MULTIBLOCK BACKWARD DIFFERENTIATION FORMULAE FOR SOLVING FIRST ORDER ORDINARY DIFFERENTIAL EQUATIONS

NOR AIN AZEANY BINTI MOHD NASIR

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By

NOR AIN AZEANY BINTI MOHD NASIR

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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DEDICATIONS

to

Madam Norjanah Jani

Mr Mohd Nasir Kamin

Madam Norazlina

and

all my family members ...

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

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November 2011

Chair: Zarina Bibi Binti Ibrahim, PhD

Faculty: Science

Block Backward Differentiation Formulae (BBDF) methods of variable order is derived to solve first order stiff ordinary differential equations (ODEs). These methods computed two approximate solutions y_{n+1} and y_{n+2} at the points x_{n+1} and x_{n+2} of the initial value problems (IVPs) concurrently in a block at each step. The numerical results are given to validate the method and the performances are being compared with the classical Backward Differentiation Formulae (BDF) method.

Furthermore, the stability properties and the stability regions for the BBDF methods are investigated to ensure the methods are useful for solving stiff ODEs. This BBDF is extended to variable order method in order to improve the efficiency of the method. A single code is developed with fixed stepsize and implemented using Microsoft Visual C++ 2008 Express Edition and compared with ode15s and ode23s which is run in MATLAB 7.1.

A parallel scheme of the BBDF is derived in order to solve large problems in ODEs using the Message Passing Interface (MPI) library run by the High Performance Computer (HPC). The efficiency of the method is justified by the numerical results given. The results generated showed that these methods produced less computational time and achieved the desired accuracy.

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

Gandaan Blok Formula Pembezaan ke Belakang untuk Menyelesaikan Peringkat Pertama Persamaan Pembezaan Biasa

Oleh

NOR AIN AZEANY BINTI MOHD NASIR

November 2011

Pengerusi: Zarina Bibi Binti Ibrahim, PhD

Fakulti: Sains

Kaedah Blok Formula Beza Ke Belakang (BFBB) pelbagai peringkat dibina untuk menyelesaikan persamaan pembezaan kaku biasa peringkat pertama (PPB). Kaedah ini menghitung dua penyelesaian anggaran y_{n+1} dan y_{n+2} pada titik x_{n+1} dan x_{n+2} dari masalah nilai awal (MNA) secara serentak dalam satu blok pada setiap langkah. Keputusan berangka diberikan untuk mengesahkan kaedah tersebut dan pelaksanaannya yang dibandingkan dengan kaedah klasik Formulasi Beza Ke Belakang (FBB).

Selanjutnya, sifat kestabilan dan rantau kestabilan untuk kaedah BFBB diselidiki bagi memastikan kaedah ini berguna untuk menyelesaikan PPB kaku. Kaedah BFBB ini diperluaskan dengan kaedah pelbagai peringkat dengan tujuan meningkatkan kecekapan kaedah. Kod tunggal dibangunkan dengan panjang langkah yang tetap dan dilaksanakan dengan menggunakan Microsoft Visual C + + 2008 Express Edition dan dibandingkan dengan ode15s dan ode23s yang dijalankan dalam MATLAB 7.1.

Satu skim selari BFBB diperolehi untuk menyelesaikan masalah besar dalam PPB menggunakan perpustakaan Mesej Antara Muka (MAM) dijalankan menggunakan Komputasi Prestasi Tinggi (KPT). Kecekapan kaedah ini dikuatkan oleh hasil berangka yang diberikan. Keputusan yang dihasilkan menunjukkan bahawa kaedah ini menghasilkan kurang masa pengkomputeran dan mencapai ketepatan yang dikehendaki.

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LIST OF ABBREVIATIONS

IVPs	Initial Value Problems
LMM	Linear Multistep Method
ODEs	Ordinary Differential Equations
BDF(3)	Backward Differentiation Formulae of order 3
BDF(4)	Backward Differentiation Formulae of order 4
BDF(5)	Backward Differentiation Formulae of order 5
BBDF(4)	Fourth order Block Backward Differentiation Formulae
BBDF(5)	Fifth order Block Backward Differentiation Formulae
BBDF(6)	Sixth order Block Backward Differentiation Formulae
VOBBDF	Variable order Block Backward Differentiation Formulae
ode15s	A variable order solver of Numerical Differentiation Formulae
ode23s	A second order of Rosenberg method
PBBDF(4)	Parallel Block Backward Differentiation Formulae of order four
MPI	Message Passing Interface
MIMD	Multiple Instruction Multiple Data
MISD	Multiple Instruction Style Data
PDEs	Partial Differential Equations
M2PG	Modified 2-point Implicit block one-step method
BDF	Backward Differentiation Formulae
BBDF	Block Backward Differentiation Formulae
RKFNC	Fixed-order Runge-Kutta method (1-5 order)
VRKF	Variable order Runge-Kutta method

