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WEIGHTED BLOCK RUNGE-KUTTA METHODS FOR SOLVING STIFF ORDINARY DIFFERENTIAL EQUATIONS

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

WEIGHTED BLOCK RUNGE-KUTTA METHODS FOR SOLVING STIFF ORDINARY DIFFERENTIAL EQUATIONS

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Weighted Block Runge-Kutta (WBRK) methods are derived to solve first order stiff ordinary differential equations (ODEs). The proposed methods approximate solutions at two points concurrently in a block at each step. Three sets of weight are chosen and implemented to the WBRK methods. Stability regions of the WBRK methods with each set of weight are constructed by using MAPLE14. Stability properties of the proposed methods with each weight show that the methods are suitable for solving stiff ODEs.

Numerical results are presented and illustrated in the form of efficiency curves. Performances of the WBRK methods in terms of maximum error and computational time are compared with the third order Runge-Kutta (RK3) and the modified weighted RK3 method based on centroidal mean (MWRK3CeM). These methods are tested with problems of single and system of first order stiff ODEs. Comparison of the proposed methods between sets of weight is also analyzed. The numerical results are obtained by using MATLAB R2011a.

Numerical results generated show that the WBRK methods obtained better accuracy and less computational time than the RK3 and MWRK3CeM method.

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

KAEDAH BLOK RUNGE-KUTTA BERPEMBERAT UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA KAKU

Oleh

SAUFIANIM BINTI JANA AKSAH

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Kaedah Blok Runge-Kutta Berpemberat (BRKB) dibina untuk menyelesaikan persamaan pembezaan biasa (PPB) kaku peringkat pertama. Kaedah yang dicadangkan ini menganggarkan penyelesaian pada dua titik serentak dalam satu blok pada setiap langkah. Tiga set pemberat dipilih dan dilaksanakan pada kaedah BRKB. Rantau kestabilan kaedah BRKB dengan setiap set pemberat dibina dengan menggunakan MAPLE14. Sifat kestabilan kaedah yang dicadangkan dengan setiap pemberat menunjukkan bahawa kaedah tersebut sesuai untuk menyelesaikan PPB kaku.

Keputusan berangka diberikan dan diilustrasikan dalam bentuk lengkungan kecekapan. Prestasi kaedah BRKB dalam bentuk ralat maksima dan masa pengiraan dibandingkan dengan kaedah Runge-Kutta peringkat ketiga (RK3) dan kaedah RK3 berpemberat yang diubah suai berdasarkan min sentroid (RK3PDMS). Kaedah-kaedah ini diuji dengan masalah PPB kaku peringkat pertama tunggal dan sistem. Perbandingan antara set-set pemberat kaedah yang dicadangkan juga dianalisis. Keputusan berangka diperoleh dengan menggunakan MATLAB R2011a.

Keputusan yang dihasilkan menunjukkan bahawa kaedah BRKB memperoleh ketepatan yang lebih baik dan masa pengiraan yang lebih cepat daripada kaedah RK3 dan RK3PDMS.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfillment 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

DEs	Differential equations
ODEs	Ordinary differential equations
PDEs	Partial differential equations
IVP	Initial value problem
LMM	Linear multistep method
RK	Runge-Kutta
BDF	Backward differentiation formula
RK3	Third order Runge-Kutta
AM	Arithmetic mean
GM	Geometric mean
HaM	Harmonic mean
HeM	Heronian mean
CoM	Contraharmonic mean
RMS	Root mean square
CeM	Centroidal mean
WBRK	Weighted block Runge-Kutta
MWRK3CeM	Modified weighted third order Runge-Kuta based on centroidal mean
BDIRK	Block diagonally implicit Runge-Kutta
BBDF	Block backward differentiation formulae
RK3CeM	Third order Runge-Kutta based on centroidal mean
MAXE	Maximum error
TIME	Computational time

WBRKI	Weighted block Runge-Kutta method with weights, $w_1 = \frac{1}{2}; w_2 = \frac{1}{2}$
WBRKII	Weighted block Runge-Kutta method with weights, $w_1 = \frac{1}{4}; w_2 = \frac{3}{4}$
WBRKIII	Weighted block Runge-Kutta method with weights, $w_1 = \frac{2}{5}; w_2 = \frac{3}{5}$
VSVO	Variable step variable order
DDEs	Delay differential equations
FDEs	Fuzzy differential equations

CHAPTER 1

INTRODUCTION

1.1 Preliminaries

Many problems in engineering, physical and social sciences are reduced to quantifiable form through the process of mathematical modeling that involved differential equations (DEs). For instance, the spread of epidemic in a population. This model enables researchers to prove the famous “Threshold Theorem of Epidemiology” which states that an epidemic will occur only if the number of people susceptible to the disease exceeds a certain threshold value (Ismail, 1999). Another example is the design of catenary curve shape of the Gateway Arch in St. Louis which is based on the solution graph of DEs (Becker, 2012). These problems are very difficult and complicated to be solved analytically, therefore researchers used numerical methods to solve them.

