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NUMERICAL SOLUTIONS OF STIFF ORDINARY DIFFERENTIAL EQUATIONS AND DIFFERENTIAL ALGEBRAIC EQUATIONS USING ONE-STEP IMPLICIT HYBRID METHODS

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By

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December 2015

Chairman : Zanariah binti Abdul Majid, PhD
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The numerical solutions of stiff ordinary differential equations and differential algebraic equations have been studied in this thesis. New one-step implicit hybrid methods are developed to solve stiff ordinary differential equations (ODEs) and semi-explicit index-1 differential algebraic equations (DAEs). These methods are formulated by using Lagrange interpolating polynomial. The developed one-step methods will solve ODEs and DAEs with the introduction of off-step points by constant step size. The source codes were written in C language.

Stiff equations in Mathematics indicate that for a certain numerical method to solve differential equations that may give unstable results unless the step size taken is extremely small. Newton's iteration is implemented together with the developed method to solve stiff equations. The numerical results showed that the performance of the methods outperformed compared to existing method in terms of maximum error and average error.

Further, this study is extended by using the developed method to solve DAEs. Semi-explicit index-1 DAEs is the system of ordinary differential equations with algebraic constrains. Newton's iteration is implemented with the developed methods to solve DAEs. The numerical results showed the performance of the developed methods is more efficient then existing methods in terms of maximum error and average error.

In conclusion, the proposed one-step implicit hybrid methods are suitable for solving stiff ordinary differential equations and semi-explicit index-1 differential algebraic equations.

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

PENYELESAIAN BERANGKA PERSAMAAN PEMBEZAAN KAKU DAN PERSAMAAN PEMBEZAAN ALGEBRA DENGAN MENGGUNAKAN KAEDAH SATU-LANGKAH HIBRID TERSIRAT

Oleh

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Penyelesaian berangka bagi persamaan pembezaan kaku dan persamaan pembezaan aljabar telah dikaji dalam tesis ini. Kaedah satu-langkah hibrid tersirat yang baharu telah dibangunkan untuk menyelesaikan persamaan pembezaan (PP) kaku dan persamaan pembezaan aljabar (PPA) semi-tak tersirat indeks-1. Kaedah ini diperolehi daripada polynomial interpolasi Lagrange. Kaedah satu-langkah ini akan menyelesaikan PP kaku dan PPA dengan memperkenalkan titik langkah luar menggunakan saiz langkah malar. Sumber kod telah ditulis dalam pengaturcaraan C.

Istilah persamaan kaku dalam Matematik menunjukkan bahawa penyelesaian daripada kaedah berangka bagi persamaan pembezaan kaku itu adalah tidak stabil kecuali pengambilan saiz langkah yang amat kecil. Lelaran Newton telah dilaksanakan bersama dengan kaedah yang dibangunkan untuk menyelesaikan persamaan pembezaan kaku. Keputusan berangka menunjukkan prestasi kaedah tersebut adalah lebih baik dari segi ralat maksimum dan ralat purata berbanding kaedah sedia ada.

Di samping itu, kajian ini diperluaskan dengan menggunakan kaedah yang dibangunkan untuk menyelesaikan PPA. PPA semi-tak tersirat terdiri daripada sistem persamaan pembezaan biasa dan persamaan aljabar. Lelaran Newton telah dilaksanakan bersama dengan kaedah yang dibangunkan untuk menyelesaikan PPA. Keputusan berangka menunjukkan prestasi kaedah yang dibangunkan memberikan keputusan yang baik dari segi ralat maksimum dan ralat purata.

Kesimpulannya, kaedah satu-langkah hibrid tersirat yang dicadangkan adalah sesuai untuk menyelesaikan persamaan pembezaan dan persamaan pembezaan aljabar semi-tak tersirat indeks-1.

