UNIVERSITI PUTRA MALAYSIA

DIRECT TWO-POINT BLOCK METHODS FOR SOLVING NONSTIFF HIGHER ORDER ORDINARY DIFFERENTIAL EQUATIONS USING BACKWARD DIFFERENCE FORMULATION

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MASTER OF SCIENCE

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By

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

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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

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September 2014

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This thesis describes the development of a Two-Point Block Backward Difference method (2PBBD) for solving system of nonstiff higher order Ordinary Differential Equations (ODEs) directly. The method computes the approximate solutions; y_{n+1} and y_{n+2} at two points x_{n+1} and x_{n+2} simultaneously within an equidistant block.

This method has the advantages of calculating the integration coefficients only once at the beginning of the integration. The relationship between the explicit and implicit coefficients has also been derived. These motivate us to formulate the association between the formula for predictor and corrector. The relationship between the lower and higher order derivative also have been established.

New explicit and implicit block methods using constant step sizes and three back values have also been derived. The algorithm developed is implemented using Microsoft Visual C++ 6.0 and run by High Performance Computer (HPC) using the Message Passing Interface (MPI) library.

The stability properties for the 2PBBD methods are analyzed to ensure its suitability for solving nonstiff Initial Value Problems (IVPs). The stability analysis shows that the method is stable.

Numerical results are presented to compare the performances of this method with the previously published One-Point Backward Difference (1PBD) and Two-Point Block Divided Difference (2PBDD) methods. The numerical results indicated that for finer step sizes, 2PBBD performs better than 1PBD and 2PBDD.

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

KAEDAH BLOK DUA-TITIK SECARA LANGSUNG BAGI MENYELESAIKAN SISTEM PERSAMAAN PEMBEZAAN BIASA TAK KAKU PERINGKAT TINGGI MENGGUNAKAN FORMULA PEMBEZAAN KE BELAKANG

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Tesis ini menerangkan tentang pembentukan kaedah Dua-Titik Blok Pembezaan Ke Belakang (2TBPB) bagi menyelesaikan sistem pembezaan biasa tak kaku peringkat tinggi secara langsung. Kaedah ini menghitung penyelesaian anggaran; y_{n+1} dan y_{n+2} pada dua titik x_{n+1} dan x_{n+2} secara serentak dalam blok yang sama jarak.

Kaedah ini mempunyai kelebihan dimana pekali kamiran yang digunakan diperoleh hanya sekali pada awal proses pengamiran. Hubungan antara pekali tersurat dan tersirat juga telah diperoleh. Maka, ia mendorong untuk merumuskan hubungan di antara peramal dan pembetul. Hubungan di antara peringkat pembezaan terendah dan tertinggi juga diperoleh.

Kaedah baru blok tersurat dan tersirat dengan menggunakan saiz langkah malar dan tiga nilai belakang dibentuk dalam tesis ini. Algoritma yang terhasil dilaksanakan dengan menggunakan Microsoft Visual C++ 6.0 dan dijalankan oleh Komputer Prestasi Tinggi (KPT) dengan menggunakan perpustakaan Mesej Antara Muka (MAM).

Sifat-sifat kestabilan bagi kaedah 2TBPB dianalisis untuk memastikan kesesuaiannya untuk menyelesaikan Masalah Nilai Awal (MNA) tak kaku. Analisis kestabilan menunjukkan bahawa kaedah ini stabil.

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I certify that a Thesis Examination Committee has met on 5 September 2014 to conduct the final examination of Hazizah binti Mohd Ijam on her thesis entitled "Direct Two-Point Block Methods for Solving Nonstiff Higher Order Ordinary Differential Equations using Backward Difference Formulation" in accordance with the Universities and University College 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 Master of Science.

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LIST OF ABBREVIATIONS

ODEs	Ordinary Differential Equations
PDEs	Partial Differential Equations
BDF	Backward Differentiation Formula
BBDF	Block Backward Differentiation Formula
IVPs	Initial Value Problems
LMM	Linear Multistep Method
$\mathcal{L}$	Linear Operator
LTE	Local Truncation Error
GE	Global Error
PECE	Predict-Evaluate-Correct-Evaluate
2PBBD	Two-Point Block Backward Difference Method
2PBDD	Two-Point Block Divided Difference Method
1PBD	One-Point Backward Difference Method
H	Step size
TS	Total Steps
MAXE	Maximum Error
AVER	Average Error
TIME	Execution Time in microseconds
HPC	High Performance Computer

CHAPTER 1

INTRODUCTION

1.1 Introduction

Many mathematical models used in science and technology are developed based on differential equations. Differential equations play a prominent role in many disciplines, for example in physics, chemistry, biology, electronics, engineering, economics e.t.c. The theory of differential equations has been developed by numerous mathematicians. In general, it can be divided into these two categories; ordinary differential equations (ODEs) and partial differential equations (PDEs). We are focusing on ODEs which can be divided in two subsystems; one stiff and the other nonstiff.

