UNIVERSITI PUTRA MALAYSIA

BLOCK MULTISTEP METHODS FOR SOLVING FIRST ORDER RETARDED AND NEUTRAL DELAY DIFFERENTIAL EQUATIONS

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By

NURUL HUDA BT ABDUL AZIZ

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

My deepest wish to my lovely husband for his great support, understanding and being a strength for my PhD journey. To my mother, father and siblings, thank you so much for all the Du'a that always encourage and support me.
Thank you so much.

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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NURUL HUDA BT ABDUL AZIZ

December 2015

Chairman: Zanariah Abdul Majid, PhD
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This thesis investigates the numerical solutions for solving first order retarded and neutral delay differential equations and its analysis in block multistep methods. The investigation begins by solving the retarded delay differential equations (RDDE) using 1-point multistep method and it then extended to the 2-point and 3-point block multistep methods. There are two strategies that have been implemented in the numerical solutions which are the variable step size and the variable step size and variable order.

In the developed algorithm, a Newton divided difference interpolation has been used in approximating a non-vanishing delay, whilst a new approach that is based on an adaptation of predictor-corrector scheme has been used to handle the vanishing delay problems. Special attention according to the numerical treatment of discontinuity in the delay solution is also presented where the techniques developed is from the adaptation of 'detect, locate and treat' strategy. The results of these strategies are shown that it can be applied in the block multistep methods and able to solve even a type of state-dependent delays.

The numerical solution of RDDE is then extended for solving the neutral delay differential equations (NDDE) of non-discontinuity and discontinuity cases. A new subroutine function has been added in the developed algorithm with the capabilities to approximate the neutral delay term using the interpolation of function evaluation. The interpolation accuracy that has been obtained from this approach is reliable and has an advantage in the less computational work.

The analysis of all numerical methods including order, error constant, consistency, zero-stability and convergence properties are also have been presented. The proposed methods have shown to have a convergence when the numerical solution approaches to the exact solution as the step size h tends to zero. From the stability properties, it has been determined that the block multistep methods of RDDE have P-stability and Q-stability regions, whilst for the NDDE has NP-stability regions as the regions shrink when the step size ratios decreased.

In conclusion, the performance of the proposed methods and the developed approaches are reliable and suitable for solving both retarded and neutral delay differential equations. Some advantages in terms of total number of steps and function calls of these proposed methods also have been identified when the comparison of the numerical results are made with the existing methods.

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

KAEDAH BLOK MULTILANGKAH BAGI PENYELESAIAN PERINGKAT PERTAMA PERSAMAAN PEMBEZAAN TUNDA LEWAT DAN NEUTRAL

Oleh

NURUL HUDA BT ABDUL AZIZ

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Tesis ini mengkaji penyelesaian berangka bagi menyelesaikan persamaan pembezaan tunda lewat dan neutral peringkat pertama dan analisisnya dalam kaedah blok multilangkah. Kajian ini dimulakan dengan menyelesaikan persamaan pembezaan tunda lewat (PPTL) menggunakan kaedah multilangkah 1-titik dan kemudiannya diperluaskan kepada kaedah blok multilangkah 2-titik dan 3-titik. Terdapat dua strategi yang telah dilaksanakan dalam penyelesaian berangka ini iaitu saiz langkah berubah, dan saiz langkah dan peringkat berubah.

Dalam algoritma yang dibangunkan, interpolasi perbezaan terbahagi Newton telah digunakan dalam menganggarkan tunda tidak terhapus, manakala satu pendekatan baru yang berasaskan kepada adaptasi skim peramal-pembetul telah digunakan untuk menangani masalah tunda terhapus. Pemerhatian khusus terhadap rawatan berangka ketidakselanjaran juga dipersembahkan di mana teknik yang dibangunkan adalah daripada penyesuaian strategi ‘mengesan, menempat dan merawat’. Hasil daripada strategi ini menunjukkan bahawa ianya boleh digunakan dalam kaedah blok multilangkah dan mampu menyelesaikan walaupun tunda jenis yang bergantung kepada keadaan.

