UNIVERSITI PUTRA MALAYSIA

BLOCK HYBRID METHODS FOR NUMERICAL TREATMENT OF DIFFERENTIAL EQUATIONS WITH APPLICATIONS

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IPM 2016 7

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By

YAP LEE KEN

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

August 2016

DEDICATIONS

To my beloved family and friends

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

BLOCK HYBRID METHODS FOR NUMERICAL TREATMENT OF DIFFERENTIAL EQUATIONS WITH APPLICATIONS

By

YAP LEE KEN

August 2016

Chairman : Professor Fudziah Binti Ismail, PhD
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This thesis focuses mainly on deriving block hybrid methods for solving Ordinary Differential Equations (ODEs). Block hybrid methods are the methods that generate a block of new solutions at the main and off-step points concurrently. The first part of the thesis is about the derivation of the explicit block hybrid methods based on Newton-Gregory backward difference interpolation formula for solving first order ODEs. The regions of stability are presented. The numerical results are shown in terms of total steps and accuracy.

The second part of the thesis describes the mathematical formulation of explicit and implicit one-point block hybrid methods for first order ODEs whereby the derivation involves the divided differences relative to main and off-step points. The stability properties are discussed. The explicit and implicit block hybrid methods are implemented in predictor-corrector mode of constant step size to obtain the numerical approximation for first order ODEs. The implementation of block hybrid methods in variable step size is also presented. Some numerical examples are given to illustrate the efficiency of the methods.

The one-point block hybrid methods are then implemented for numerical solution of first order delay differential equations (DDEs). The Q-stability of the methods is investigated. Since the block hybrid methods include the approximate solution at both the main and additional off-steps points, more computed values that surrounding the delay term can be used to provide a better estimation in interpolating the delay term.

The third part of the thesis is mainly focused on block hybrid collocation methods for obtaining direct solution of second-, third- and fourth-order ODEs. The derivation involves interpolation and collocation of the basic polynomial. The stability properties are investigated. Illustrative examples are presented to demonstrate the efficiency of the methods. The block hybrid collocation methods are also applied to solve the physical problems such as Lane-Emden equation, Van Der Pol oscillator, Fermi-Pasta-Ulam problem, the nonlinear Genesio equation, the problem in thin film flow and the fourth order problem

from ship dynamics.

As a whole, the block hybrid methods for solving different orders of ordinary differential equations have been presented. The illustrative examples demonstrate the accuracy advantage of the block hybrid methods.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

KAEDAH BLOK HIBRID UNTUK RAWATAN BERANGKA PERSAMAAN PEMBEZAAN DENGAN APLIKASI

Oleh

YAP LEE KEN

Ogos 2016

Pengerusi : Professor Fudziah Binti Ismail, PhD
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Tumpuan utama tesis ini adalah untuk menerbitkan kaedah blok hibrid untuk menyelesaikan Persamaan Pembezaan Biasa (PBB). Kaedah blok hibrid adalah kaedah yang menghasilkan satu blok penyelesaian baru di titik utama dan titik separa secara serentak. Bahagian pertama tesis ini adalah mengenai terbitan kaedah blok hibrid tak tersirat berdasarkan rumus interpolasi beza ke belakang Newton-Gregory untuk menyelesaikan PBB peringkat pertama. Rantau kestabilan dipersembahkan. Keputusan berangka ditunjukkan dari segi jumlah langkah dan kejituan.

Bahagian kedua menerangkan rumus matematik kaedah blok hibrid satu-titik tak tersirat dan tersirat untuk PBB peringkat pertama di mana terbitan melibatkan beza bahagi yang relatif kepada titik utama dan titik separa. Ciri kestabilan dibincangkan. Kaedah blok hibrid tak tersirat dan tersirat dilaksanakan dalam mod peramal-pembetul dengan saiz langkah malar untuk mendapatkan penghampiran berangka bagi PBB peringkat pertama. Pelaksanaan kaedah blok hibrid dalam panjang langkah berubah juga dipersembahkan. Beberapa contoh berangka diberi untuk menunjukkan keberkesanan kaedah tersebut.