The problem of determining the charge or current in an electric circuit, the problem of determining the vibrations of a wire or membrane and the reactions of chemicals can be formulated into differential equations. Since many differential equations have no analytic solution, hence a numerical approximation to the solution is often suggested.

To solve ODEs numerically, there are two general classes of numerical methods, for instance single step method and multistep method. The single step method is a method which uses only one previous computed value to obtain the next value. Euler's method and Runge-Kutta method are examples of single step methods. On the contrary, the multistep method is a method which requires starting values from several previous steps. This method can be found in Adams formula and Backward Differentiation Formula (BDF).

1.2 The Initial Value Problems (IVPs)

For the sake of simplicity of discussion and without loss of generality, we will discuss the single equation

$$y^{(d)} = f\left(x, \tilde{Y}\right) \tag{1.1}$$

with $\tilde{Y}(a) = \tilde{\eta}$ in the interval $a \leq x \leq b$ where

$$\tilde{Y}(x) = \left(y, y', y'', \dots, y^{(d-1)}\right)$$

$$\tilde{\eta} = \left(\eta, \eta', \eta'', \dots, \eta^{(d-1)}\right).$$

With regard to (1.1), we make an assumption that for each $f\left(x, \tilde{Y}\right)$, it satisfies the following conditions;

a) $f(x,\tilde{Y})$ is defined and continuous in the interval $a \leq x \leq b, -\infty < y < \infty$, where a and b are finite.
b) There exists a constant L, known as *Lipschitz constant*, such that for arbitrary $x \in [a,b]$ and any $\tilde{Y}$ and $\tilde{Y}^*$, $\left|f(x,\tilde{Y}) - f(x,\tilde{Y}^*)\right| \leq L\left\|\tilde{Y} - \tilde{Y}^*\right\|$. This condition is known as *Lipschitz condition.*

Theorem 1.1 (Existence and Uniqueness)

If the equation (1.1) satisfies the condition in a) and b), then there exists a unique solution of $y(x)$ with the following three properties:

i) $y(x)$ is continuous and d times differentiable for $x \in [a,b]$,
ii) $y^{(d)}(x) = f(x,\tilde{Y})$ for $x \in [a,b]$,
iii) $\tilde{Y}(a) = \tilde{\eta}$.

The proof for the first order case was given by Henrici (1962). For the case of higher order system $(d > 1)$, the problem (1.1) is reduced to a system of first order equations and then the theorem applies.

For the following discussion, we will consider the IVPs for the single equation, which can be written in the form

$$y' = f(x,y), \quad y(a) = \eta, \;\; a \leq x \leq b. \tag{1.2}$$

1.3 Linear Multistep Method (LMM)

These methods require the information computed from the previous steps to approximate the solution at the current step. For example, in the k-step method the values of y computed at the previous k step i.e. at $x_{n+j} = x_n + jh, j = 0,1, \dots, k-1$ are used to calculate x_{n+k}. The general LMM is given by

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=o}^{k} \beta_j f_{n+j} \tag{1.3}$$

where α_j and β_j are constants. We also assume that $\alpha_k \neq 0$ and that not both α_0 and β_0 are zero. If $\beta_k = 0$, y_{n+k} occurs only on the left side of (1.3), the method is called an explicit method. If $\beta_k \neq 0$, y_{n+k} is present on both sides of (1.2) and the method is known as an implicit method.

Lambert (1973) discusses the specific linear multistep methods can be derived using Taylor expansions, numerical integration and interpolation.

Definition 1.1

The LMM (1.3) is *convergent* if for all initial value problems (1.2) subject to the hypotheses of Theorem 1.1, we have

$$\lim_{\substack{h\to 0\\ nh=x-a}} y_n = y(x_n)$$

holds for all $x \in [a,b]$, and for all solution $\{y_n\}$ of the difference equation (1.3) satisfying starting conditions $y_\mu = \eta_\mu(h)$ for which $\lim_{h\to 0} \eta_\mu(h) = \eta,\ \mu = 0,1,\ldots,k-1$.

