UNIVERSITI PUTRA MALAYSIA

SECOND DERIVATIVE BLOCK METHODS FOR SOLVING FIRST AND HIGHER ORDER ORDINARY DIFFERENTIAL EQUATIONS

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By

MOHAMMED YOUSIF TURKI

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

September 2018

DEDICATION

To:
My late father
A strong and gentle soul who taught me to trust in Allah, believe in hard work, and that so much could be done with little
My mother,
Whose affection, love, encouragement, and prayers of day and night make me able to get such success and honor
My beloved wife,
For her great patience, support in all my life
My beloved daughter Rinad
My Brothers, and sister,
For their love, support and encouragement
My respected Teachers.

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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By

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September 2018

Chair:Professor Fudziah Binti Ismail, PhD
Faculty: Science

Traditionally, higher order ordinary differential equations (ODEs) are solved by reducing them to an equivalent system of first order ODEs. However, it is more cost effective if they can be solved directly by numerical methods. Block methods approximate the solutions of the ODEs at more than one point at one time step, hence faster solutions can be obtained. It is rather well-known too that a more accurate numerical results can be obtained by having extra derivatives in the method. Based on these arguments, we are focused on developing block methods with extra derivatives for solving first, second and third ODEs. The study in the thesis consists of three parts.

The first part of the thesis described the derivation of two and three point implicit and semi implicit block methods with second derivative for solving first order ODEs. Absolute stability for both implicit and semi implicit second derivative block methods are also presented. Numerical results clearly show that the new proposed methods are more efficient in terms of accuracy and computational time when compared with well-known existing methods.

The second part of the thesis is focused on the derivation of two and three point implicit and semi implicit second derivative block methods for directly solving second order ODEs. The zero-stability of the new methods are also given. The numerical results revealed that the new methods are more accurate as compared to the existing methods and it is also illustrated that the new second derivative block methods require less computational time when solving second order ODEs.

Finally, the last part of the thesis concerned with the construction of two and three point implicit and semi implicit second derivative block multistep methods for directly solving third order ODEs. The zero-stability for the new methods are also presented. Numerical results show that new methods are more efficient than the existing methods.

In conclusion, accurate and required less computational time have potential to be a good tools for solving first, second and third order ODEs respectively.

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

KAEDAH JENIS RUNGE-KUTTA UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA PERINGKAT KETIGA DAN MASALAH AYUNAN PERINGKAT PERTAMA

Oleh

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Secara tradisinya, persamaan pembezaan biasa (PPB) peringkat yang lebih tinggi dapat diselesaikan dengan menurunkan ke sistem PPB peringkat pertama yang setara. Bagaimanapun, adalah lebih kos efektif jika ia dapat diselesaikan secara langsung oleh kaedah berangka. Kaedah blok menghampiri penyelesaian PPB pada lebih daripada satu titik pada satu langkah, maka penyelesaian yang lebih cepat dapat diperolehi. Umum mengetahui bahawa hasil berangka yang lebih tepat boleh diperolehi dengan mempunyai terbitan tambahan dalam kaedah tersebut. Berdasarkan hujah-hujah ini, kami memberi tumpuan kepada membangunkan kaedah blok dengan terbitan tambahan untuk menyelesaikan PPB peringkat pertama, kedua dan ketiga. Kajian dalam tesis terdiri daripada tiga bahagian.

Bahagian pertama tesis menerangkan bagaimana menerbitkan kaedah tersirat dan semi tersirat blok dua dan tiga titik dengan dengan terbitan kedua untuk menyelesaikan PPB peringkat pertama. Kestabilan mutlak untuk kedua-dua kaedah tersirat dan semi tersirat blok dengan terbitan kedua juga dipersembahkan. Keputusan berangka menunjukkan dengan jelas bahawa kaedah baru yang dicadangkan, lebih cekap dari segi ketepatan dan masa pengiraan apabila dibandingkan dengan kaedah sedia ada.

Bahagian kedua tesis memberi tumpuan kepada cara menerbitkan kaedah tersirat dan semi tersirat blok dua dan tiga titik dengan terbitan kedua untuk menyelesaikan secara langsung PPB peringkat kedua. Kestabilan sifar kaedah baru juga diberikan. Keputusan berangka mendedahkan bahawa kaedah baru lebih cekap dibandingkan dengan kaedah yang sedia ada dan ia juga menggambarkan bahawa kaedah blok dengan terbitan kedua yang baru adalah lebih tepat dan cekap apabila menyelesaikan

PPB peringkat kedua.

