UNIVERSITI PUTRA MALAYSIA

DIAGONAL R-POINT VARIABLE STEP VARIABLE ORDER BLOCK METHOD FOR SOLVING SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS

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By

NOORAINI BINTI ZAINUDDIN

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

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DEDICATIONS

This thesis is dedicated to

my parents and family members,

for their endless love and continuous support.

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

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November 2016

Chairman : Zarina Bibi Binti Ibrahim, PhD
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This thesis focuses on solving the initial value problems of stiff second order Ordinary Differential Equations (ODEs) directly by methods of 2-point Diagonal Block Backward Differentiation Formula (2DBBDF) and 3-point Diagonal Block Backward Differentiation Formula (3DBBDF). The 2DBBDF and 3DBBDF give two and three approximated solutions respectively for each integration step. The coefficients of these methods are derived by utilizing the error constants of the linear difference operators obtained from the general form of each method. The convergence and stability properties of the 2DBBDF and 3DBBDF methods are also discussed in details.

The proposed 2DBBDF and 3DBBDF methods are implemented with fixed step size in order to justify the numerical efficiency of the proposed methods. Subsequently, the computation of variable step size of 2DBBDF and 3DBBDF methods of order two, three and four are presented and finally they are implemented in variable step variable order scheme. The detailed algorithms on the selection of step sizes and orders are discussed. Conclusively, numerical results obtained while comparing the proposed methods with the existing variable step methods show the efficiency in reducing the number of function evaluations as well as the number of total steps. Further implementation of the 2DBBDF and 3DBBDF methods in variable step variable order scheme displays comparable results with other variable step variable order methods. These findings conclude that the proposed methods can serve as an alternative solver for solving stiff second order ODEs directly.

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

KAEDAH R-TITIK BLOK PEPENJURU SAIZ LANGKAH BERUBAH PERINGKAT BERUBAH UNTUK PENYELESAIAN PERSAMAAN PEMBEZAAN BIASA PERINGKAT KEDUA

Oleh

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Tesis in tertumpu kepada penyelesaian masalah nilai awal Persamaan Pembezaan Biasa (PPB) kaku peringkat kedua secara terus dengan menggunakan kaedah 2-titik Blok Pepenjuru Formula Pembezaan ke Belakang (2BPFPB) dan 3-titik Blok Pepenjuru Formula Pembezaan ke Belakang (3BPFPB). Kaedah 2BPFPB dan 3BPFPB masing-masing memberikan dua dan tiga penyelesaian untuk setiap langkah penyelesaian. Pekali-pekali bagi kaedah-kaedah ini diterbitkan dengan menggunakan pemalar ralat operator beza linear yang diperolehi daripada bentuk umum bagi setiap kaedah. Ciri-ciri penumpuan dan kestabilan bagi kaedah 2BPFPB dan 3BPFPB juga turut dibincangkan dengan terperinci.

Kaedah 2BPFPB dan 3BPFPB diimplementasikan dengan saiz langkah tetap untuk menjustifikasikan keberkesanan berangka bagi kaedah yang ditawarkan. Seterusnya, pengiraan kaedah 2BPFPB dan 3BPFPB dengan saiz langkah berubah peringkat dua, tiga dan empat diberikan dan akhirnya diimplementasikan dengan skim saiz langkah berubah peringkat berubah. Perincian algoritma mengenai pemilihan saiz langkah dan peringkat dibincangkan. Kesimpulannya, keputusan berangka yang diperoleh apabila kaedah yang diusulkan dibandingkan dengan kaedah sedia ada menunjukkan keberkesanan dalam mengurangkan nombor penilaian fungsi dan juga jumlah langkah. Pelaksanaan selanjutnya bagi kaedah 2BPFPB dan 3BPFPB dengan skim saiz langkah berubah peringkat berubah memberikan keputusan yang setanding dengan kaedah saiz langkah berubah peringkat berubah sedia ada. Penemuan ini menyimpulkan bahawa kaedah yang dicadangkan boleh berfungsi sebagai penyelesai terus alternatif kepada PBB kaku peringkat kedua.

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I certify that a Thesis Examination Committee has met on 7 November 2016 to conduct the final examination of Nooraini binti Zainuddin on her thesis entitled "Diagonal R–Point Variable Step Variable Order Block Method For Solving Second Order Ordinary Differential Equations" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the degree of Doctor of Philosophy.

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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 Methods
BDF	Backward Differentiation Formulae
2DBBDF	2-Point Diagonal Block BDF methods for solving second order ODEs directly
3DBBDF	3-Point Diagonal Block BDF methods for solving second order ODEs directly
2DBBDF(2)	Second order variable step 2DBBDF
2DBBDF(3)	Third order variable step 2DBBDF
2DBBDF(4)	Fourth order variable step 2DBBDF
3DBBDF(2)	Second order variable step 3DBBDF
3DBBDF(3)	Third order variable step 3DBBDF
3DBBDF(4)	Fourth order variable step 3DBBDF
Yatim(VSVO)	Variable Step Variable Order Block Backward Differentiation Formulae for solving second order ODEs by Yatim(2013)
2D(VSVO)	2DBBDF implemented in variable step variable order scheme
3D(VSVO)	3DBBDF implemented in variable step variable order scheme
ode15s	A variable order method of Numerical Differentiation Formulae (NDFs) of order 1-5
ode23s	A fixed order method of new modified Rosenbrock (2,3) pair
RLC	Second order circuit build together with an inductor and a capacitor

CHAPTER 1

INTRODUCTION

1.1 Introduction

Ordinary Differential Equations (ODEs) arises naturally in the field of science and engineering. The problems of second order ODEs involve the second derivatives of dependent variable with respect to one independent variable. Such problems are Van der Pol Oscillator, electric circuit and the swinging pendulum, to mention a few. Some carefully chosen problems can be treated directly with the fundamentals of calculus and algebra. However, many realistic mathematical problems involving ODEs are impossible to solve analytically, and therefore the computational approach is sought for the numerical approximation.