Define the linear difference operator $\mathcal{L}$ associated with (1.3) as

$$\mathcal{L}[y(x);h] = \sum_{j=0}^{k}\left[\alpha_j y(x+jh) - h\beta_j y'(x+jh)\right] \tag{1.4}$$

where $y(x)$ is an arbitrary function continuously differentiable on $[a,b]$. Expanding $y(x+jh)$ and $y'(x+jh)$ in (1.4) as Taylor series about x yields

$$\mathcal{L}[y(x);h] = C_0 y(x) + C_1 h y'(x) + \cdots + C_q h^q y^{(q)}(x) + \cdots \tag{1.5}$$

where,

$$\begin{aligned}
C_0 &= \alpha_0 + \alpha_1 + \cdots + \alpha_k\\
C_1 &= \alpha_1 + 2\alpha_2 + \cdots + k\alpha_k - (\beta_1 + \beta_2 + \cdots + \beta_k)\\
&\ \ \vdots \qquad\qquad \vdots \qquad\qquad \vdots\\
C_q &= \frac{1}{q!}(\alpha_1 + 2^q\alpha_2 + \cdots + k^q\alpha_k)\\
&\quad - \frac{1}{(q-1)!}\left(\beta_1 + 2^{(q-1)}\beta_2 + \cdots + k^{(q-1)}\beta_k\right)\\
&\quad q = 2,3,\ldots
\end{aligned} \tag{1.6}$$

Definition 1.2

The difference operator (1.4) and the associated LMM (1.3) are said to be of the order p if $C_0 = C_1 = \cdots = C_p = 0, C_{p+1} \neq 0$. The first of non-vanishing coefficient, C_{p+1} is called the error constant.

Definition 1.3

The local truncation error (LTE) at x_{n+k} of the linear multistep method (1.3) is the linear difference operator $\mathcal{L}[y(x);h]$ as defined in (1.4) when $y(x)$ is the exact solution of the IVP (1.2).

In order to compute LTE at x_{n+k}, we made the localizing assumption that no previous truncation errors have been made, that is $y_{n+j} = y\left(x_{n+j}\right)$, $j = 0,1,\dots,k-1$. If no such assumption is made, then the difference between the exact and computed solution, i.e. $y(x_{n+k}) - y_{n+k}$ gives the global error (GE).

Definition 1.4

If the LMM (1.3) has order $p \geq 1$ the method is then said to be *consistent*. Referring to (1.6), the method (1.3) is consistent if and only if

$$\sum_{j=0}^{k} \alpha_j = 0 \text{ and } \sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_j \tag{1.7}$$

The equation $\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j$ and $\sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j$ are defined to be the first and second characteristic polynomials respectively. It follows from (1.7) that the linear multistep method is consistent if and only if $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$. Therefore, the first characteristic polynomial $\rho(\xi)$ always has a root at 1 for a consistent method. This root is better known as the *principal root* and denoted by ξ_1. The other roots, $\xi_s, s = 2,3,\dots,k$, are called *spurious roots*. Since consistency controls only the principal and not the spurious roots, it implies that a consistent method is not necessarily convergent.

Definition 1.5

The LMM (1.3) is *zero-stable* if the first characteristic polynomial $\rho(\xi)$ has no root whose modulus is greater than 1 and every root with modulus 1 is simple.

Definition 1.6

The method (1.3) is said to be *absolutely stable* in a region $\Re$ of the complex plane if, for all $\hat{h} \in \Re$, all roots of the stability polynomial $\pi \;\; r, \hat{h}$ associated with the method, satisfy $\left|r_s\right| < 1, s = 1, 2, \dots, k$.

Theorem 1.2

A LMM is *convergent* if and only if it is consistent and zero-stable. The proof of the theorem can be found in Henrici (1962).

Definition 1.7 (Block Method)

According to Hall (1976), *r*-point block method is a method which simultaneously produce a block of approximations $y_{n+1}, y_{n+2}, \ldots, y_{n+r}$.

Generally, ODEs can be classified into 2 types that is; stiff and nonstiff. Here we use the definition given by Lambert (1991).

Definition 1.8

The systems of ODEs (1.1) is said to be *stiff* if

(i) Re $\lambda_t < 0, t = 1, 2, \ldots, m$ and

(ii) $\max_t |\text{Re } \lambda_t| >> \min_t |\text{Re } \lambda_t|$ where λ_t are the eigenvalues of the Jacobian matrix, $J = \left(\frac{\partial f}{\partial y} \right)$.

Otherwise it is defined as nonstiff.

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