Kaedah blok hibrid satu-titik tersebut dilaksanakan untuk penyelesaian berangka Persamaan Pembezaan Lengah (PBL) peringkat pertama. Kestabilan-Q kaedah tersebut dikaji. Kaedah blok hibrid melibatkan penyelesaian anggaran untuk kedua-dua titik utama dan titik separa, lebih banyak nilai-nilai yang dikira sekitar sebutan lengah boleh digunakan untuk memberikan anggaran yang lebih baik dalam interpolasi sebutan lengah.

Bahagian ketiga tesis memberi tumpuan utama kepada kaedah blok hibrid kolokasi untuk penyelesaian PBB peringkat kedua, ketiga dan keempat secara langsung. Penerbitan melibatkan interpolasi dan kolokasi daripada polinomial asas. Ciri kestabilan kaedah dikaji. Contoh-contoh ilustrasi dipersembahkan untuk menunjukkan kecekapan kaedah. Kaedah blok hibrid kolokasi juga digunakan untuk menyelesaikan masalah fizikal seperti persamaan Lane-Emden, pengayun Van Der Pol, masalah Fermi-Pasta-Ulam, persamaan tidak linear Genesio, masalah dalam aliran filem nipis dan masalah peringkat keempat dari dinamik kapal.

Secara keseluruhannya, kaedah blok hibrid untuk menyelesaikan persamaan pembezaan biasa pada peringkat yang berbeza telah dipersembahkan. Contoh-contoh ilustrasi menunjukkan kelebihan kejituan kaedah blok hibrid.

ACKNOWLEDGEMENTS

First and foremost, I would like to show my deepest appreciation and gratitude to the Chairman of the Supervisory Committee, Professor Dr. Fudziah Binti Ismail for her invaluable assistance, advice and guidance throughout the duration of the studies. I also wish to express my sincere thank to Yang Berbahagia Professor Dato Dr. Mohamed Bin Suleiman, Professor Dr. Mohamed Bin Othman and Dr. Norazak Senu for their guidance and assistance.

Great appreciation goes to my beloved family especially my parents for their unconditional love, support and understanding throughout the course of my research. Last but not least, special thanks to all my friends and also colleagues from Universiti Tunku Abdul Rahman who kindly provided valuable and helpful comments during my studies.

I certify that a Thesis Examination Committee has met on 22 August 2016 to conduct the final examination of Yap Lee Ken on her thesis entitled "Block Hybrid Methods for Numerical Treatment of Differential Equations with Applications" 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 Doctor of Philosophy.

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LIST OF ABBREVIATIONS

DDEs	Delay Differential Equations
IVPs	Initial Value Problems
ODEs	Ordinary Differential Equations
NDDEs	Neutral delay differential equations
RDDEs	Retarded delay differential equations
E1PB	Explicit 1-point with 1 off-step point block method
E2PB	Explicit 2-point with 2 off-step points block method
E3PB	Explicit 3-point with 3 off-step points block method
I1PO3	Implicit 1-point block hybrid method of order three
I1PO4	Implicit 1-point block hybrid method of order four
I1PO5	Implicit 1-point block hybrid method of order five
BHCM2	Block hybrid collocation method for second order ODEs
BHCM3	Block hybrid collocation method for third order ODEs
BHCM4	Block hybrid collocation method for fourth order ODEs

CHAPTER 1

INTRODUCTION TO NUMERICAL ORDINARY AND DELAY DIFFERENTIAL EQUATIONS

Ordinary differential equations (ODEs) are equations that involve an unknown function with independent variable and one or more of its derivatives. ODEs arise in many contexts of engineering and science such as fluid dynamics, radioactive decay and population growth. Many theoretical and numerical studies for such equations have appeared in the literature. The analytical way of solving ODEs is via application of integration technique. However, it is difficult or impossible to determine the anti-derivatives for most of the realistic systems of ODEs. Thus, numerical methods for ODEs have attracted considerable attention.

1.1 Numerical Methods for ODEs

Here, we consider the nth order ordinary differential equations

$$y^{(n)} = f(x, y, \ldots, y^{(n-1)}), \quad \text{where } n = 1, 2, 3, 4 \tag{1.1}$$

with initial conditions

$$y(a) = y_0 \text{ and } y^{(i)}(a) = \eta_i, \quad 0 < i < n-1, \quad x \in [a, b].$$

In first order ODEs, the quantity being differentiated, y is named as the dependent variable, while the quantity with respect to which y is differentiated, x is named as independent variable.