Penyelesaian berangka bagi PPTL kemudiannya diperluaskan untuk menyelesaikan persamaan pembezaan tunda neutral (PPTN) bagi kes keselanjaran dan ketidakselanjaran. Satu fungsi subrutin baru telah ditambah dalam algoritma yang dibangunkan dengan keupayaan untuk menganggar istilah tunda neutral dengan menggunakan interpolasi daripada penilaian fungsi. Ketepatan interpolasi yang diperoleh daripada pendekatan ini boleh dipercayai dan mempunyai faedah dalam mengurangkan kerja komputasi.

Analisis bagi semua kaedah termasuk ciri-ciri peringkat, pemalar ralat, konsistensi, kestabilan-sifar dan penumpuan juga turut dipersembahkan. Kaedah-kaedah yang dicadangkan telah menunjukkan bahawa ia mempunyai penumpuan apabila penyelesaian berangka menghampiri penyelesaian sebenar bagi saiz langkah h yang cenderung kepada sifar. Daripada ciri-ciri kestabilan, ia telah ditentukan bahawa kaedah blok multilangkah bagi PPTL mempunyai kawasan kestabilan-P dan kestabilan-Q, manakala bagi PPTN ia mempunyai kawasan kestabilan-NP iaitu kawasan kestabilan mengecil apabila nisbah saiz langkah berkurang.

Kesimpulannya, prestasi bagi kaedah-kaedah yang dicadangkan dan pendekatan yang dibangunkan adalah boleh dipercayai dan sesuai bagi menyelesaikan kedua-dua persamaan pembezaan tunda jenis lewat dan neutral. Beberapa kelebihan darisegi jumlah bilangan langkah dan penilaian fungsi daripada kaedah-kaedah yang dicadangkan juga dikenal pasti apabila perbandingan keputusan berangka dibuat dengan kaedah yang sedia ada.

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I certify that a Thesis Examination Committee has met on 9 December 2015 to conduct the final examination of Nurul Huda Bt Abdul Aziz on her thesis entitled "Block Multistep Methods for Solving First Order Retarded and Neutral Delay 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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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

DDEs	Delay Differential Equations
RDDE	Retarded Delay Differential Equation
NDDE	Neutral Delay Differential Equation
NFDE	Neutral Functional Differential Equation
ODEs	Ordinary Differential Equations
RODEs	Retarded Ordinary Differential Equations
IVP	Initial Value Problem
VS	Variable Step Size
VSVO	Variable Step Size and Variable Order
PPT	Persamaan Pembezaan Tunda
SLB	Saiz Langkah Berubah
SLPB	Saiz Langkah dan Peringkat Berubah
DTE	Discontinuity Tracking Equation
ERKM	Embedded Runge-Kutta Method
LMM	Linear Multistep Method
MOS	Method of Steps
LOB	Lower Bound
UPB	Upper Bound

CHAPTER 1

INTRODUCTION

1.1 Introduction

Delay Differential Equations (DDEs) play an important roles in the history of scientific areas. It is known as a central of mathematical models that used to describe many phenomena in real life. For instance, the delay can be represented as a transport delay (a signal to travel to the controlled object; driver reaction time), dengue fever epidemics (the delay exist from the time of a bite to the time at which the human is infective), biological processes (the time for the body to produce red blood cells and the cell devision time), and physiological and pharmaceutical kinetics (the body's reaction to CO_2) (Lumb, 2004). Indeed, the use of the time delays are found in many processes whether natural or man made, as quoted by Kuang (1993),

> "Like it or not, time delays occur so often, in almost every situation, that to ignore them is to ignore the reality."

In mathematics, DDEs are defined as a differential equations in which the derivatives of some unknown functions at present time are dependent on the values of the functions at previous time. It is also called as a time-delay systems, hereditary systems, equations with deviating argument or differential-difference equations. Some authors refer to DDEs as 'ordinary differential equations with time lags' or 'retarded ordinary differential equations' (RODEs) where the terminology for DDEs has yet to be standardized. However, all names of DDEs above belong to the class of functional differential equations (Driver, 1977).

In the elementary theory of initial value problems, ordinary differential equations (ODEs) and DDEs are said to have a few similarities in terms of obtaining a unique solution and both problems originating from the study of physical phenomena that can be solved exactly. Despite the obvious similarities, there are some important differences between ODEs and DDEs as has been highlighted in Table 1.1.