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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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- the research conducted and the writing of this thesis was under our supervision;
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LIST OF ABBREVIATIONS

ODEs	Ordinary Differential Equations
DAEs	Differential Algebraic Equations
RK	Runge-Kutta
HM1	Hybrid method with an off-step point at $y_{n+\frac{5}{4}}$
HM2	Hybrid method with an off-step point at $y_{n+\frac{3}{2}}$
HM3	Hybrid method with an off-step point at $y_{n+\frac{7}{4}}$
2OBBDF	2-point block BDF method with off-step points of order 5
3BEBDF	3-point block extended backward formula
BDF	Classical one-point backward differentiation formula
BBDF(5)	Fifth order block backward differentiation formula
1BDF	1-point sequential BDF
2BDF	2-point block BDF method
3BDF	3-point block BDF method

CHAPTER 1

INTRODUCTION

1.1 Introduction

Mathematical models are often developed to facilitate the understanding of physical phenomena in the disciplines of science and engineering. One of the common mathematical problems that arise from the formulations of these mathematical models in the field of science and engineering is differential equation.

A differential equation in which the unknown is a function of a single independent variable is prevalently referred to as ordinary differential equations (ODEs). The general form of an ODEs is as follows:

$$y' = f(x, y), \qquad y(a) = y_0, \qquad a \le x \le b. \tag{1.1}$$

Stiffness occurs when some components of the solution decay much more rapidly than the others (Lambert, 1991). When ODEs have different decaying time dependencies, then the ODEs can be classified as stiff ODEs. Stiff ODEs have to be solved by using small step size to get a stable and accurate solution unless an A-stability properties method is used.

A differential algebraic equation (DAE) is an equation that involves an unknown function and its derivatives. A DAE is an equation that involves algebraic equations and is generally difficult to solve. DAEs can be classified by using index number. A higher index number indicates a higher difficulty in solving it.

The application of DAEs arises in a variety of applications in scientific and engineering area. These include chemical process, electric circuit design, chemical, and optimal control. Most commonly, ODEs and DAEs arises from the modeling of physical phenomena and there are no exact solutions. Therefore, the development of numerical methods is essential in order to find the approximate solutions for ODEs and DAEs.

The numerical method is a differential equation involving a number of consecutive approximations $y_{n+j}, j = 0,1, \quad k$ from which it will be possible to compute sequentially the sequence $\{y_n \mid n = 0,1,2, \quad , N\}$; naturally, this differential equation will also involve the function f (Lambert, 1991). The numerical methods estimate solutions by consecutive approximation steps, using iteration process.

Generally, there are two classes of methods, prevalently known as are one-step method and multistep method. The one-step method uses information from only one of the previous points to determine the next approximate point. The multistep method uses information that more than one previous point to determine the approximate value at the next point. This research will focus on using one-step method to solve stiff ODEs and DAEs.

1.2 Objective of the Thesis

The main objective of this thesis is to develop three new one-step implicit hybrid methods for the numerical solutions of stiff ODEs and DAEs. These objectives can be achieved by:

1. Deriving three one-step implicit hybrid methods to solve stiff ODEs and semi-explicit index 1 DAEs by using constant step sizes.

2. Analyzing basic properties of the developed methods which include order, error constant and region of absolute stability.

3. Developing the algorithm of implicit hybrid methods to solve stiff ODEs and semi-explicit index 1 DAEs by using constant step sizes.

1.3 Stiff Differential Equations

A stiff equation is a differential equation that gives unstable result and it is a predicament to solve. Based on Curitess (1952), a stiff equation is exceedingly difficult to solve by ordinary numerical procedures.

Definition 1

If a numerical method with a finite region of absolute stability, applied to a system with any initial conditions, is forced to use in a certain interval of integration with 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.

Stiff equations in mathematics indicate that for certain numerical methods, solving differential equation will be numerically unstable, unless the step size taken is extremely small. Based on Lambert (1991), a linear constant coefficient system is stiff if all of its eigenvalues have negative real parts and the stiffness ratio is large.

$$y(t) = e^{-\lambda t}. \tag{1.2}$$

Most commonly, the stiffness of the differential equation can be identified by the values of the negative part of the eigenvalues. The higher the value of λ , the more stiff the equation is. The equation will be moderately stiff if $\lambda = 1$ and the equation will be highly stiff if $\lambda = 1000$.