LTE	Local Truncation Error
LTE(4)	Local Truncation Error of BBDF(4)
LTE(5)	Local Truncation Error of BBDF(5)
LTE(6)	Local Truncation Error of BBDF(6)
NDF	Numerical Differentiation Formulae
2PEB	2-point explicit block method
3PEB	3-point explicit block method
SISD	single-instruction single-data
SIMD	single-instruction multiple-data
HPC	High Performance Computing
MBBDF	Multiblock Backward Differentiation Formulae
DDEs	Delay Differential Equations
DAEs	Differential Algebraic Equations
FDEs	Fuzzy Differential Equations

CHAPTER 1
INTRODUCTION

1.1 Introduction

Engineers, scientists and physicians are frequently confronted with mathematical modelling problems that involved differential equations which are complicated to be solved analytically. For instance, problems in physics such as projectile motion of a satellite which involves accelerations and velocities, determining the time of death of John Doe using the temperature of the dead body and the surrounding, and chemical kinetics may be modelled by differential equations. The differential equations can be divided into two categories, which are ordinary differential equations (ODEs) and partial differential equations (PDEs).

In order to solve ODEs numerically, there are two classes of numerical methods such as the single step method and the multistep method. The single step method is a method which uses the computed previous value to calculate the next value, for example Eulers method and Runge-Kutta method. On the other hand, the multistep method is a method that requires other method such as the single step method to compute the backvalues. The examples of multistep methods are Adams method and Backward Differentiation Formulae (BDF).

In this chapter, we briefly introduce the problems and basic definitions related to ODEs.

1.2 The Initial Value Problem

The initial value problems (IVPs) for a system of m first order ordinary differential equations (ODEs) is defined by

$$Y' = F\left(x, Y\right), Y\left(a\right) = \eta \tag{1.1}$$

where $Y = \left[y_1, y_2, ..., y_m\right]^T, F = \left[f_1, f_2, ..., f_m\right]^T, \eta = \left[\eta_1, \eta_2, ..., \eta_m\right]^T$ and $a \leq x \leq b$.

The following theorem states the conditions on $F\left(x, Y\right)$ which guarantee the existence of a unique solution of the IVPs (1.1).

Theorem 1.1

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

$$\left|F\left(x, Y\right) - F\left(x, Y^*\right)\right| \leq L\left|y - y^*\right| \tag{1.2}$$

Proof: see Henrici (1962).

The requirement (1.2) is known as a *Lipschitz condition*, and the constant L as a *Lipschitz constant*.

The next section discusses the basic theory of linear multistep method (LMM) which is given by Lambert (1991).

1.3 Linear Multistep Method (LMM)

In LMM, we find the approximate solution for (1.1) on the set of points $x_{n+1} = x_n + h, n = 0, 1, 2, \dots, n-1, x_0 = a$ and $x_n = b$ where h is the stepsize. The general form of LMM can be written as

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

where α_j and β_j are constants subject to the conditions $\alpha_k = 1$, $|\alpha_0| + |\beta_0| \neq 0$. The method (1.3) is explicit if $\beta_k = 0$, and is implicit if $\beta_k \neq 0$.

1.4 Block Method

The block method is a method which uses computed previous k blocks to calculate the current block where each block contains r points. The general form for r point k block was given by Ibrahim et al. (2008) as

$$\sum_{j=0}^{k} A_j y_{n+j} = h \sum_{j=0}^{k} B_j f_{n+j} \tag{1.4}$$

where A_j and B_j are r by r matrices.

The advantages of the block method are:-

- to generate solutions at several points concurrently
- able to reduce the computational time and total number of steps while maintaining the accuracy.

1.5 Convergence

It is important that an acceptable LMM generates the solution y_n should converge to the exact solution $y(x)$ as the stepsize h tends to zero. In order to ensure the method proposed converges, the method must satisfy the following theorem given by Lambert (1973, 1991).