Akhir sekali, bahagian akhir tesis adalah berkenaan dengan pembinaan kaedah tersirat dan semi tersirat blok dua dan tiga titik untuk menyelesaikan secara langsung PPB peringkat ketiga. Kestabilan sifar untuk kaedah baru juga dibentangkan. Hasil berangka menunjukkan bahawa kaedah baru lebih berkesan daripada kaedah yang sedia ada.

Kesimpulannya, kaedah dan kod baru yang dibangunkan berdasarkan kaedah yang terhasil ini sesuai untuk menyelesaikan PPB peringkat pertama, kedua dan ketiga masing-masingnya.

ACKNOWLEDGEMENTS

Firstly, All praise is to Allah the lord of the world, The Beneficent, The Merciful who in His infinite mercy gives me life, good health, strength, hope, guidance and perseverance to pursue this program to the successful completion. May Allah's Mercy and Peace be upon our noble prophet Muhammad Rasulillah Sallallahu Alaihi Wasallam, his family and companions. My deepest appreciation and gratitude goes to the chairman of the supervisory committee, Prof. Dr. Fudziah Binti Ismail for her invaluable assistance, advice and guidance throughout the duration of the studies. This work would not have been completed without her help that I received in various aspects of the research.

I am also grateful to the member of the supervisory committee, Associate Prof. Dr. Norazak bin Senu and Associate Professor Dr. Zarina Bibi Ibrahim. I aslo wish to express my thanks to my friends especially Firas Adel Fawzi and Kasim Abbas Hussain during my study in Universiti Putra Malaysia. Moreover, I would like to thank all staffs of the Department of Mathematics. I thank AL-Anbar University and Ministry of Higher Education and Scientific Research in Iraq for providing me scholarship and support me.

My biggest thanks goes to my mother, brothers (Hutheifa, Mohaned, and Muaath), and sisters for their patience, encouragement and for supporting me along.

Finally, I cannot put into words how much I appreciate the continuous support, understanding and patience of my kind wife, Tiba , and beloved daughter, Rinad.

I certify that a Thesis Examination Committee has met on 24 September 2018 to conduct the final examination of Mohammed Yousif Turki on his thesis entitled "Second Derivative Block Methods for Solving First and Higher 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 Doctor of Philosophy.

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LIST OF ABBREVIATIONS

ODEs	Ordinary Differential Equations
IVPs	Initial Value Problems
LTE	Local Truncation Error
MAXE	Maximum Error
New 2PSDBI	2-point implicit block method for first order
New 2PSDBE	2-point semi implicit block method for first order
New 23PSDBI	3-point implicit block method for first order
New 3PSDBE	3-point semi implicit block method for first order
New 2PSDBI(2)	2-point implicit block method for second order
New 2PSDBE(2)	2-point semi implicit block method for second order
New 23PSDBI(2)	3-point implicit block method for second order
New 3PSDBE(2)	3-point semi implicit block method for second order
New 2PSDBI(3)	2-point implicit block method for third order
New 2PSDBE(3)	2-point semi implicit block method for third order
New 23PSDBI(3)	3-point implicit block method for third order
New 3PSDBE(3)	3-point semi implicit block method for third order

CHAPTER 1

INTRODUCTION

1.1 Ordinary Differential Equations

Ordinary differential equation(ODE) is a differential equation that contains only ordinary derivatives of one or more unknown functions with respect to a single independent variable.

The $d-$th order ODEs can be written as:

$$y^{(d)} = f\left(x, y, ..., y^{(d-1)}\right), \tag{1.1}$$

with initial conditions:
$y(a) = y_0$ and $y^{(i)}(a) = \eta_i$, $0 < i \leq d-1$, $x \in [a,b]$,
while the first order ODEs can be written as:

$$\frac{dy}{dx} = f\left(x, y(x)\right), y(a) = y_0 \tag{1.2}$$

where $x \in [a,b]$.
In (1.2), the quantity being differentiated, y is called the dependent variable, while the quantity with respect to y which is differentiated, x is called the independent variable.

1.2 The Initial Value Problems to ODEs

The initial value problems (IVPs) of system first order differential equation is defined as:

$$\mathbf{y}'(x) = \mathbf{f}(x, \mathbf{y}), \tag{1.3}$$

with initial conditions

$$\mathbf{y}(x_0) = \mathbf{y}_0, \quad \mathbf{y}'(x_0) = \mathbf{y}'_0, \quad x \in [a,b]$$

where

$$\mathbf{y}(x) = [y_1(x), y_2(x), ..., y_s(x)]^T$$
$$f(x, \mathbf{y}) = [f_1(x, \mathbf{y}), f_2(x, \mathbf{y}), ..., f_s(x, \mathbf{y})]^T,$$

and $\mathbf{y}_0$ is a given vector of initial conditions. The initial value problems (IVPs) of general second order is defined as:

$$y''(x) = f(x, y, y'), \tag{1.4}$$

with initial conditions

$$y(x_0) = y_0, \quad y'(x_0) = y'_0,$$

where $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$, and $y_0, y'_0 \in \mathbb{R}^d$.
The initial value problems (IVPs) of general third order is defined as:

$$y'''(x) = f(x, y, y', y''), \tag{1.5}$$

with initial conditions

$$y(x_0) = y_0, \quad y'(x_0) = y'_0, \quad y''(x_0) = y''_0,$$

where $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$, and $y_0, y'_0, y''_0 \in \mathbb{R}^d$.