An example of a stiff ODE model from science application is shown as follows:
1. Flame propagation

$$y' = y^2 - y^3,$$
$$y(0) = o, \qquad (1.3)$$
$$0 < t < \frac{2}{o}.$$

Where initial radius of the flaming ball is o.

1.4 Differential Algebraic Equations

Generally, there are two forms of differential algebraic equations (DAEs), which are fully implicit DAEs and semi-explicit DAEs. The general forms of DAEs are shown as follows:

1. Fully implicit DAEs

$$F(y, y', z) = 0. \qquad (1.4)$$

2. Semi-explicit DAEs

$$y' = f(y, z),$$
$$0 = g(y, z). \qquad (1.5)$$

A fully implicit DAE is a system of ODEs in which the partial derivative $\left(\frac{\partial F}{\partial y'}\right)$ is singular. The unknowns are y and z which represent differential variables and algebraic variables respectively. A semi-explicit DAE is a system of ODEs with algebraic constraints. Examples of DAE models from engineering application are shown as follows:

1. Simple pendulum

$$x_1' = x_3,$$
$$x_2' = x_4,$$
$$x_3' = -\frac{F}{ml} x_1, \qquad (1.6)$$
$$x_4' = g\frac{F}{l} x_2,$$
$$0 = x^2 + y^2 - l^2.$$

2. An RLC circuit

$$
\begin{aligned}
&V_C' = \frac{1}{C} i_L, \\
&V_L' = \frac{1}{L} i_L, \\
&0 = V_R + R i_E, \\
&0 = V_E + V_R + V_C + V_L, \\
&0 = i_L - i_L.
\end{aligned}
\tag{1.7}
$$

A remark is that every ODE is a DAE, but not every DAE is an ODE (Petzold, 1982). Fully implicit DAEs can always be transformed into semi-explicit DAEs.
Example: Consider the following ODEs

$$
\begin{aligned}
&(y')^3 - y^2 = 0, \\
&y(0) = 1.
\end{aligned}
\tag{1.8}
$$

Letting $y' = z$, we get

$$
\begin{aligned}
&y' = z, \\
&0 = z^3 - y^2.
\end{aligned}
\tag{1.9}
$$

DAEs can be categorized by using index. The index of a DAE is the minimum number of differentiation steps required to transform DAEs into ODEs. Gear et al. (1984) stated that the higher the index of DAEs, the more complex it is to solve it. This research will only focus on solving semi-explicit index 1 DAEs.

1.5 Scope of Study

This thesis will be pivot around solving stiff ODEs and semi-explicit index 1 DAEs. Three one-step implicit hybrid methods involving adding different positions of future off-step points will be implemented in this thesis. These methods will solve ODEs and '$(VWKHFRPELQDWLRQRI1ZWRQWHWLRQKRG7KHSRGHPHWKRGZOO solve ODEs and DAEs using constant step size.

1.6 Outline of the Thesis

In Chapter 1, the objectives, a brief introduction of stiff differential equations and differential algebraic equations and the scope of study have been presented. The structure of the thesis has also been described in Chapter 1.

Basis definitions and properties related to hybrid method and Lagrange interpolation polynomial will be discussed in Chapter 2. Related preliminary mathematical concepts, background research and the review of previous work also presented in the following chapter.

The derivations of one-step implicit hybrid methods involving additional off-step point, stability and order of the new derived methods are also determined and presented in Chapter 3.

In Chapter 4, the implementations and algorithm of the new hybrid methods with 1RQVWLII2'(VDUHXWLOLQ7KHREOHPRIVWLII2'(VDWWH with the derived methods and the numerical results are shown.

,QSWHUWKHLPSOHPHQWDWLRQRIWKHQUGPHWKRGZLWK1RQVWDWLRQ for solving DAEs are presented. The algorithm to solve DAEs using the new hybrid method is discussed and the numerical results are given.

The summary of the entire thesis, conclusion and recommendation for future research are presented in Chapter 6.

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