UNIVERSITI PUTRA MALAYSIA

DIRECT METHODS VIA MULTIPLE SHOOTING TECHNIQUE FOR SOLVING BOUNDARY VALUE PROBLEMS

PHANG PEI SEE

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By

Phang Pei See

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

May 2015

DEDICATIONS

To

The Dear Teachers

And

My Beloved Family

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

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By

PHANG PEI SEE

MAY 2015

Chair: Zanariah Abdul Majid, Ph.D.

Faculty: Science

In this thesis, nonlinear two-point second order boundary value problems (BVPs) are solved using the one-point, two-point block and three-point block direct method. Subsequently, the two-point direct block method is extended to solve third order BVPs. It also elaborates on the computational complexity, stability analysis, consistency, convergent and the order of the methods.

Multiple shooting technique via the three-step iterative method is implemented in order to solve the BVPs. This approach can avoid the sensitive BVPs when choosing the wrong initial guessing value and converge faster compared to the existing method. Variable step size strategy is adapted for solving second order and third order BVPs respectively. Furthermore the variable step size and order strategy is developed to solve second order BVPs directly. Besides that, a two-point direct block method is proposed to solve three applications of BVPs in fluid dynamics. These applications

are modelled as third order BVPs and system with combination of third and second order BVPs.

Numerical results showed that the performance of the developed methods can obtain better results in terms of maximum error, total step, total function calls and execution time when compared to existing method. In conclusion, the proposed direct block methods in this thesis are appropriate for solving second order and third order nonlinear boundary value problem.

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

KAEDAH TERUS MELALUI TEKNIK PENEMBAKAN BERBILANG UNTUK MENYELESAIKAN MASALAH NILAI SEMPADAN

Oleh

PHANG PEI SEE

MAY 2015

Pengerusi: Zanariah Abdul Majid, Ph.D.

Fakulti: Sains

Dalam tesis ini, masalah nilai sempadan (MNS) dua titik tak linear akan diselesaikan oleh kaedah terus satu-titik, blok dua-titik dan blok tiga-titik. Seterusnya, kaedah terus blok dua-titik dilanjutkan untuk menyelesaikan MNS peringkat ketiga. ia juga menghuraikan tentang kerumitan pengiraan, analisis kestabilan, konsistensi, penumpuan dan peringkat untuk kaedah.

Teknik penembakan berbilang melalui kaedah tiga langkah lelaran dilaksanakan untuk menyelesaikan MNS. Pendekatan ini boleh mengelakkan MNS yang sensitif apabila memilih nilai tekaan yang salah telah dilakukan dan membolehkan penumpuan yang lebih cepat berbanding dengan kaedah yang sedia ada. Strategi saiz langkah berubah digunakan untuk menyelesaikan peringkat kedua dan ketiga MNS masing-masing. Tambahan pula strategi saiz langkah dan peringkat berubah dibangunkan untuk menyelesaikan MNS peringkat kedua secara langsung. Selain itu, kaedah terus dua-titik blok dicadangkan untuk menyelesaikan tiga aplikasi MNS dalam dinamik

bendalir. Applikasi ini dimodelkan sebagai MNS berperingkat tiga dan sistem gabungan MNS peringkat dua dan tiga.

Hasil berangka menunjukkan bahawa prestasi kaedah yang dibangunkan boleh mendapatkan keputusan yang lebih baik dari segi ralat maksimum, jumlah langkah, jumlah fungsi panggilan dan masa pelaksanaan. Kesimpulannya, kaedah blok terus yang dicadangkan dalam tesis ini adalah sesuai untuk menyelesaikan peringkat kedua dan ketiga masalah nilai sempadan tak linear .

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I certify that a Thesis Examination Committee has met on **18 May 2015** to conduct the final examination of **Phang Pei See** on her thesis entitled "**Direct Methods Via Multiple Shooting Technique For Solving Boundary 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 **Degree of Doctor of Philosophy**.