1.3 Existence and Uniqueness

The solutions to higher order ODEs can be obtained by reducing the ODEs to the systems of first order ODEs and direct methods. The following two theorems can be stated: Theorem 1.1 discusses about the existence and uniqueness of first order ODEs and Theorem 1.2 guarantees the uniqueness of higher order ODEs.

Theorem 1.1 **:** *Henrici (1962)*
Let $f(x,y)$ be defined and continuous $\forall$ points $\big(x,y\big)$ in a domain D defined by $x \in [a,b], y \in (-\infty,\infty)$, containing initial values $\big(x_0,y_0\big)$, a and b are finite. Let there exists a constant L called Lipschitz constant such that for any $x \in [a,b]$ and for any pairs y_1, y_2 for which $\big(x,y_1\big)$, $\big(x,y_2\big)$ are both in D $\mid f\big(x,y_1\big) - f\big(x,y_2\big) \mid \leq L \mid y_1 - y_2 \mid$. Then for any given number $x \in [a,b]$, the first order initial vale problem has a unique solution $y(x)$.

Theorem 1.2 **:** *Wend (1969)*
Let D be the region defined by the inequalities $x_0 \leq x \leq x_0 + a, \mid s_j - c_j \mid \leq b, j = 0,1...,d-1 (a > 0, b > 0)$. Suppose $F(x, s_0, ..., s_{d-1})$ is defined in D and in addition
(1) F is nonnegative and nondecrensing in each of $x, s_0, ..., s_{d-1}$ in D,
(2) $F(x, c_0, ..., c_{d-1}) > 0$ for $x_0 \leq x \leq x_0 + a$,
(3) $c_k \leq 0, k = 1,2,...,d-1$.
then the d-th order intial value problem has aunique solution in D.

1.4 Linear Multistep Method

Linear multistep method of step k is the computational method for determining the sequence $y(x)$ for a function $f(x, y, ..., y^{d-1}) = y^d(x)$ which consists of a linear relationship between $y_{n+j}, f_{n+j}, j = 0, 1, .., k$.

$$\sum_{j=0}^{k} \alpha_j \, y_{n+j} = h \sum_{j=0}^{k} \beta_j \, y'_{n+j} + ... + h^d \sum_{j=0}^{k} \gamma_j \, f_{n+j}, \tag{1.6}$$

where d is the order of the differential equation, α_j, β_j and γ_j are constants and assume that $\alpha_k \neq 0$. This method is implicit if $\beta_k \neq 0$ and $\gamma_k \neq 0$ and explicit if $\beta_k = 0$ and $\gamma_k = 0$

Definition 1.1 *(Gear (1971), Fatunla (1991) and Lambert (1991))*
The linear difference operator L associated with the (1.6)*, is defined by*

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

where d is the order of the differential equation and $y(x)$ *is an orbitary function that is continuous and differentiable on [a,b]. Using the the Taylor series at point x to expand* $y(x_n + jh)$ *and* $y^d(x_n + jh)$ *in* (1.7) *gives*

$$L[y(x);h] = C_0 y(x) + C_1 h y'(x) + ... + C_p h^p y^p + C_{p+1} h^{p+1} y^{p+1} + ...$$

where

$$C_0 = \sum_{j=0}^{k} \alpha_j,$$

$$C_1 = \sum_{j=0}^{k} (j\alpha_j - \beta_j),$$

$$.$$

$$.$$

$$.$$

$$C_p = \sum_{j=0}^{k} (\frac{j^p}{p!}\alpha_j - \frac{j^{p-1}}{(p-1)!}\beta_j - ... - \frac{j^{p-d}}{(p-d)!}\gamma_j).$$

The multistep (1.6) *is said to have order p if* $C_0 = C_1 = ... = C_p = C_{p+1} = ... = C_{p+(d-1)} = 0, C_{(p+d)} \neq 0$. *Therefore,* $C_{(p+d)}$ *is the error constant and* $C_{(p+d)} h^{(p+d)} y^{(p+d)}(x_n)$ *is the principal local truncation error at the point* x_n.