From Table 1.1, it shows that the numerical solution of ODEs require only the initial value at initial point, $x = a$ in order to obtain the sequence of the solution $y(x)$. Unlike DDEs, two extra steps are required in the process before obtained the approximate solution $y(x)$. The numerical solution of DDEs start by finding the location of the delay terms, $\alpha_i = x_i - \tau(x_i, y(x_i))$ that may lies within the interval at point, $x = x_i$ for $i = 0, 1, 2, \ldots, n$. After the location of the delays are known, the decision in approximating $y(\alpha_i) = y(x_i - \tau(x_i, y(x_i)))$ will be made.

If the delays, α_i lies in between $[-\tau, 0]$, the initial function will be used as $y(\alpha_i) = \phi(\alpha_i)$. Otherwise, if the delays are in between $[a, b]$ where b is the end point, then an

Table 1.1: **The differences between ODEs and DDEs**

ODEs	DDEs
Standard form: $y'(x) = f(x, y(x))$, a system that ignores the presence of delays	**Standard form:** $y'(x) = f(x, y(x), y(x - \tau(x, y(x))))$, a system with the presence of delays
Solution: The differential equations are all evaluated at certain time x	**Solution:** The differential equations are all evaluated at both current time x and prior time $(x - \tau(x, y(x)))$
Needs an **initial value** at point $y(a) = y_0$ to determine a unique solution $y(x)$	**Needs** an **initial function** $y(x) = \phi(x)$ to determine a unique solution $y(x)$

interpolation procedure must be performed in finding the solution of the delays. The detailed description in which the properties of DDE systems are different from those of ODE systems can be seen in Martin and Ruan (2001) and Raghothama and Narayanan (2002).

1.2 Delay Differential Equations

DDEs can be divided into four different classes which are retarded DDE (Baker, 2000), distributed DDE (Augeraud-Veron and Leandri, 2014), neutral DDE (Jackiewicz and Lo, 2006) and stochastic DDE (Fan, 2011) where the retarded type has become the most well-known class of DDEs. In this thesis, the DDEs of retarded and neutral types will be considered for solving in block multistep methods.

A retarded delay differential equations (RDDE) is an ordinary differential equation that involved the solution of the delay term $y(x - \tau(x, y(x)))$, given by

$$\begin{aligned} y'(x) &= f(x, y(x), y(x - \tau(x, y(x)))), \quad && x \in [a, b], \\ y(x) &= \phi(x), && x \leq a. \end{aligned} \tag{1.1}$$

A neutral delay differential equations (NDDE) is an ordinary differential equation that involved both solutions of the delay term $y(x - \tau(x, y(x)))$ and its derivative $y'(x - \sigma(x, y(x)))$, given by

$$\begin{aligned} y'(x) &= f(x, y(x), y(x - \tau(x, y(x))), y'(x - \sigma(x, y(x)))), \quad && x \in [a, b], \\ y(x) &= \phi(x), && x \leq a, \\ y'(x) &= \phi'(x), && x \leq a. \end{aligned} \tag{1.2}$$

Here, the delays or lags τ and σ are measurable as a physical quantities that is a scalar in a function. It is always non-negative and the function f is assumed to be continuous and satisfies the Lipschitz condition in $y(x)$ for all $x \in [a, b]$. $\phi(x)$ is the given initial function which is understood to be defined in $[\rho, x_0]$, where

$$\rho = \min_{1 \le i \le n} \{ \min_{x \ge x_0} (x - \tau_i) \}. \quad (1.3)$$

There are three conditions that the delay can be represent which are a constant (the *constant* delay case), a functions of x, $\tau_i = \tau_i(x)$ (the *variable* or *time-dependent* delay case) and a functions of both x and y, $\tau_i = \tau_i(x, y(x))$ (the *state-dependent* delay case) (Bellen and Zennaro, 2003; Hayashi, 1996).

1.3 Problem Statement

In the numerical solution of DDEs, there are three essential issues that one needs to be considered. First, the approximation of the retarded argument $y(x - \tau(x, y(x)))$; second, handling the problem arising from the vanishing delays; third, the numerical treatment of derivative discontinuities in the solution. Some authors has classified the second and third issues as a main challenges in solving DDEs numerically (Yagoub et al., 2011; Carver, 1978; Oberle and Pesch, 1981).

The vanishing delays occur when $\tau(x, y(x)) \to 0$ as $x \to x^*$ for some x^*. This is due to the delay values $x - \tau(x, y(x))$ that are smaller than the step size and caused it lies in the current step. The difficulties arise when there is no current solution of $y(x)$ available at the current point to approximate the solution of the delay term $y(x - \tau(x, y(x)))$.