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Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Chairperson)

Norihan bt Md Arifin, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Leong Wah June, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Siraj-Ul-Islam, PhD
Professor
Department of Basic Science
University of Engineering and Technology
Pakistan
(External Examiner)

This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy. The members of the Supervisory Committee were as follows:

Zanariah Abdul Majid, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Chairperson)

Fudziah Ismail, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

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Khairil Iskandar Bin Othman, PhD
Associate Professor
Universiti Teknologi Mara
(Member)

NORITAH OMAR, PhD
Associate Professor and Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date:

BUJANG BIN KIM HUAT, PhD
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date:

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This is to confirm that:
- the research conducted and the writing of this thesis was under the supervision;
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Name of
Chairman of
Supervisory
Committee: ____________________

Signature: ____________________
Name of
Member of
Supervisory
Committee: ____________________

Signature: ____________________
Name of
Member of
Supervisory
Committee: ____________________

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LIST OF ABBREVIATIONS

BVPs:	Boundary Value Problems
IVPs:	Initial Value Problems
ODEs:	Ordinary Differential Equations
VS:	Variable step size strategy
VSVO:	Variable step size and order strategy
bvp4c :	Matlab solver with fourth order collocation method.
bvp5c :	Matlab solver with fifth order collocation method.
mshoot:	Mathematica solver with shooting method.
dsolve :	Maple solver with numeric for bvp.
NLBVS :	One-point direct block method with multiple shooting technique using variable step size strategy.
2PNLBVS :	Two-point direct block method with multiple shooting technique using variable step size strategy.
3PNLBVS:	Three-point direct block method with multiple shooting technique using variable step size strategy.
2PNLBVSVO:	Two-point direct block method with multiple shooting technique using variable step size and order strategy.
2P3BVS :	Two-point direct block method to solve third order boundary value problem with variable step size strategy.

CHAPTER 1

INTRODUCTION

1.1 Introduction

In engineering and the physical sciences, problems in heat transfer equation and boundary layer equation that are modelled as boundary value problems (BVPs), are often encountered. Therefore, various studies have been done to find solutions for the BVPs. In the case where the BVPs are linear, the analytic solution can be obtained and solved using the analytic method. Unfortunately, most of the real world problems are modelled as nonlinear BVPs. In this case, it is impossible to identify analytic solutions to these problems. Even if the analytic solutions do exist, the evaluation involves a tedious process; thus, triggering rigorous studies in determining the approximate solutions of the BVPs to be carried out in recent years.

Since there is a high demand to improve the performance of the methods used to solve the BVPs numerically,the development of a quick method is essential in this research area. Many numerical methods have been developed such as the finite different method, collocation method and initial value method to solve BVPs numerically. The most popular of the initial value method is to solve BVPs indirectly by reducing the higher order differential equation to the first order equation system. This approach is easy to implement, but it will enlarge the equation system and make the process more costly. In this research, a more efficient method that can solve the higher order BVPs directly is developed. The higher order BVPs will be treated as the original form without being reduced to the system of first order the equation. The initial value method developed in this research is a multistep method which is called the block method. The block method has an advantage as it can approximate more than one solution in a single step.

The selection of the step size to solve BVPs by the numerical method is important in obtaining more accurate and efficient results. Smaller step sizes will produce a more accurate result, but it lengthens the execution time. Most existing research for solving BVPs use constant step size; however, this research implements the use of the variable step size strategy and the variable step size and order strategy. These strategies assure the accuracy and efficiency of the proposed code.

The shooting technique is required to transform the boundary condition to the initial condition with generate the guessing value. This research implemented the multiple shooting techniques and replace the root finding method from the Newton method with the three-step iterative method in order to achieve a faster convergent.

The problem in fluid dynamic is often modelled as the system of combination for the second and third order of the BVPs. When using the existing BVPs solver, many researchers face the difficulty to obtain the second solution when the dual solution exists. Researchers are required to test various initial guessing values to obtain the second solution. This research presents a code which is a combination of the second and third order BVPs adapted with multiple shooting technique via a three-step iterative method. The advantage of the proposed code is that with two initial guessing values, the researcher can obtain both the first and second solutions for a problem.

1.2 Objectives of the Thesis

The main objective of this thesis is to develop one-point and block direct method adapted with multiple shooting technique via a three-step iterative method to solve non-linear two-point BVPs. The objectives can be accomplished by:

1. deriving one-point direct method and implementing the method to solve second order BVPs using the variable step size strategy;
2. deriving two-point and three-point direct block methods and implementing these methods to solve the second order of BVPs using the variable step size strategy;
3. deriving two-point direct block method of different orders and implementing the method to solve the second order of BVPs using the variable step size and

order strategy;

4. deriving two-point direct block method and implementing the method for solving the third order of BVPs using the variable step size strategy; and

5. developing an algorithm which consists of a combination of the second and third order BVPs, and implementing the algorithm to solve the applications of BVPs in fluid dynamic.