The following standard theorem asserts the sufficient conditions for a unique solution to exist. We shall assume that the hypotheses of this theorem are satisfied.

Theorem 1.1 :(Existence and Uniqueness)
Let $f(x,y)$ be defined and continuous for all points (x,y) in the region D defined by $a \leq x \leq b$, $-\infty < y < \infty$, where a and b are finite, and let there exists a constant L such that for any $x \in [a,b]$ and any two numbers y and y^*,

$$|f(x,y) - f(x,y^*)| \leq L|y - y^*|.$$

This condition is known as Lipschitz condition. Then there exists exactly one function $y(x)$ with the following three properties:

i. $y(x)$ *is continuous and differentiable for* $x \in [a,b]$,
ii. $y' = f(x, y(x))$, $x \in [a,b]$,
iii. $y(a) = \eta$.

The proof is given by Henrici (1962).

Basically, the numerical methods for ODEs are classified as one-step method and multistep method. One-step method requires the information from only one previous point, x_n to find the approximation at the mesh point, x_{n+1}. On the other hand, multistep method requires the usage of information from more than one previous points to find the next approximation.

In general, the linear k-step method for first order ODEs can be written as

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \tag{1.2}$$

where α_j and β_j are constants with the conditions $\alpha_k \neq 0$ and $|\alpha_0| + |\beta_0| > 0$. Since (1.2) can be multiplied by the same constant without altering the relationship, the coefficient α_j and β_j are arbitrary to the extent of a constant multiplier. This arbitrariness has been removed by assuming that $\alpha_k = 1$. Method (1.2) is explicit if $\beta_k = 0$ and implicit if $\beta_k \neq 0$.

According to Lambert (1973), hybrid method is the modified linear multistep method which incorporate the function evaluation at off-step point. It retaining certain characteristic of linear multistep method whilst it has the property in utilizing data at off-step points besides the standard step points.

Following Lambert (1973), the k-step hybrid method for first order ODEs can be defined as

$$\sum_{j=0}^{k} \alpha_j y_{n+j} + \sum_{j=1}^{k} \alpha_{\nu_j} y_{n+\nu_j} = h \left(\sum_{j=0}^{k} \beta_j f_{n+j} + \sum_{j=1}^{k} \beta_{\nu_j} f_{n+\nu_j} \right) \tag{1.3}$$

where α_0 and β_0 are not both zero, $\alpha_k = 1$ and ν_j is not integer.

Definition 1.1 : *[See Lambert (1973)]*
The linear difference operator L associated with the hybrid method (1.3) is defined by

$$L[y(x);h] = \sum_{j=0}^{k} \left[\alpha_j y(x+jh) - h\beta_j y'(x+jh) \right] + \sum_{j=1}^{k} [\alpha_{\nu_j} y(x+\nu_j h) - h\beta_{\nu_j} y'(x+\nu_j h)] \tag{1.4}$$

where $y(x)$ is an arbitrary function that is sufficiently differentiable on $[a,b]$. Expanding the test function and its first derivative as Taylor series about x and collecting the terms to obtain

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

where the coefficients C_q are constants independent of $y(x)$. In particular,

$$\begin{aligned}
C_0 &= \sum_{j=0}^{k} \alpha_j + \sum_{j=1}^{k} \alpha_{v_j} \\
C_1 &= \sum_{j=1}^{k} j\alpha_j + \sum_{j=1}^{k} v_j \alpha_{v_j} - \left(\sum_{j=0}^{k} \beta_j + \sum_{j=1}^{k} \beta_{v_j} \right) \\
C_2 &= \frac{1}{2!} \left[\sum_{j=1}^{k} j^2 \alpha_j + \sum_{j=1}^{k} v_j^2 \alpha_{v_j} - 2 \left(\sum_{j=1}^{k} j\beta_j + \sum_{j=1}^{k} v_j \beta_{v_j} \right) \right] \\
&\vdots \\
C_q &= \frac{1}{q!} \left[\sum_{j=1}^{k} j^q \alpha_j + \sum_{j=1}^{k} v_j^q \alpha_{v_j} - q \left(\sum_{j=1}^{k} j^{q-1} \beta_j + \sum_{j=1}^{k} v_j^{q-1} \beta_{v_j} \right) \right].
\end{aligned}$$

Definition 1.2 :
The hybrid method (1.3) and the associated linear difference operator defined by (1.4) are said to be of order p if

$$C_0 = C_1 = C_2 = \ldots = C_p = 0 \text{ and } C_{p+1} \neq 0.$$

The first non-vanishing coefficient, C_{p+1}, is called the error constant.

