UNIVERSITI PUTRA MALAYSIA

FIFTH ORDER 2-POINT IMPLICIT BLOCK METHOD WITH AN OFF-STAGE FUNCTION FOR SOLVING FIRST ORDER STIFF INITIAL VALUE PROBLEMS

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By

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December 2014

Chairman: Dato' Mohamed Suleiman, PhD

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Numerical solution schemes are often referred to as being explicit or implicit. However, implicit numerical methods are more accurate than explicit for the same number of back values in solving stiff Initial Value Problems (IVPs). Hence, one of the most suitable methods for solving stiff IVPs is the Backward Differentiation Formula (BDF).

In this thesis, a new two−point implicit block method with an off-stage function (2P4BBDF) for solving first order stiff Ordinary Differential Equations (ODEs) is developed. This method computes the approximate solutions at two points simultaneously based on equidistant block method. The proposed new formula is different from previous studies because it has the advantage of generating a set of formulas by varying a value of the parameters within the interval (-1,1). In this thesis we use $\frac{1}{2}$ and $-\frac{1}{4}$ as the parameter.

The stability analysis for the method derived namely; $\zeta = \frac{1}{2}$ and $\zeta = -\frac{1}{4}$ show that the method is almost A-stable. Numerical results are given to compare the competitiveness of the new method with an existing method. The new method is compared numerically with a fifth order 3−point BBDF method by Ibrahim et al (2007). It is seen that the new method is marginally better than the 3−point BBDF in terms of accuracy and computational times. We also investigate the convergence and order properties of the 2P4BBDF method. The zero stability and consistency which are necessary conditions for convergence of the BBDF method are established. The algorithm for implementing the method will also developed.

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

KAEDAH BLOK TERSIRAT 2−TITIK DENGAN FUNGSI LUAR TAHAP PERINGKAT KELIMA BAGI MENYELESAIKAN MASALAH NILAI AWAL PERINGKAT PERTAMA

Oleh

SITI ZHAFIRAH ZAINAL

Disember 2014

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Skim penyelesaian berangka sering dirujuk sebagai tak tersirat atau tersirat. Walau bagaimanapun, kaedah berangka tersirat adalah lebih jitu daripada yang tak tersirat bagi nilai belakang yang sama dalam menyelesaikan Masalah Nilai Awal (MNA) kaku. Oleh itu, salah satu kaedah yang paling sesuai untuk menyelesaikan MNA kaku adalah Rumus Pembezaan Ke Belakang (RPK).

Dalam tesis ini, kaedah baru blok dua titik menggunakan blok empat titik kebelakang (2T4RPKB) untuk menyelesaikan peringkat pertama Persamaan Pembezaan Biasa (PPB) jenis kaku diterbitkan.Kaedah ini mengira penyelesaian anggaran pada dua titik yang sama berdasarkan kaedah blok sama jarak. Formula baru yang dicadangkan adalah berbeza daripada kajian sebelum ini kerana ia mempunyai kelebihan menjana satu set formula dengan mengubah nilai parameter dalam selang (-1,1). Di mana dalam tesis ini kita menggunakan $\zeta = \frac{1}{2}$ dan $\zeta = -\frac{1}{4}$ sebagai parameter.

Analisis kestabilan untuk kaedah yang telah diterbitkan iaitu $\zeta = \frac{1}{2}$ dan $\zeta = -\frac{1}{4}$ menunjukkan bahawa kaedah ini hampir A-stabil. Keputusan berangka diberikan untuk membandingkan daya saing kaedah baru dengan kaedah yang sedia ada. Kaedah baru dibandingkan secara berangka dengan Rumus Pembezaan Ke Belakang Blok 3−titik (3RPKB) peringkat kelima oleh Ibrahim dan rakan-rakan lain (2007). Ia dilihat bahawa kaedah baru adalah lebih baik sedikit daripada Rumus Pembezaan Ke Belakang Blok 3−titik (3RPKB) peringkat kelima dari segi ketepatan dan masa pengiraan. Dibincangkan juga kestabilan dan kekonsistenan kaedah 2T4RPKB. Ini kerana sifat-sifat tersebut merupakan ciri-ciri yang diperlukan untuk penumpuan kaedah RPKB. Algoritma untuk menerbitkan kaedah ini juga dibangunkan.

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I certify that a Thesis Examination Committee has met on **3 December 2014** to conduct the final examination of **Siti Zhafirah Binti Zainal** on his (or her) thesis entitled "**FIFTH ORDER 2−POINT IMPLICIT BLOCK METHOD WITH AN OFF−STAGE FUNCTION FOR SOLVING FIRST ORDER STIFF INITIAL VALUE PROBLEMS**" 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 **Master of Science**.