1.2 Differential Equation

A DE is an equation that involves one or more derivatives of some unknown function or functions. There are various types of DEs. Some of the commonly known are ordinary differential equations (ODEs) and partial differential equations (PDEs). ODEs involve ordinary derivatives which contains a single independent variable and one or more dependent variables as shown

$$f\left(x, y, \frac{dy}{dx}, \frac{d^2y}{dx^2}, \ldots, \frac{d^ny}{dx^n}\right) = 0.$$

Usually, the independent variable is denoted by x and the dependent variable is y.
On the other hand, PDEs involve partial derivatives with more than one independent variable and one or more dependent variables of the form

$$f\left(x_1, \ldots, x_n, y, \frac{\partial y}{\partial x_1}, \ldots, \frac{\partial y}{\partial x_n}, \ldots, \frac{\partial^2 y}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 y}{\partial x_1 \partial x_n}, \ldots\right) = 0 .$$

One characteristic of DE is the order which is the highest derivative appearing in the equation represent by n as shown in the above functions.

1.3 Problem Statement

This research focuses in solving problems of first order stiff ODEs of the form

$$y'(x) = f(x,y), \qquad y(a) = \eta \tag{1.1}$$

where $y = [y_1(x), y_2(x), ..., y_n(x)]^T$ and $f = [f_1(x,y), f_2(x,y), ..., f_n(x,y)]^T$ with $\eta = [\eta_1, \eta_2, ..., \eta_n]^T$ is a known vector.

Throughout this research, we shall assume that $f(x,y)$ satisfies the following theorem that guarantees the existence of a unique solution of Eq. (1.1) as stated by Lambert (1973).

Theorem 1.1
Let $f(x,y)$ be defined and continuous for all points (x,y) in the region D defined by $a \le x \le b$, $-\infty < y < \infty$, a and b finite, and let there exist a constant L such that, for every x, y, y^* such that (x,y) and (x,y^*) are both in D,

$$|f(x,y) - f(x,y^*)| \le L|y - y^*|. \tag{1.2}$$

Proof: see Henrici (1962).

Then, if η is any given number, there exists a unique solution $y(x)$ of the initial value problem (IVP) (1.1), where $y(x)$ is continuous and differentiable for all (x,y) in D. The requirement (1.2) is known as Lipschitz condition, and the constant L as a Lipschitz constant.

1.4 Numerical Methods

The exact solution of IVP (1.1) can be approximated by using numerical method. Generally, there are two classes of methods; a one-step method and a linear multistep method (LMM). One-step method uses the solution of current point for example, y_n, as initial value to compute solution at the next point, y_{n+1}. On the other hand, multistep method uses information from the previous steps to calculate the next value.

Euler's method is the easiest and widely used numerical method for solving IVP (1.1). It is written as

$$y_{n+1} - y_n = hf\left(x_n, y_n\right) \equiv hf_n .$$

The Euler's method is an explicit one-step method that does not requires any additional starting values. It is also readily permits a change of steplength during the computation. The most famous family of one-step method is Runge-Kutta (RK) methods.

By referring to IVP (1.1), we indicate the solution by $y(x)$. Next, we consider the sequence points $\{x_n\}$ defined by $x_n = a + nh,\ n = 0,1,2,...$ where h is the step size. Let y_n be an approximation to the theoretical solution x_n, that is, to $y\left(x_n\right)$, and let $f_n \equiv f\left(x_n, y_n\right)$. If a computational method for determining the sequence $\{y_n\}$ takes the form of a linear relationship between y_{n+i} and f_{n+i} with $i = 0,1,...,k,$ we call the method as LMM of step number k.

The general LMM can be written as

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i}$$

where α_i and β_i are constants. The method is explicit when $\beta_k = 0$ and implicit when $\beta_k \neq 0$. Iterative methods such as Newton's method are often used to solve the implicit formula.

In certain cases, an explicit LMM is used to "predict" the value of y_{n+i}. That value is then used in an implicit formula to "correct" the value. The result is a predictor-corrector method. There are three families of LMM; Adams-Bashforth methods, Adams-Moulton methods, and the backward differentiation formula (BDF). Further information on LMM can be found in Lambert (1973).

1.5 Runge-Kutta Methods

RK methods assumed that correct value of the slope over the step can be written as a linear combination of function $f(x, y)$ evaluated at certain points at the step. RK methods may be regarded as a particular case of the general explicit one-step method of the form

$$y_{n+1} - y_n = h\phi(x_n, y_n, h). \tag{1.3}$$

Definition 1.1
Eq. (1.3) is said to have order p if p is the largest integer for which

$$y(x+h) - y(x) - h\phi(x, y(x), h) = O(h^{p+1})$$

holds, where $y(x)$ is the theoretical solution of the IVP shown in Eq. (1.1).