To deal with this difficulty, various computational methods such as linear multistep methods (LMM) and Runge-Kutta are widely used and its advancement is extensively proposed. Variety of implementation techniques such as variable step and variable step variable order are applied in order to improve the efficiency of the numerical computations. Some are made available in readily software such as ode15s in MATLAB which apply the technique of variable step variable order for the computational approach.

These numerical methods are carefully chosen when dealing with the problem of ODEs, which can be classified as stiff and nonstiff. The popular numerical method for stiff ODEs is backward differentiation formulae (BDF) which sometimes known as Gear's formulae and Adams formulae for nonstiff ODEs.

Through this thesis, the numerical methods which are in the form of BDF are proposed to cater the problem of stiff second order ODEs.

1.2 Objectives of the Thesis

This thesis proposed second order ODEs solver which belongs to the family of BDF. The following objectives are made compulsory to be accomplished by the end of this thesis.

1. To derive the 2-pointand 3-point diagonal block BDF (rDBBDF, r = 2, 3) methods of constant step for solving second order ODEs.
2. To construct variable step sizes of rDBBDF, r = 2, 3 methods of order two, three, and four.
3. To establish the convergence and stability properties of rDBBDF, r = 2, 3 methods.

4. To develop the code of rDBBDF, r = 2, 3 methods by using Microsoft Visual Studio C++ programming language. The implementation will be starting with constant step size, followed by varying the step sizes and finally by varying the step sizes and orders.
5. To evaluate the efficiency of the rDBBDF, r = 2, 3 methods on solving the problem of second order ODEs directly.
6. To verify the efficiency of the proposed method on solving second order ODE obtained from RLC circuit.

1.3 Scope of the Thesis

This thesis focuses on solving directly the initial value problems of stiff second order ODEs. The proposed method known as diagonal block backward differentiation formulae are derived to give the approximated solutions at two and three points concurrently. The method is developed to give the solutions by the means of constant step, variable step and finally variable step variable order scheme. The given conclusions are restricted only to the selected tested problems and their numerical performances.

1.4 Problems Statement

This thesis is devoted on solving the initial value problem of second order ODEs. The systems of s second order ODEs are defined as:

$$y_i'' = f_i\left(x, \tilde{Y}\right), \quad i = 1, 2, ,.s, \quad \tilde{Y}(a) = \tilde{\eta}, \qquad x \in [a, b], \tag{1.1}$$

where

$$Y(x) = \left(y_1, y_1', ,.y_s, y_s'\right), \quad \eta = \left(\eta_1, \eta_1', ,\eta_s, \eta_s'\right).$$

Throughout the thesis, the following theorem which states the conditions on $f\left(x, \check{Y}\right)$ that guarantee the existence of a unique solution of (1.1).

Theorem 1.1
Let $f\left(x, \check{Y}\right)$ be defined and continuous for all points $\left(x, \check{Y}\right)$ in the region D defined by $a \leq x \leq b$, $\left\|\check{Y}\right\| < \infty$, where a and b are finite, and let there exists a constant L known as *Lipschitz constant* such that for every $x, \check{Y}$ and $\check{Y}^*$ such that $\left(x, \check{Y}\right)$ and $\left(x, \check{Y}^*\right)$ are both in D,

$$\left\| f\left(x, Y\right) - f\left(x, Y^*\right)\right\| \leq L \left\| Y - Y^* \right\|. \tag{1.2}$$

Then if η is any given number, there exist a unique solution $\tilde{Y}(x)$ of the initial value problem (1.1) where $\tilde{Y}(x)$ is continuous and differentiable for all $(x, \tilde{Y})$ in D.

The requirement (1.2) is known as *Lipschitz condition*. For the proof, see Henrici (1962). This assumption establishes the existence of a unique solution of (1.1).

1.5 Outline of the Thesis

Chapter 1 provides a brief introduction on the second order ODEs which is going to be covered in this thesis.

In Chapter 2, previous research finding and complexities on the studies related to stiff ODEs and block methods are pointed out. Theories and definitions related to the proposed methods are given to support this study.

Chapter 3 gives the details derivation of the constant step 2-point and 3-point diagonal block BDF (rDBBDF, r = 2, 3) methods. Numerical results are given to support the early progress of the proposed methods.

The methods derived in Chapter 3 are extended to variable step rDBBDF, r = 2, 3 methods. The details of the derivation, convergence and stability properties of these methods are discussed throughout Chapters 4 and 5. Given D = 2, 3, and 4, Chapter 4 is dedicated to variable step D^{th} order 2DBBDF method, and variable step D^{th} order 3DBBDF method is devoted in Chapter 5.

Chapter 6 discusses the details implementation approach of variable step rDBBDF, r = 2, 3 methods. The necessary condition for when the methods need to maintain its current step size or not is discussed here. Numerical results are presented to justify the efficiency of the proposed variable step rDBBDF, r = 2, 3 methods.

The following Chapter 7 focuses on the implementation of variable step variable order rDBBDF, r = 2, 3 methods. The algorithm on varying the step as well as the order is elaborated in details. In order to justify the numerical performances of this approach, the problem of second order ODEs given in Chapter 6 is recalculated by using the mentioned methods and the comparison are made with other variable step variable order methods.

Chapter 8 provides the case study when the proposed methods solve the problems of second order ODE in RLC circuit.

Lastly, Chapter 9 concludes the research concerning this topic. Recommendations for future research are also put forward.

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