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LIST OF ABBREVIATIONS

ODEs	Ordinary Differential Equations
BDF	Backward Differentiation Formula
LMM	Linear Multistep Method
L	Linear Operator
NS	Number of Step
2P4BBDF	2−point Implicit Block Method with an off-stage function
3BBDF	Fifth Order 3−point Block Backward Differentiation Formula
λ	Lagrange Multiplier
IVP	Initial Value Problem
MAXE	Maximum Error
TIME	Computation Time in Second
RKF	Runge-Kutta Formula
INF	Fail to Complete

CHAPTER 1

INTRODUCTION

Numerical Ordinary Differential Equation (ODE) is the part of numerical analysis which studies the numerical solution of Ordinary Differential Equations (ODEs). ODEs frequently occur as mathematical models in many branches such as in Chemistry, Physics, Economics and Biology. As an example, differential equation has been used in Physics through the Newton's Second Law of Motion and the Law of Cooling. It is also used in Hooke's Law for modelling the motion of a spring or in representing models for population growth and money flow in circulation. Also, differential equations are often used to model problems in engineering either as first order or higher order systems of differential equations. For example, mathematical models of electrical circuits, mechanical systems, chemical processes and etc. are described by systems of ODEs. Besides that, the problems of the bending of a thin clamped beam, the motion of projectiles and some problems in control theory are formulated in terms of higher order differential equations.

ODEs are equations to be solved in which the unknown element is a functional, rather than a number. Further, information is known about the derivative function. Besides that ODEs are the derivatives where all are with respect to single independent variable, often representing time.

In this study, the numerical solution of Initial Value Problems (IVPs) for system of first order Ordinary Differential Equations (ODEs) are discussed. The ODEs are given by

$$y^d = F(x, y, y', y'', ..., y^{(d-1)}) \tag{1.1}$$

where d represents the highest derivative; y is a function of x, $y^{'}$ is the first derivative with respect to x and $y^{(d-1)}$ is the $(d-1)$th derivative with respect to x.

Many of the differential equations cannot be solved analytically and hence the use of numerical methods are proposed. Basically, these problems are categorized as stiff and nonstiff. The stiff equations arise in many applications and are due to the existence of differing time dependencies. The numerical solution of stiff system is more challenging compared to the nonstiff ones and thus attracted the attention of many researchers. Initial value problems for which this is likely to occur are called as stiff equations and are quite common, particularly in the study of vibrations, chemical kinetics, nuclear reactors, control theory and electrical circuits theory. Generally speaking, whenever there involves a quickly changing dynamics, there is stiffness.

Many of these ODEs in (1.1) are stiff ODEs and are difficult to solve, since some of the numerical methods have stability restriction on the step size. Moreover, stiff equation needs the Jacobian to be calculated and subsequently solve the resulting system. Many stiff problems are effectively non-stiff during the initial phase. An approach to solve such problems involving stiffness is to integrate the stiff part implicitly and the non-stiff part explicitly. The codes that are commonly used for solving nonstiff ODEs are based on the explicit Runge-Kutta

Formulas (RKFs), Adams formulas or extrapolation method. While for stiff ODEs, the most commonly used multistep method are based on Backward Differentiation Formulas (BDFs).

Most numerical methods for solving differential equations produce only one new approximation value at each step of the integration. Method for solving stiff ODEs include non-block methods like the implicit Runge-Kutta and the BDF methods. There are some earlier research on computing the solution of (1.1) at one point per step to two or more points called Block method that have been discussed by Milne (1953). Sequential block method is based on the idea of simultaneously producing a block of approximations $y_{n+1}, y_{n+2}, y_{n+3}, \dots y_{n+k}$, at each iteration of the algorithm.