Definition 1.2
Eq. (1.3) is consistent with the IVP (1.1) if

$$\phi(x, y, 0) \equiv f(x, y).$$

Definition 1.3
Eq. (1.3) is convergent by the following properties:

(i) Let the function $\phi(x, y, h)$ be jointly continuous as a function of its three arguments, in the region D defined by $x \in [a,b], y \in (-\infty, \infty)$, and $h \in [0, h_0]$ with $h_0 > 0$.

(ii) Let $\phi(x, y, h)$ satisfy a Lipschitz condition of the form $|\phi(x, y^*, h) - \phi(x, y, h)| \leq M|y^* - y|$ for all points (x, y^*, h) and (x, y, h) in D.

Eq. (1.3) is convergent if and only if it is consistent (Lambert, 1973).

In addition, Lambert also considers that conditions (i) and (ii) are satisfied if the function satisfies the condition stated in Theorem 1.1. It is also mentioned that there is no requirement regarding the zero stability, since no parasitic solutions can arise with a one-step method.

In this research, we are using explicit third order RK (RK3) methods as the basic for development of the proposed method. The formula below shows the general form of classical RK3 methods as shown in Lambert (1973).

$$y_{n+1} - y_n = \frac{h}{6}(k_1 + 4k_2 + k_3), \tag{1.4}$$

where

$$k_1 = f(x_n, y_n),$$
$$k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1),$$
$$k_3 = f(x_n + h, y_n - hk_1 + 2hk_2).$$

1.6 Stability of Runge-Kutta Methods

The stability theory in numerical analysis is concerned with the growth of numerical errors in computed solution of the DE. The linear stability and accuracy of explicit RK methods are characterized completely by the stability function of the method, which in turn dictates the acceptable stepsize as stated by Butcher (2008b). The following stability analysis for explicit RK methods and proof for the stated theorem are shown in Hairer and Wanner (1991).

Definition 1.4

The function $R(z)$ is called the stability function of the method. It can be interpreted as the numerical solution after one step for

$$y' = \lambda y, \qquad y_0 = 1, \qquad z = h\lambda,$$

the famous Dahlquist test equation. The set

$$S = \left\{ z \in C; \left| R(z) \right| \le 1 \right\}$$

is called the stability domain of the method.

Theorem 1.2

If RK method is of order p, then

$$R(z) = 1 + z + \frac{z^2}{2!} + \ldots + \frac{z^p}{p!} + O\left(z^{p+1}\right)$$

with $h\lambda = z.$

As referred in Rahim (2004), absolute stability can also be defined as follows.

Definition 1.5

By letting $z = h\lambda$, then $R(z)$ is known as the stability function of the method. Hence, $y_n \to 0$ as $n \to 0$ if and only if

$$|R(z)| < 1 \tag{1.5}$$

and the method is absolutely stable for those value of z for which Eq. (1.5) holds. The region $\Re_A$ of the complex $z-$plane which Eq. (1.5) holds is the region of absolute stability of the method.

Burden *et al.* (2015) stated that a method can be applied effectively to a stiff equation only if $h\lambda$ is in the region of absolute stability of the method which will results in a restriction on the size of h. The condition also applies for the approximation to decay to zero and the growth of error to be under control. The absolute criterion forces h to remain small.

1.7 Stiff Systems of Ordinary Differential Equations

Many fields of application, notably chemical engineering and control theory yield IVPs that sometimes exhibit a phenomenon known as stiffness (Akanbi *et al.*, 2011). There has been various definition of stiffness used by former researchers as mention in the literature with respect to the linear system of first order equation which defined as below

$$\tilde{y}' = A\tilde{y} + \tilde{\phi}(x), \qquad \tilde{y}(a) = \tilde{\eta}, \qquad a \le x \le b \tag{1.6}$$

where $\tilde{y}^T = (y_1, y_2, ..., y_m)$, $\tilde{\eta}^T = (\eta_1, \eta_2, ..., \eta_m)$, and A is an $m \times m$ matrix with the eigenvalues $\lambda_i, i = 1, 2, ..., m$. In this research, we used the most widely accepted definition of stiffness given by Lambert (1973).

Definition 1.6
The linear system (1.6) is said to be stiff if

(i) $\operatorname{Re}(\lambda_i) < 0,\ i = 1, 2, ..., m$ and

(ii) $\max_i |\operatorname{Re}(\lambda_i)| >> \min_i |\operatorname{Re}(\lambda_i)|$, where λ_i are the eigenvalues of A, and the ratio $S = \dfrac{\max_i |\operatorname{Re}(\lambda_i)|}{\min_i |\operatorname{Re}(\lambda_i)|}$ is called the stiffness ratio. By following the definition above, stiff problem has $S >> 1$.