Definition 1.3 :
The hybrid method (1.3) is said to be consistent if it has order at least one. It follows that the method (1.3) is consistent if and only if

$$\sum_{j=0}^{k} \alpha_j + \sum_{j=1}^{k} \alpha_{v_j} = 0 \tag{1.5}$$

and

$$\sum_{j=1}^{k} j\alpha_j + \sum_{j=1}^{k} v_j \alpha_{v_j} = \sum_{j=0}^{k} \beta_j + \sum_{j=1}^{k} \beta_{v_j}. \tag{1.6}$$

The first and second characteristic polynomials of the hybrid method (1.3) are defined as follows

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j + \sum_{j=1}^{k} \alpha_{v_j} \xi^{v_j}$$

$$\sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j + \sum_{j=1}^{k} \beta_{v_j} \xi^{v_j}.$$

It follows from (1.5) and (1.6) that the hybrid method is consistent if and only if

$$\rho(1) = 0 \ \text{ and } \ \rho'(1) = \sigma(1).$$

Thus, the first characteristic polynomial $\rho(\xi)$ always has a root at one for a consistent method. The root is named as principal root and labelled as ξ_1. The remaining roots, ξ_s, $s = 2, 3, \ldots k$ are known as spurious roots.

Definition 1.4 :
The hybrid method (1.3) is said to be zero-stable if no root of the first characteristic polynomial $\rho(\xi)$ has modulus greater than one, and if every root with modulus one is simple.

Detailed in Lambert (1973).

Theorem 1.2 :
The necessary and sufficient conditions for a method to be convergent are that it be consistent and zero-stable.

The proof of the theorem can be found in Butcher (1966).

Definition 1.5 :
The hybrid method is said to be absolutely stable for a given $\overline{h}$ if all roots ξ_s of stability polynomial, $\Pi(\xi, \overline{h}) = \rho(\xi) - h\sigma(\xi) = 0$, where $\overline{h} = h\lambda$ satisfy $|\xi_s| < 1$, $s = 1, 2, \ldots, k$, and to be absolutely unstable otherwise. The region of absolute stability consists of all $\overline{h}$ in the complex plane for which the method is absolutely stable.

1.2 Delay Differential Equations

Most of the numerical methods for solving first order initial value problems (IVPs) are adapted to solve delay differential equations (DDEs). From mathematical point of view, DDEs are similar to ODEs except that DDEs involve the past values of the dependent variable and derivatives. DDEs arise in many area of mathematical modelling such as infectious diseases, population dynamics and driver reaction time. In general, DDEs can be classified as retarded and neutral delay differential equations.

Retarded delay differential equations (RDDEs) are the ODEs that involve the solution of the delay terms given by

$$\begin{aligned} y'(x) &= f(x, y(x), y(x - \tau_1(x, y(x))), y(x - \tau_2(x, y(x))), \ldots, \\ &\qquad y(x - \tau_\nu(x, y(x)))) \qquad \text{for } \ x > x_0 \\ y(x) &= \varphi(x) \qquad \text{for } \ x \leq x_0 \end{aligned} \tag{1.7}$$

where y, f and φ are N-vector functions and τ_i for $i = 1, 2, \dots \nu$ are scalar functions that represent the delay. If the delay is a constant, we call it a constant delay. If the delay is a function of time x only, it is called a time dependent delay. If the delay is a function of time x and the solution $y(x)$, it is called the state dependent delay. A delay argument that passes the current time, $(x - \tau(x, y(x))) > x$, is called an advanced delay.