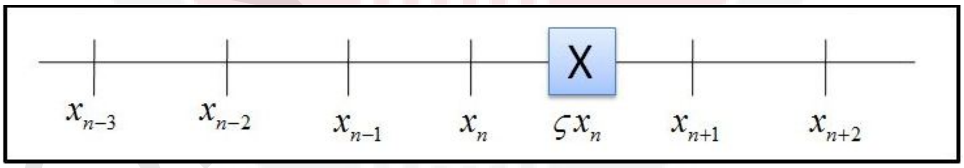
This research proposed a new implicit block method for solving (1.1). The BBDF in Ibrahim et al. (2007) and Ibrahim (2006) has the form

$$\sum_{j=0}^{5} \alpha_{j,i} y_{n+j-1} = h\beta_{k,i} f_{n+k}, \qquad k = 1, 2, \qquad i = k \tag{1.2}$$

where the solution is computed at 2 and 3 different points concurrently.
Our new formula will take the form :

$$\sum_{j=0}^{5} \alpha_{j,i} y_{n+j-3} = h\beta_{k,i}(f_{n+k} - \zeta f_{n+k-1}) \tag{1.3}$$

$k = 1, 2, \quad i = k$. See Musa (2013).
where α_j and β_j are constants subject to conditions $\alpha_k = 1, |\alpha_0| + |\beta_0| \neq 0$.



The point $x_{n-3}, \dots, x_{n+2}$ are the on stage point. The point in the box is an off-stage point. The on stage points are used in the classical BDF formula. An off-stage point will be introduced in the new formula.

The new proposed formula will be different from (1.2) by considering the free parameters, ζ which is restricted to $[-1, 1)$ to ensure stability of the method and note that the last term of the new formula has added the additional point f_{n+k-1}.
A similar form of (1.3) has been considered by Musa (2013) in a variable step size mode. The main difference with that in Musa (2013) is that our scheme is fifth order with a fixed step size and has four back values when compared with the formula in Musa (2013) where the scheme is third order with two back values only.

1.1 Motivation of the study

Currently, there are several works on implicit block methods developed for the solution of stiff IVPs. There are only a small number of researchers who solve stiff IVPs using block method such as Ibrahim (2006) and Nasir et al. (2012). Partly because in stiff method, we have to calculate Jacobian which is costly and difficult. Therefore we are motivated by the development by Musa (2013) and Ibrahim (2006) to develop at least a competitive method. In order to achieve this, we introduce a new implicit block method for solving ODEs which is a new form of the 2−point BBDF as given in Ibrahim (2006). This is achieved by adding additional back values and an off-stage function evaluation. Furthermore, we intend to improve the accuracy of the 2-point BBDF even when it has the same order with our scheme.

1.2 Objective

The objectives of this study are:
i. To develop a new fifth order implicit block method suitable for integrating stiff Initial Value Problems (IVPs).
ii. To discuss and investigate the convergence properties of the method developed.
iii. To develop an algorithm for implementing the method developed.

1.3 Problem to be solved

The study will be for a system of first order IVPs of the form

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

where $y = (y, y_1, ..., y_k)$, $\eta = (\eta, \eta_1, ..., \eta_k)$ and $a \leq x \leq b$.

Suppose that the real function $f(x, y)$ satisfies the following conditions:
i. $f(x, y)$ is defined and continuous in the strip $a \leq x \leq b, -\infty < y < \infty$, where a and b are finite.
ii. There exists a constant L such that for any $a \leq x \leq b$ and any two numbers y and y^*

$$|f(x, y) - f(x, y^*)| \leq L\,|y - y^*| \tag{1.5}$$

1.4 Basic Definition

Definition 1.1(The Initial Value Problem)

It is often the case in Physics that one is interested in only one solution among all solutions to a differential equation. One way to select a particular solution is to require that $y(a) = y_0$, that is, the solution at a given point a takes the given value y_0. The point a is called the initial point, and the condition $y(a) = y_0$ is called the initial condition. An Initial Value Problems (1.1) is the following. Given the function f and the constants x_0, y_0 find all functions y which are solution of

$$\frac{dy}{dx}(x) = f(x), \qquad y(x_0) = \eta \qquad \eta = [\eta_1, .., \eta_m] \tag{1.6}$$

Theorem 1.1 (Existence and Uniqueness)

The requirement of (1.5) is called Lipschitz condition.
Let $f(x, y)$ satisfies condition (i) and (ii) above and let η be a given number. Then there exists exactly one function $y(x)$ with the following properties:
(a) $y(x)$ is continuous and differentiable for $a \leq x \leq b$;
(b) $y^{'}(x) = f(x, y(x))$, $a \leq x \leq b$;
(c) $y(a) = \eta$;

The proof is given in Henrici (1962).

Definition 1.2 (Stiff Systems for Ordinary Differential Equations)

Stiffness is a property of the mathematical problem in the numerical solution of ODEs and arises in many applications including the study of spring and damping system, analysis of control system, problem in chemical kinetics and chemical reactions such as Oregenator reaction between $HBrO^2$, Br, and Ce(IV).