The particular issue that caused to inaccurate or inefficient in the numerical method are mostly originate from the nature of discontinuity in DDEs. It is occurs when the local truncation error that form the basis of most step size control algorithms may no longer be valid in the region of such discontinuities and derivative discontinuities (Paul, 1991). This observation motivated us to study in more detail associated with the numerical solution of retarded and neutral type of DDEs with the difficulties treatment in block multistep methods.

1.4 Objectives of the Thesis

This thesis will be focused on the following objectives:

1. to develop new algorithms for solving non-vanishing and vanishing delays of RDDE in 1-point multistep method, 2-point block multistep method and 3-point block multistep method.
2. to develop new algorithms for discontinuity treatment of RDDE in 2-point block multistep method and 3-point block multistep method.
3. to analyse the properties of RDDE in 1-point multistep method, 2-point block multistep method and 3-point block multistep method including order, consistency,

zero-stability, convergence and stability.

4. to develop new algorithms for solving non-discontinuity and discontinuity cases of NDDE in 2-point block multistep method and 3-point block multistep method.
5. to analyse stability of NDDE in 2-point block multistep method and 3-point block multistep method.

1.5 Scope and Limitations

This thesis concentrates on the numerical solution of block multistep methods for solving first order retarded and neutral delay differential equations. There are three methods that will be implemented to solve both types of DDEs which are 1-point multistep method, 2-point block multistep method and 3-point block multistep method. The analysis of these methods including order, consistency, zero-stability, convergence and stability are also discussed in this thesis. In implementing the step size control mechanism, two strategies of the variable step size (VS) and the variable step size and variable order (VSVO) will be adapted in the numerical solution.

1.6 Outline of the Thesis

This thesis is organized as follows. In Chapter 1, a brief introduction associated with the DDEs in the real life applications and its difference with ODEs are presented.

In Chapter 2, some of the basic assumptions and definitions that are necessary for the numerical method of DDEs are introduced. Then, followed by the discussion of the numerical difficulties that may arise in solving DDEs. A review of previous works in both retarded and neutral type of DDE and the block method are also presented in this chapter.

The numerical solution of 1-point multistep method for solving the non-vanishing delay and vanishing delay of retarded DDE is discussed in Chapter 3. In this chapter, the strategy of Newton divided difference interpolation and assigning the current predictor-corrector solution for handling the non-vanishing and vanishing delays, respectively are highlighted. The developed algorithm is implemented in the variable step size strategy that requires the step size ratios to be constant, halved or doubled. The analysis of the order, consistency, zero-stability, convergence and stability are also been discussed.

In Chapter 4, the 2-point and 3-point block multistep methods are presented. These methods are used to solve problems with non-vanishing delay and vanishing delay presented in Chapter 3. Comparisons are made in order to illustrate the advantage of this block multistep methods. The same strategy of Newton divided difference interpolation and assigning the current predictor-corrector solution are adapted in 2-point and 3-point block multistep methods.

In Chapter 5, the implementation of variable step size and variable order strategy in 2-point block multistep method is developed for solving the problems of retarded DDE. The range of the order is started from order 4 and up until order 9 depending on the local truncation error condition. In this implementation, the algorithm is designed to detect the number of interpolation points involved is proportional to the current order of the method. A detailed discussion associated with this strategy is discussed in this chapter.

The investigation associated with the numerical treatment of derivative discontinuities and its propagation for retarded DDE is discussed in Chapter 6. There are three steps in treating the discontinuities such as ‘detect’ the derivative discontinuities, ‘locate’ the discontinuity points to include in mesh points and ‘treat’ the discontinuities are described. This strategy is adapted in 2-point and 3-point block multistep methods and the detailed of the implementation is described in Section 6.4.

Then, in Chapter 7, the numerical solution of neutral DDE for the case of non-discontinuity and discontinuity using the variable step size implementation are presented. In this chapter, the strategy of how to approximate the derivative solution of the delay term $y'(x-\sigma(x,y(x)))$ using the interpolation of function evaluation is described. Meanwhile, the strategy in treating the discontinuities in neutral DDE are adapted from the strategy that has been implemented in Chapter 6.

Finally, Chapter 8 summarizes the findings and highlights some potential future researches in this study.

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