1.3 Motivation and Contribution of the Thesis

Boundary value problem has wide application therefore much attention has been paid on finding the solution of the BVPs. Along with the development of computer technology, the usage of numerical methods has been popularized and there are a large number of numerical methods available to be utilized in solving the BVPs. Famous example are the collocation method which is the based algorithm in bvp4c, bvp5c and COLNEW codes. The limitation of these codes are the collocation method cannot solve the BVPs directly, therefore these solvers are expensive in term of execution time. This is the motivation of this study to developed new codes which can solve the BVPs directly. It is worth to mention that most of the available BVP solvers is implement adapted with simple shooting technique. For example the matlab solver, dsolve and the mathematica solver, mshoot are based on the simple shooting technique. Unfortunately, simple shooting technique may fail to converge when there is a sensitive BVPs or a bad initial guessing value was chosen. Therefore, multiple shooting technique has been used in this research. Besides that, to improve the efficiency for solving the BVPs, the block method was chosen. This is because the block method can solve the higher order BVPs directly and approximated the solutions more than one points. It is not surprising that the block method has been used to solve the BVPs by others researches. So far, all the block method to solve the BVPs is implement with the constant step size. The contribution of this research is to develop new algorithms of direct block method for solving second and third order BVPs with variable step size (VS) and variable step size and order (VSVO) strategy.

1.4 Scope of the Thesis

This thesis concentrates on the development of new algorithms to solve the second order and third order of the boundary value problems (BVPs) directly. Three numerical methods, i.e. the one-point direct method, the two-point direct block method and the three-point direct block method will be derived and discussed in this thesis. The properties of this method will be analysed in terms of order, consistence, convergence, zero-stable and computational complexity. These methods are adapted with the multiple shooting technique via the three-step iterative method to solve the second order and third order of the BVPs. Two strategies implemented in this thesis are variable step size strategy, and variable step size and order strategy. The application problems of BVPs in fluid dynamic will be solved.

1.5 Boundary Value Problem

Boundary value problems (BVPs) are defined as differential equations subject to a set of additional restrictions on boundaries, which are known as boundary conditions. One of the subdivisions of BVPs is between linear and non-linear problems, dependent on the type of function in the differential equation consisting of BVPs. The n^{th}-order BVPs is linear if the differential equation is as follows:

$$y^{(n)} = P_n(x)y^{(n-1)} + ... + P_3(x)y'' + P_2(x)y' + P_1(x)y + R(x),$$

where $R(x), P_1(x), P_2(x), ..., P_n(x)$ are functions of x or constants.
The n^{th}-order nonlinear BVPs consists of the differential equation as follows:

$$y^{(n)} = f(x, y, y', y'', ..., y^{n-1}).$$

In this research, second and third order nonlinear BVPs are the focus.
The general second order two-point nonlinear BVPs are as follows:

$$y'' = f(x, y, y'), \quad a \leq x \leq b, \tag{1.1}$$

subject to the three common type of boundary conditions:

1. Dirichlet boundary condition: all conditions for the primary dependent variable
$$y(a) = \alpha, \quad y(b) = \beta, \tag{1.2}$$
where a, b, α and β are constants.

2. Neumann boundary condition: all conditions for the derivative of the primary dependent variable
$$y'(a) = \alpha, \quad y'(b) = \beta, \tag{1.3}$$
where a, b, α and β are constants.

3. Mixed boundary condition:
$$c_1 y + c_2 y'(a) = \alpha, \quad c_3 y + c_4 y'(b) = \beta, \tag{1.4}$$
where a, b, α and β are constants; and c_1, c_2, c_3 and c_4 are simple function of x or constants.

The general third order nonlinear BVPs are as follows:
$$y''' = f(x, y, y', y''), \quad a \leq x \leq b, \tag{1.5}$$
subject to various boundary conditions. Below are a list of some boundary conditions for third order BVPs:

1. Type I boundary condition:
$$y(a) = \alpha, \quad y'(a) = \gamma, \quad y(b) = \beta. \tag{1.6}$$

2. Type II boundary condition:
$$y(a) = \alpha, \quad y'(a) = \gamma, \quad y'(b) = \beta. \tag{1.7}$$

3. Type III boundary condition:

$$y(a) = \alpha, \quad y''(a) = \gamma, \quad y(b) = \beta. \tag{1.8}$$

In this research, the Dirichlet and Neumann type second order BVPs will be focused. For third order BVPs of type I, II and type III boundary conditions will be covered . The solution to the BVPs is a solution to the differential equation which also satisfies the boundary conditions. The following theorem gives the general conditions to ensure that the solution to a n^{th}-order BVPs exists and unique.