There are many variations of the definition for stiffness given in the literature with respect to the linear system of first order equations,

$$\tilde{y}' = A\tilde{y} + \tilde{\phi}(x),\ \tilde{y}(a) = \tilde{\beta},\ a \leq x \leq b \tag{1.7}$$

where $\tilde{y}^T = (y_1, y_2, ..., y_s)$, $\tilde{\beta^T} = (\beta_1, \beta_2, ..., \beta_s)$ and A is an $s \times s$ matrix while $\tilde{\phi}$.
Here we choose the definitions given by Lambert (1973). The system is said to be stiff if

(i) For all eigenvalues λ_i, $\text{Re}(\lambda_i) < 0$, i=1,...,s

(ii) $\underset{i}{max}\,|Re(\lambda_i)| >> \underset{i}{min}\,|Re(\lambda_i)|$ where λ_i are the eigenvalues of A, and the ratio $\frac{\underset{i}{max}|Re(\lambda_i)|}{\underset{i}{min}|Re(\lambda_i)|}$ is called the stiffness ratio or stiffness index.

The general solution to (1.7) is of the form

$$\tilde{y}(x) = \sum_{i=1}^{s} k_i e^{\lambda_i x} \tilde{u}_i + \tilde{\psi}(x) \tag{1.8}$$

where $\sum_{i=1}^{s} k_i e^{\lambda_i x} \tilde{u}_i$ is the transient solution and $\tilde{\psi}(x)$ is the steady state solution.

Definition 1.3 (Linear Multistep Method)

Linear Multistep Methods constitute an important class of numerical integrators for Ordinary Differential Equations (ODEs). Some particular methods are well suited for solving non-stiff and some for stiff equations, see Suleiman (1979) and Majid (2004). In contrast to one step methods, multistep method increase efficiency by using the information from several previous solution approximation. In particular, multistep methods require the back values of $y_n, y_{n+1}, ..., y_{n+k-1}$ to determine y_{n+k} where $y_{n+i} \approx y(x_{n+i}), 0 \leq i \leq k$. The Linear Multistep

Method (LMM) or linear $k-$step method can be represented in standard form by an equation

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \tag{1.9}$$

where α_i and β_i are constants and assuming that $\alpha_k \neq 0$ and not both α_0, β_0 at the same instance while $y_{n+j} \approx y(x_{n+j})$ and $f_{n+j} \equiv f(x_{n+j}, y_{n+j})$. For any k step method α_k is normalised to 1.

Definition 1.4 (Taylor's Series Expansion)

The Taylor's series expansion of $y(x_n + h)$ about x_n is defined by

$$y(x_n + h) = y(x_n) + hy'(x_n) + \frac{h^2}{2!}y'' + ... \tag{1.10}$$

where

$$y^m = \frac{\mathrm{d}^m y}{\mathrm{d}x^m} \quad m = 1, 2, ...$$

Definition 1.5

The linear difference operator L associated with the linear multistep (1.9) is defined by

$$L[y(x); h] = \sum_{j=0}^{k} [\alpha_j y(x + jh) - h\beta_j y'(x + jh)] \tag{1.11}$$

where $y(x)$ is an arbitrary function, continuously differentiable on [a,b].

Expanding the test function $y(x+jh)$ and its derivative $y^{'}(x+jh)$ about x, and collect terms in (1.13) to obtain

$$L[y(x); h] = C_0 y(x) + C_1 h y^{(1)}(x) + .. + C_q h^q y^{(q)}(x) + ... \tag{1.12}$$

where C_q are constants given by

$$\begin{aligned}
C_0 =& \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 + ... + \alpha_k \\
C_1 =& \alpha_1 - 2\alpha_2 + 3\alpha_3 + .. + k\alpha_k - (\beta_0 + \beta_1 + ... + \beta_k) \\
&. \\
&. \\
&. \\
C_q =& \frac{1}{q!}(\alpha_1 + 2^q\alpha_2 + 3^3\alpha_3 + .. + k^q\alpha_k) - \frac{1}{(q-1)!}(\beta_1 + 2^{q-1}\beta_2 + ... + k^{q-1}\beta_k) \\
q =& 2, 3, .., k
\end{aligned} \tag{1.13}$$

Definition 1.6 (Convergence)

The Linear Multistep Method in (1.9) is said to be convergent if, for all initial value problems satisfying the hypotheses of Theorem (1.1) we have that

$$\lim_{\substack{h \to 0 \\ n \to \infty}} y(n) = y(x) \tag{1.14}$$

where $n = (x - a)/h$ holds for all $x \in [a, b]$ and for all solutions y_n of the difference equation in (1.9) satisfying the condition $y_\mu = \eta_\mu(h)$ for which $\lim_{h \to 0} \eta_\mu(h) = \eta$, $\mu = 0, 1, ..., k - 1$. For proof, see Henrici (1962).