Neutral delay differential equations (NDDEs) are the ODEs that involve both the solution and the derivative of the delay terms as follows

$$\begin{aligned} y'(x) = f(x, y(x), y(x - \tau_1(x, y(x))), y(x - \tau_2(x, y(x))), \dots, y(x - \tau_\nu(x, y(x))), \\ y'(x - \tau_{\nu+1}(x, y(x))), \dots y'(x - \tau_{\nu+\omega}(x, y(x)))) \qquad \text{for } x \geq x_0 \\ y(x) = \varphi(x), \quad y'(x) = \varphi'(x) \qquad \text{for } x \leq x_0 \end{aligned}$$

where y, f, φ and φ' are N-vector functions and τ_i for $i = 1, 2, \dots \nu + \omega$ are scalar functions.

1.3 Problem Statement

It is possible to solve the first order ODEs (1.1) by applying various multistep methods in the literature, the numerical methods consist of the main and off-step points can be derived via numerical integration using divided differences. These approaches should provide significant improvement in accuracy.

We consider the simple RDDEs (1.7) with single delay term. The conventional approach for solving RDDEs is to adapt the standard ODEs solver and incorporates the interpolation technique. One of the major difficulties is the severe limitation of the points that surrounding the delay argument for interpolation. Hence, larger interpolation errors occur and affect the accuracy. With the inclusion of off-step points in the block hybrid methods, we aim to improve the accuracy.

The conventional multistep methods for direct solution of higher order ODEs (1.1) require the subroutine to provide the starting values. It lead to complicated computational work. Here, we propose the block hybrid collocation methods which can be implemented as self-starting methods for solving higher order ODEs (1.1) directly. These approaches should provide significant improvement in accuracy and decrease in computational work.

1.4 Objective of the Studies

The main objective of the research is to derive the block hybrid methods for solving ordinary differential equations. The implementation of block hybrid methods are expected to generate the approximation of y at both the main and off-step points simultaneously. These approaches should provide significant improvement in accuracy. The objective of the thesis can be accomplished by:

1. deriving the explicit block hybrid methods for first order ODEs based on Newton-Gregory backward difference interpolation formula.

2. deriving the implicit block hybrid methods for first order ODEs based on divided differences that incorporate the main and off-step points and implementing in constant step size and also variable step size.

3. adapting the implicit block hybrid methods for the numerical treatment of first order DDEs.

4. deriving the block hybrid collocation methods for second-, third- and fourth-order ODEs via interpolation and collocation of the basic polynomial.

5. investigating the stability properties of the methods.

6. comparing the performances of the newly proposed methods with the existing methods.

7. applying the newly proposed methods to solve physical problems.

1.5 Outline of the Thesis

The brief description for the organization of the thesis will be provided here. Chapter 1 discusses the brief overview of ODEs and DDEs. The theories and definitions that are related to the proposed methods are provided.

Chapter 2 reviews some of the previous works on the numerical solutions of ODEs and DDEs. In Chapter 3, the formulation of explicit block hybrid methods based on Newton backward difference formula is provided. The newly proposed methods include explicit 1-point with 1 off step point method, 2-point with 2 off-step points method and 3-point with 3 off-step points method.

Chapter 4 comprises the implicit block hybrid methods of order three, four and five for first order ODEs. The derivation of the methods is based on the divided difference relative to main and off-step points. The stability of the these methods is also discussed in this chapter. The implementation of the implicit block hybrid methods for first order ODEs using constant step size and the numerical treatment using variable step size technique are presented. Chapter 5 is concerned with the application of implicit block hybrid methods for the solution of first order retarded DDEs. The analysis of the Q-stability for one-point block hybrid methods is presented.

Chapters 6, 7 and 8 deal with the block hybrid collocation method for higher order ODEs. The derivation involves the interpolation and collocation of basic polynomial. Chapter 6 focuses on the five point block hybrid collocation method for direct solution of second order ODEs. In Chapter 7, the three point block hybrid collocation method with two off-step points for solving third order ODEs directly is discussed. The four point block hybrid collocation method with three off-step points for fourth order ODEs is developed and presented in Chapter 8. The applications of these block hybrid methods for solving some well-known physical problems are shown.

Finally, Chapter 9 summarizes the thesis. Future work is also recommended.

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