Theorem 1.1 *(Existence and Uniqueness, Edwards et al. (2008))*
Suppose the function, $f(x, y, y', y'', ..., y^{(n)})$ in the BVPs is continuous on the set,

$$D = \{(x, y, y', y'', ..., y^{(n)}) | a \leq x \leq b, -\infty < y, y', y'', ..., y^{(n)} < \infty\}.$$

The BVPs have a unique solution when the following properties have been fulfilled:

i) $f(x, y, y', y'', ..., y^{(n)}) \in D$ *is continuous function.*
ii) $f(x, y, y', y'', ..., y^{(n)}), f_x(x, y, y', y'', ..., y^{(n)}), f_y(x, y, y', y'', ..., y^{(n)}),$
$f_{y'}(x, y, y', y'', ..., y^{(n)}), ..., f_{y^{(n)}}(x, y, y', y'', ..., y^{(n)})$ *are bounded.*
iii) $f(x, y, y', y'', ..., y^{(n)}) > 0$ *on* $[a, b] \in D$.

1.6 Preliminary Concepts

In this section, the preliminary concepts to be used throughout this thesis are established. The general initial value methods for solving BVPs may be categorized as either a single step or multistep method. The single step method is a self-starting method, as only one back value is needed, such as the Euler and Runge-Kutta method. The multistep method uses more than one back value to determine the next mesh point. Generally, the one-step method will be employed to obtain these initial values. The initial value methods developed in this thesis are direct method of Adams type, which is a subfamily of the linear multistep method (LMM). Lambert (1991) and Fatunla (1991) stated the following definitions of LMM. The general form of the k step LMM may written as follows:

$$\begin{aligned}\sum_{j=0}^{k}\alpha_{v_j}y_{n+v_j} &= h\sum_{j=0}^{k}\beta_{v_j}y'_{n+v_j}+h^2\sum_{j=0}^{k}\gamma_{v_j}y''_{n+v_j}+...+h^d\sum_{j=0}^{k}\delta_{v_j}f_{n+v_j},\\ j &= 0,1,...,k,v_j=\sum_{i=0}^{j}r_i,\end{aligned}$$

where α_j, β_j, γ_j and δ_j are constants, r_j is the ratio of the step size and assume that $\alpha_k \neq 0$. The linear operator L associated with the LMM is defined by the following:

$$\begin{aligned}L[y(x);h] &= \sum_{j=0}^{k}[\alpha_{v_j}y(x+v_jh)-h\beta_{v_j}y'(x+v_jh)-\\ &\quad h^2\gamma_{v_j}y''(x+v_jh)-...-h^n\theta_{v_j}y^{(n)}(x+v_jh)],\\ j &= 0,1,...,k,v_j=\sum_{i=0}^{j}r_i,\end{aligned} \tag{1.9}$$

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

To determine the order of the method, the term in Eq. (2.9) is expanded using Taylor polynomials as follows:

$$L[y(x);h]=C_0y(x)+C_1hy^{(1)}(x)+...+C_ph^py^{(p)}(x)+\cdots, \tag{1.10}$$

where $C_0,C_1,...,C_p$ are constants satisfying:

$$
\begin{aligned}
C_0 &= \sum_{j=0}^{k} \alpha_{v_j} \\
C_1 &= \sum_{j=0}^{k} v_j \alpha_{v_j} + \sum_{j=0}^{k} \beta_{v_j} \\
C_2 &= \sum_{j=0}^{k} \frac{v_j^2}{2} \alpha_{v_j} + \sum_{j=0}^{k} v_j \beta_{v_j} + \sum_{j=0}^{k} \gamma_{v_j} \\
C_3 &= \sum_{j=0}^{k} \frac{v_j^3}{3!} \alpha_{v_j} + \sum_{j=0}^{k} \frac{v_j^2}{2} \beta_{v_j} + \sum_{j=0}^{k} v_j \gamma_{v_j} + \sum_{j=0}^{k} \sigma_{v_j} \\
&\vdots \\
C_p &= \sum_{j=0}^{k} \frac{v_j^p}{p!} \alpha_{v_j} + \sum_{j=0}^{k} \frac{v_j^{p-1}}{(p-1)!} \beta_{v_j} + \sum_{j=0}^{k} \frac{{v_j}^{p-2}}{(p-2)!} \gamma_{v_j} + \sum_{j=0}^{k} \frac{{v_j}^{p-3}}{(p-3)!} \sigma_{v_j},
\end{aligned}
\tag{1.11}
$$

where $j = 0, 1, ..., k, v_j = \sum\limits_{i=0}^{j} r_i,\ p = 4, 5, 6, ...$

Definition 1.6.1 The LMM is order of p if $C_0 = C_1 = ... = C_{p+r-1} = 0$ and $C_{p+r} \neq 0$ where r is the order of the equation.

Definition 1.6.2 The LMM is of order p is said to have error constant C_{p+r} where r is the order of the equation.

