t, $t = 1, 2, \cdots, m$, *are the eigenvalues of* A. *The ratio*

$$\left[\max_{t=1,2,\cdots,m} |Re(\lambda_t)|\right] : \left[\min_{t=1,2,\cdots,m} |Re(\lambda_t)|\right]$$

is called stiffness ratio.

In the following section, a brief review about the linear multistep method (LMM) will be given and some basic definitions related to the study are provided.

1.3 Linear Multistep Method

General linear of k-step method which are given by Lambert (1973) is written as

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \tag{1.3}$$

where α_j and β_j are constants by assuming that $\alpha_k \neq 0$ and both of α_0 and β_0 are not zero. Method (1.3) is explicit if the value of $\beta_k = 0$ and implicit when $\beta_k \neq 0$. The LMM (1.3) can be derived using interpolating polynomial, generating function and Taylor's series expansion. In this research, we are going to use Taylor's series expansion to obtain the coefficient values of proposed method. Therefore, the following definitions that will be considered in the construction of method are provided.

Definition 1.2 *The Taylor's series expansion of $y(x_n+h)$ about x_n is defined by*

$$y(x_n+h) = y(x_n) + hy'(x_n) + \frac{h^2}{2!}y''(x_n) + \cdots + \frac{h^q}{q!}y^{(q)}(x_n) \tag{1.4}$$

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

Definition 1.3 *The linear difference operator, L associated with LMM (1.3) is defined as*

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

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

Expanding $y(x_n+jh)$ and $y'(x_n+jh)$ using the Taylor's series expansion (1.4) about x_n and collecting terms in $y(x_n)$, $y'(x_n)$, $y''(x_n)$, $\cdots$ yields the following equation.

$$L[y(x_n);h] = C_{0,i}y(x_n) + C_{1,i}hy'(x_n) + \cdots + C_{q,i}h^q y^{(q)}(x_n) = 0, \tag{1.6}$$

where $i = 1, 2, \cdots, N$ is number of point and

$$\begin{aligned}
C_{0,i} &= \sum_{j=0}^{k} \alpha_j, \\
C_{1,i} &= \sum_{j=0}^{k} \left[j\alpha_j - \beta_j\right], \\
&\vdots \\
C_{q,i} &= \sum_{j=0}^{k} \left[\frac{j^{(q)}}{q!}\alpha_j - \frac{j^{(q-1)}}{(q-1)!}\beta_j\right], \qquad q = 2, 3, \cdots, N.
\end{aligned} \tag{1.7}$$

For a LMM (1.3) to be convergent it must be consistent and zero-stable (Buchanan and Turner (1992)). Theorem 1.1 is given to support the statement.

Theorem 1.1 *The necessary and sufficient conditions for a LMM (1.3) to be convergent are that it be consistent and zero-stable.*

Definition 1.4 *The LMM (1.3) is consistent if and only if the following conditions are satisfied:*

$$\sum_{j=0}^{k} \alpha_j = 0, \tag{1.8}$$

$$\sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_j. \tag{1.9}$$

Definition 1.5 *The LMM (1.3) is said to be zero-stable if no root of the first characteristic polynomial $\rho(t)$ has modulus greater than one, and every root with modulus one is simple.*

1.4 Problem Statement

This thesis considered to solve first order stiff ODEs in the form of equation (1.2) by assuming that the equation has satisfied the following theorem to assure that the existence of a unique solution to the initial value problems (IVPs).

Theorem 1.2 *Let $\tilde{f}(x,\tilde{y})$ be defined and continuous for all points $(x,\tilde{y})$ in the region D defined by $a \le x \le b$, $-\infty < \tilde{y} < \infty$, a and b finite and let there exist a constant L such that, for every x, $\tilde{y}$, $\tilde{y}^*$ such that $(x,\tilde{y})$ and $(x,\tilde{y}^*)$ are both in D,*

$$\left|\tilde{f}(x,\tilde{y}) - \tilde{f}(x,\tilde{y}^*)\right| \le L\left|\tilde{y} - \tilde{y}^*\right|. \tag{1.10}$$

Then, if $\tilde{\eta}$ is any given number, there exists a unique solution $\tilde{y}(x)$ of the initial value problem (1.2), where $\tilde{y}(x)$ is continuous and differentiable for all $x,\tilde{y}$ in D.

The requirement (1.10) is known as a Lipschitz condition and the constant L is a Lipschitz constant. See Henrici (1962) for further details proving.

1.5 Objective of the Thesis

In this research, we developed the formulas based on Block Backward Differentiation Formula (BBDF) method with fixed step size for solving first order stiff ODEs. The objectives of this thesis are

1. to extend the derivation of 2-point Block Backward Differentiation Formula method by Musa et al. (2013b) with a new set of coefficients to improve the accuracy and computational time,
2. to construct a new set coefficients of 3-point block method by extending objective 1,
3. to investigate stability and convergence properties of the derived methods by determining the stability region, zero stability and consistency,
4. to implement the derived methods by using Newton's iteration for solving the problems, and
5. to apply the derived methods on solving an application problem of the SIR model.

1.6 Scope of the Thesis

This thesis focuses on the derivation of a new formulas of 2-point and 3-point block methods for solving first order ODEs. The derived methods will be constructed using constant step size to give the approximated solutions at two and three points simultaneously. It is limited to solve first order stiff ODEs. To illustrate the performance of the derived method on solving the stiff problem, the numerical results obtained will be compared with the existing methods in terms of the accuracy and computational time. The given conclusions are restricted only to the selected test problems and their numerical performances. In addition, the SIR model of Influenza A(H3N2) is solved using the derived methods to show the capability of the method on solving the application problem.

1.7 Outline of the Thesis

This thesis consists of seven chapters. In Chapter 1, a brief introduction regarding the systems of ODEs and some definitions related to the study are provided. The objectives of the research are stated in this chapter.

Chapter 2 discusses about the previous researches on one step method and multistep method. The related literature on the stability and convergence properties of the block method is also reviewed.

The derivation of 2-point block methods of third and fifth order are presented in Chapter 3. Order and error constant of the methods are determined. Implementation of the methods using Newton's iteration for solving the first order stiff ODEs is presented. Numerical results obtained in this chapter will be compared with some known results to illustrate the performance of the derived methods in terms of the accuracy and efficiency.

Discussion on the stability characteristics of the methods is discussed in Chapter 4. Consistency and zero stability of the methods are investigated for the purpose of convergence properties.

The formulation of an implicit 3-point BBDF method for solving stiff ordinary differential equation is presented in Chapter 5. Order and error constant of the method are verified. Stability region and convergence properties of the 3-point block method are analysed. Newton's iteration is used for the implementation of method to solve the first order stiff ODEs. The numerical results obtained are tabulated and compared with the existing methods to measure its performance.

Ability of the derived methods are tested in Chapter 6 by solving an application problem. The method is used to solve the problem of first order ODEs in the Influenza A(H3N2) disease related to the SIR model. The numerical results obtained will be described and its performance will be compared with the approximation value obtained by MAPLE2015 solver. Finally, Chapter 7 will be summarized the findings of the research based on the listed objectives and recommendations for future work are presented.

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