Definition 1.2 *(see Lambert (1991)) The multistep method is said to be consistent if it has order $p \geqslant 1$. The method is consistent if and only if*

$$\sum_{j=0}^{k} \alpha_j = 0$$

and

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

The first and second characteristic polynomials of the linear multistep method are defined as

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \, \xi^j,$$

$$\sigma(\xi) = \sum_{j=0}^{k} \beta_j \, \xi^j.$$

The multistep method 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 $\xi_s, s = 2,3,..,k$, are called spurious roots. The characteristic polynomial of the method may be written as follows:

$$\pi(r,\bar{h}) = \rho(r) - \bar{h}\,\sigma(r) = 0,$$

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

Definition 1.3 *(see Lambert (1991)) The linear multistep method is said to be zero stable if no root of the first characteristic polynomial $\rho(\xi)$ has modulus greater than one, and every root with modulus one is simple.*

Definition 1.4 *(see Henrici (1962)) The linear multistep method (1.6) is said to be zero stable if the root of the first characteristic polynomial $\rho(\xi)$ has modulus less than or equal to one, and that the multiplicity of the roots with modulus one be at most two.*

Theorem 1.3 : *Henrici (1962)*
The necessary and sufficient conditions for a method to be convergent are that it be consistent and zero-stable.

Definition 1.5 *(see Stoer and Bulirsch (1991))*
If given $x_0, x_0, \ldots, x_n$ are (n+1) distinct numbers and f is a function whose values are given at these numbers, then there exists a unique polynomial P of degree at most n with property that

$f(x_i) = P(x_i) \qquad$ *for each* $i = 0, 1, .., n.$
The Hermite interpolating polynomial P is given by

$$P(x) = \sum_{i=0}^{n} \sum_{k=0}^{m_{i-1}} f^{(k)}(x_i) L_{i,k}(x), \tag{1.8}$$

where $L_{i,k}(x)$ *is the generalized Lagrange polynomial which can be defined by*

$$L_{i,m_{i-1}}(x) = \ell_{i,m_{i-1}}(x),\ i = 0, 1, ..., n,$$

$$\ell_{i,k}(x) = \frac{(x-x_i)^k}{k!} \prod_{j=0, j\neq i}^{n} \left(\frac{x-x_j}{x_i-x_j}\right)^m j, i = 0, 1, ..., n, k = 0, 1, ..., m_{i-1}.$$

and recursively for $k = m_i - 2, m_i - 3, ..., 0.$

$$L_{i,k}(x) = \ell_{i,k}(x) - \sum_{v=k+1}^{m_i - 1} \ell_{i,k}^{(v)}(x_i) L_{i,v}(x).$$

1.5 Problem Statement

Initial value problems (IVPs) of first, second and third order (ODEs) often arise in many fields of applied sciences such as mathematics, chemistry, physics, electricity and nuclear.

The common technique for solving general second and general third order ODEs is by transforming the problems into a system of first order ODEs and solving it using a suitable numerical method in the literature. The disadvantage of this techique is that it needed more computional time.

The aim of this research is to develop efficient numerical methods in terms of accuracy and computational time for directly solving general second order ODEs and general third order ODEs.

1.6 Scope of Study

The study focuses on methods for the solution of first, second and third order ODEs directly using extra derivative block methods.

1.7 Objectives of the Study

The main objective of the thesis are:

- To derive two and three point implicit and semi implicit second derivative block methods for directly solving first order $y' = f(x,y)$,second order $y'' = f(x,y,y')$ and third order $y''' = f(x,y,y',y'')$ ODEs by using Hermite interpolating polynomial.
- To establish the order conditions and zero-stability of the methods.
- To perform numerical comparison of the proposed methods with other existing methods.

1.8 Outline of Thesis

This thesis is divied into six chapters which are organized as follows:

In Chapter 1, an introduction on the ordinary differential equations, basic theory and definitions of multistep methods are given.

Chapter 2, deals with the review of previous works on numerical methods for solving the first order, general second order and general third-order ODEs.

Chapter 3, described the derivation of the two and three point implicit and semi implicit second derivative block multistep methods for solving first order ODEs. The zero-stable and order of the new methods are also presented. The numerical results obtained are compared with other well-known existing methods.

In Chapter 4, the derivation of two and three point implicit and semi implicit second derivative block multistep methods for solving general second order ODEs are given. The zero-stable and order of the new methods are discussed. Numerical results based on the methods are presented and compared with existing methods.

In Chapter 5, construction and derivation of two and third point implicit and semi implicit second derivative block multistep methods for solving general third order ODEs are explained in detail. The zero-stability and order of the new methods are obtained. Numerical results are presented and performance of the methods compared with existing methods are discussed.

Lastly, the summary of the entire thesis, conclusions and future studies are given in Chapter 6.

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