Theorem 1.2

The necessary and sufficient conditions for a LMM to be convergent are that it be consistent and zero-stable.

Proof: see Henrici (1962).

Definition 1.1

The LMM (1.3) is said to be consistent if it has order $p \geq 1$.

Lambert (1973, 1991) states that the method (1.3) is consistent if and only if satisfies the Definition 1.2.

Definition 1.2

$$\sum_{j=0}^{k} \alpha_j = 0; \sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_j \tag{1.5}$$

and the linear difference operator L for LMM (1.3) is defined by

$$L\left[y(x);h\right] = \sum_{j=0}^{k} \left[\alpha_j y(x+jh) - h\beta_j f(x+jh)\right]. \tag{1.6}$$

Definition 1.3

The difference operator (1.6) and the associated LMM (1.3) are said to be of order p if $C_0 = C_1 = ... = C_p, C_{p+1} \neq 0$.

The general formula for C_q is as follows.

$$C_q = \left[\frac{1}{q!} \sum_{j=0}^{k} j^q \alpha_j - \frac{1}{(q-1)!} \sum_{j=0}^{k} j^{q-1} \beta_j \right] \tag{1.7}$$

where α_j and β_j are the coefficients in equation (1.3).

1.6 Stability Theory of Block Method

It is stated in Shampine and Watts (1969), the stability problem would appear to be the most serious limitation of block methods when used as a predictor-corrector type combination (Chu and Hamilton, 1987). The stability properties of the proposed method should be analysed and their relevance in solving stiff problems is demonstrated.

Definition 1.4

The LMM (1.3) is said to be zero-stable if no root of the first characteristic polynomial $\rho(t)$ has modulus greater than one, and if every root with modulus one is simple.

Definition 1.5

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 $\pi\left(r, \hat{h}\right)$ associated with the method, satisfy $|r_s| < 1$, $s = 1, 2, \ldots, k$.

Based on Dahlquist (1963), a numerical method is able to solve stiff systems if it satisfies the definitions below.

Definition 1.6

A numerical method is said to be A-stable if its region of absolute stability contains the whole of the left-hand half-plane $Re(h\lambda) < 0$.

However, Gear (1969) has given an alternative slackening of the A-stability requirement in the following definition by Lambert (1973, 1991).

Definition 1.7

A numerical method is said to be stiffly stable if

(i) its region of absolute stability contains $\Re_1$ *and* $\Re_2$ *and*

(ii) it is accurate for all $h \in \Re_2$ *when applied to the scalar test equation* $y' = \lambda y$, λ *a complex constant with* $Re(h\lambda) < 0$, *where* $\Re_1 = \{h\lambda | Re(h\lambda) < -a\}$, $\Re_2 = \{h\lambda | -a \le Re(h\lambda) \le b, -c \le Im(h\lambda) \le c\}$ *and* a, b *and* c *are positive constants.*

1.7 Stiff Problems

There is no generally accepted definition of a stiff problem but the definition given by Lambert (1973, 1991) is widely used.

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

1.8 Literature Review

Numerous researchers have proposed numerical methods for solving ODEs. The numerical methods can be categorized as one-step method and multistep method. The famous one-step method is Runge-Kutta method and as for the multistep method is Adams method.

The earliest one-step method is known as Euler's method which has been introduced by Leonhard Euler. It is not commonly used since there are several other methods that are more efficient (Rao, 2002). After a few years pass by, many researchers such as Jain et al. (1979), Chang and Gnepp (1984) and Chawla et al.

(1995) have proposed several one-step methods to improve the efficiency of the numerical method. In 2003, Majid et al. (2004) has established the 2-point block one-step method to solve non-stiff ODEs. The method uses the latest values of approximation solutions for computing the approximation solution for the next iteration. The previous iteration formulae are one order less from the next iteration formulae. This technique is called the Gauss Seidel style. Consequently, the method has given less number of steps, execution time and produced better approximation solutions. Mehrkanoon et al. (2010) has extended the method Majid et al. (2004) suggested and it is called modified 2-point implicit block one-step (M2PG) method for solving first order ODEs. In M2PG, the improvement is done at the predictor formula for the second approximate solution, whereby the predictor formula has added one frontvalue, x_{n+1} to compute the second approximate solution. Hence, this formula is one order more than the predictor formula for the first approximate solution. Consequently, the method has produced less number of steps without losing the accuracy of the solutions.