Next, we will discuss on mean and introduce some of the means that commonly used in mathematics. These means are then represented in a trapezoid to show the connection between each means.

1.8 Mean

According to Umberger (2000), there are many types of mean in mathematics represent by different equations. However, most people memorize these equations without making a relation to geometrical form of the means. Umberger had presented seven types of mean –arithmetic mean (AM), geometric mean (GM), harmonic mean (HaM), heronian mean (HeM), contraharmonic mean (CoM), root mean square (RMS) and centroidal mean (CeM)- and shows how to construct them in a trapezoid.

Figure below is an example of trapezoid containing all seven means.

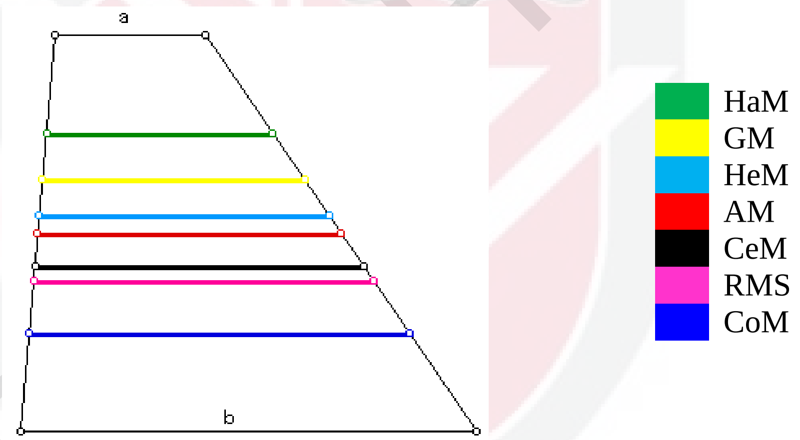

Figure 1.1: Trapezoid with Means.

As for this research, we are focusing on CeM. CeM is the length of a segment which is parallel to the bases a and b of the trapezoid, and also passes through the centroid area of the trapezoid as shown in Figure 1.1. CeM of any two real numbers a and b can be represented by the following equation.

$$CeM = \frac{2\left(a^2 + ab + b^2\right)}{3\left(a+b\right)}.$$

A detailed step-by-step construction of each means in a trapezoid can be found in Umberger (2000).

1.9 Objective of the Thesis

In this research, we develop a block method based on RK method for solving first order stiff ODEs. The aims in developing a block method are to reduce the computational time and improve accuracy of the proposed methods when compared with existing methods.

Objectives of this thesis are

i. to develop weighted block RK (WBRK) methods for solving first order stiff ODEs,

ii. to implement the new developed methods on stiff ODEs problems in order to test the performance of the methods,

iii. to construct the stability regions of the WBRK methods with different sets of weight and analyze their stability properties to indicate that the methods are suitable for solving first order stiff ODEs, and

iv. to determine the accuracy and efficiency of the WBRK methods between weights and between the existing methods.

1.10 Planning of the Thesis

In Chapter 1, we give some introductions on DE that related to the research. Then, a brief statement regarding the problem that need to be solved is also included. Numerical methods that are commonly used in solving ODEs problems are discussed. This leads to introduction on the RK method and its stability properties. Definition of stiff system for solving ODEs is presented. Means in a trapezoid is defined in this chapter. The objective and planning of the thesis are also discussed.

In Chapter 2, we review on the literature of the classical RK methods and stiffness. Some historical background of mean and block methods related to the research are also discussed.

Derivation of CeM by Pushpam & Dhayabaran (2011), and modified weighted RK3 based on CeM (MWRK3CeM) method by Sharmila & Amirtharaj (2011) are discussed in the beginning of Chapter 3. Then, we present the modification of MWRK3CeM to form the new proposed methods called the WBRK methods. The general form of the methods is presented in the chapter. Implementation of the chosen sets of weight to the WBRK methods can be found in the subsections of Chapter 3.

In Chapter 4, we study the stability of the WBRK methods with different sets of weight. In order to do so, we construct the stability regions of the methods for each weight from the stability polynomial of the proposed methods. Then, we analyze the stability properties of each set of weight.

Numerical results are presented in Chapter 5. In the chapter, we present the problems of single and system of first order stiff ODEs. These problems are tested with different stepsizes to see the relationship between the stepsizes and the accuracy of the proposed methods. Comparisons are made with the RK3 method and MWRK3CeM in terms of maximum error and computational time of the proposed methods with the comparing methods to analyze the performances of the methods. The comparison is also made between the sets of weight implemented. Results are presented in table form and illustrated in efficiency curve. The results are analyzed and discussed.

Finally, Chapter 6 will summarize the findings of the research and suggestions for related future studies.

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