Definition 1.7 (Order)

The difference operator in (1.11) and the associated linear multistep method (1.9) are said to be of order p, if in (1.12),

$$C_0 = C_1 = .. = C_p = 0, C_{p+1} \neq 0$$

Definition 1.8 (Local Truncation Error)

The local truncation error (LTE) at x_{n+k} is defined to be the expression $L[y_(x_n); h]$ given by (1.11), when $y(x)$ is the theoretical solution of the given IVP.

Definition 1.9 (Characteristic Polynomial)

The first characteristic polynomial, $\rho(\phi)$ is the polynomial of degree k where the coefficients are α_j and the second characteristic polynomial, $\sigma(\phi)$ where the coefficients are β_j. The first characteristic polynomial and the second characteristic polynomial associated with the LMM (1.9) is defined as

$$\rho(\phi) = \sum_{j=0}^{k} \alpha_j \phi^j \tag{1.15}$$

$$\sigma(\phi) = \sum_{j=0}^{k} \beta_j \phi^j$$

Thus for a consistent method, the first characteristic polynomial has root at $+1$. This root is called the principal root and label as ϕ_1. The remaining roots are $\phi_s, s = 2, 3, .., k$ are spurious roots and arise only when the step number of the method is greater than one. The characteristic polynomial of the method (1.9) is given by

$$\pi(r, \bar{h}) = \rho(r) - \bar{h}\sigma(r) = 0 \tag{1.16}$$

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

Definition 1.10 (Consistency)

The Linear Multistep Method (LMM) (1.9) is said to be consistent if it has order $p \geq 1$. From (1.13) it follows that the method (1.9) is consistent if and only if

$$\begin{aligned} \sum_{j=0}^{k} \alpha_j &= 0 \\ \sum_{j=0}^{k} j\alpha_j &= \sum_{j=0}^{k} \beta_j \end{aligned} \qquad (1.17)$$

It follows form (1.17) that the LLM (1.9) is consistent if and only if

$$\begin{aligned} \rho(1) &= 0 \\ \rho'(1) &= \sigma(1) \end{aligned} \qquad (1.18)$$

See Lambert (1973).

Definition 1.11 (Zero Stability)

The Linear Multistep Method (1.9) is said to be zero stable if no root of the first characteristic polynomial $\rho(\phi)$ has a modulus greater than one, and all roots with modulus one is a simple root.

Definition 1.12 (Absolute Stability)

The LMM (1.9) is said to be absolutely stable for a given h if for that h all the roots r_s of the stability polynomial satisfy $|r_s| < 1,\ s = 1, 2, .., k$ and to be absolutely unstable for that h otherwise. An interval (α, β) of the real line is said to be an interval of absolute stability if the method is absolutely stable for all $h \in (\alpha, \beta)$. If the method is absolutely unstable for all h it is said to have no interval of absolute stability.

Definition 1.13 (A−Stable)

A method is said to be A−Stable if all numerical approximations tend to zero as $n \to \infty$ when applied to the differential equation $y' = \lambda y$ with a fixed positive h and a complex constant λ with negative real part.

1.5 Outline of the thesis

The following is the outline of the thesis.
Chapter I provide the introduction of numerical ODEs with an overview of the problems and the formula used in the later chapters. The chapter also define the stability properties that are relevant when solving stiff problems. This chapter also includes the motivation and the objectives of the study.

Over the years several implicit methods have been discussed, developed and implemented extensively in the literature. Hence, Chapter II contains review of literatures of related work.

In chapter III, the formulation of the 2−point implicit block method with an off-stage function (2P4BBDF) is developed. For absolute stability of the method, we will choose ζ in the interval $(-1, 1)$. In this study we choose $\zeta = \frac{1}{2}$ and $\zeta = -\frac{1}{4}$. Such choice of ζ are based on empirical evidence. Further, the absolute stability region of the method are also determined. Next, some test problems are solved numerically. Comparison of the performance are made with the existing block BDF in Ibrahim (2007).

Chapter IV investigates the convergence properties namely; the order and zero stability of the 2−point implicit block method with an off-stage function (2P4BBDF). Zero stability and consistency conditions of the method are also established in this chapter.

Chapter V concludes the main finding in relation to the objectives of the study and recommendations for future research are also included.

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