The classical approach for numerical method is computing a solution in each step. The block method is proposed to reduce the overhead of computing the solutions. Thus, this method has been used by several researchers, for example Rosser (1967), Shampine and Watts (1969) and Chu and Hamilton (1987). Fatunla (1990) has derived 1-block r point by determining the order of the method. The method will produce r solution simultaneously in a block. Voss and Abbas (1997) proposed one-step fourth-order block method with variable stepsize for solving ODEs. The method is based on the composite Simpson rule when applied in $P(EC)^1E$ mode. Even though the order of the method has increased, the error is still within the given tolerance. Ken et al. (2008), has introduced explicit and implicit r point block methods that have been derived using linear difference operator. The

Newton-Gregory backward interpolation formula is implemented using constant stepsize.
The popular multistep methods are Adams method and Backward Differentiation Formulae (BDF). The Adams method is commonly used to solve non-stiff problems. The Adams-Bashforth which is one of the families of the Adams method, is among the earliest multistep method. This method requires one-step method to calculate the backvalues just before using the method. Given in Henrici (1962), Moulton (1926) has improved the efficiency of the method by constructing Adams Moulton method. The Adams Moulton method is an implicit method while the Adams-Bashforth is an explicit method. In 1976, the work of Hull et al. (1972) is extended by Enright and Hull (1976) to test several methods that would fulfil the requirement of the desired accuracy. The methods tested are extrapolation methods, variable-order Adams methods and Runge-Kutta-Fehlberg method. The results showed that the variable-order Adams method produced the least number of function evaluation than the others. It is found that when derivative evaluations are relatively expensive, the variable-order Adams method are best (Enright and Hull, 1976). Nevertheless, there are many other methods proposed by others researchers such as Burrage (1993), Omar (1999) and Majid (2004). Majid and Suleiman (2006) have extended the work by Omar (1999) in purpose to reduce the computation costs by storing all the coefficients of the integration in their codes.

Curtiss and Hirschfelder (1952) have introduced the BDF, although at that time they have not given the name for the method (Henrici, 1962). The BDF is a method that have been widely used by Gear (1974) to solve various stiff problems. Unfortumately, the order of the formulae used in these methods must be restricted to be six at most (Sacks-Davis, 1980). To overcome these difficulties, Enright et al. (1975), Jackson and Sacks-Davis (1980), Sacks-Davis (1980) and Lebedev

(1998) have formulated a new method to improve the efficiency for solving stiff ODEs. Ibrahim (2006) has introduced Block BDF (BBDF) method for solving stiff ODEs. The implementation of the method is using Newton's two stages iteration and stored all coefficient of differentiations to save the computational time.

In addition, there are many approaches and techniques that have been proposed and implemented to enhance the efficiency of the methods. The ideas are to use all the information in the literature to improve the method and to increase the efficiency. Hence, the intention of this study is to extend the method developed by Ibrahim (2006) to variable order BBDF method for solving stiff ODEs.

1.9 Objective of the Study

The objectives of this study are

- to formulate the BBDF corrector formulae for fourth order, fifth order and sixth order BBDF method.
- to investigate the stability properties of the derived method.
- to develop the codes for all formulae using fixed stepsize and extend the method to variable order method.
- to compare the performance in terms of maximum error and computational time.
- parallelization of the fourth order BBDF method.

1.10 Planning of the Thesis

The thesis comprises the following:
In chapter 1, we briefly introduce the IVPs and definitions that can be used to solve the problems. The problem is solved using block multistep method and the convergence of the method is discussed. The definition of stiff ODEs is also mentioned in the last part of the chapter.

In Chapter 2, the formulations of the fourth order, fifth order and sixth order BBDF method are presented. This chapter also discusses the 2-point block method which means that the solutions are computed at two points concurrently and the implementation of the method is derived. Numerical results are being discussed based on the performance of the existing methods.

The stability properties of the derived methods are elaborated further in Chapter 3. The regions of the methods are plotted and discussed. We will seek the restriction on the stepsize of the method in order to achieve a user-friendly criterion, in choosing the right stepsize.

The methods are extended to variable order method in Chapter 4. The strategy of the method will be discussed further. In the chapter, the performance of the method will be compared with ode15s and ode23s in MATLAB. Parallelization of the fourth order method will be carried out in Chapter 5 to increase the efficiency of the method.

Finally, Chapter 6 will summarize the conclusion of the research and the future work will be suggested.

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