Definition 1.6.3 The LMM is zero stable provided the roots $R_j, j = 0(1)k$ of the first characteristic polynomial $\rho(R)$ specified as $\rho(R) = \det \left[\sum_{i=0}^{k} A^{(i)} R^{k-i}\right] = 0$, satisfy $|R_j| \leq 1$ and the multiciplicity for the $|R_j| = 1$ must not exceed the order of the equation.

Definition 1.6.4 The LMM is said to be consistent if it has order greater or equal to 1, $(p \geq 1)$.

Definition 1.6.5 The LMM is said to be convergent if it is consistent and zero stable.

1.7 Predictor-Corrector Method

A predictor-corrector method involves a combination of an explicit and implicit methods. When β_0, γ_0 and δ_0 for a k-step method in the Eq.(2.4) is zero, the method is called an explicit method. Meanwhile, when the values of β_0, γ_0, and δ_0 are not equal to 0, the method is implicit. The explicit method is called as the predictor and the implicit method is called the corrector. This is because the explicit method is used to predict the approximate solution, y at point x, while the implicit method is used to improve the accuracy of the solution, y at point x. Usually, the corrector method used is more accurately than the predictor method. In this thesis, the corrector formulae is one order higher than the predictor.
The predictor-corrector scheme use in this thesis is $PE(CE)^t$, which involves iteration to convergence as follows:
P: Evaluate the approximate solution, $y_{k+1}^{(0)}$ using predictor formulae.
E: Evaluate the function.
C: Evaluate the approximate solution, $y_{k+1}^{(1)}$ using corrector formulae.
E: Evaluate the function.
If $|y_{k+1}^{(t)} - y_{k+1}^{(t-1)}| > TOL$, $t = 1, 2, 3, ...$ repeat the step (CE).
Since the predictor-corrector method in this thesis cannot be self-starting, the one-step method was chosen as the starting method to obtain the initial value. The one-step method is also implemented the $PE(CE)^t$ mode. The one-step methods used in this thesis are the Euler and modified Euler method.
The predictor formula is written as:

$$y(x_{n+1}) = y(x_n) + hf(x_n). \tag{1.12}$$

The corrector formula is written as:

$$y(x_{n+1}) = y(x_n) + \frac{h}{2}(f(x_{n+1}) + f(x_n)). \tag{1.13}$$

1.8 Outline of the Thesis

The research work presented in the thesis consists of nine chapters. Below is the summary of each chapter:

Chapter 1 begins with an introduction of the research. The objectives, motivation, contribution and the scope of the thesis are stated. The introduction of the boundary value problems (BVPs) which includes the existence and uniqueness of BVPs are presented. Some preliminary concepts and the predictor corrector method will be discussed.

Chapter 2 consists of a review of the earlier research on BVPs. It also includes the literature review of the block methods and the shooting technique.

Chapter 3 describes the derivation of the one-point direct method and analyses its properties including the stability and order. It also introduces the multiple shooting technique and its adaptation to the direct method in order to solve the second order of the BVPs using the variable step size strategy. It also introduces the algorithm developed and discusses the numerical results based on the eight problems tested.

Chapter 4 takes into consideration the use of the direct block method to solve the second order of BVPs.It shows the derivations of the two-point and three-point block methods and presents the stability and the order of the methods. It also explains the proposed methods that are implemented with the multiple shooting technique via the three step iterative method using the variable step size strategy. Finally, it shows and discusses the numerical results based on the algorithms 2PNLBVPVS and 3PNLBVPVS which were developed and tested with eight problems of the second order of BVPs.

Chapter 5 analyses the computational complexity of the one-point direct method and the block direct method which is determined based on the number of arithmetic operations performed in the algorithm. The results show that the computational complexity of these methods is reliable in estimating the cost of these methods.

Chapter 6 shows the derivation of the two-point direct block method. It presents the stability and the order of the method. The implementation of the variable step size and variable order strategy adapted with the multiple shooting technique are used to solve the second order BVPs. It then presents and discusses the numerical results.

Chapter 7 covers the solution of the third order BVPs. It presents the derivation, stability and order of the two-point direct block method to solve the third order BVPs. The multiple shooting technique via the three-step iterative method is implemented to solve the third order BVPs using variable step size strategy. It shows and discusses the numerical results of eight problems tested.

Chapter 8 focuses on the solutions to the application of BVPs in fluid dynamic. It discusses the formulation of the problem and the implementation to solve the problem. It displays and compares the numerical results with the existing methods.

Chapter 9 summarizes and suggests the future work in this research.

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