UNIVERSITI PUTRA MALAYSIA

SOLVING BOUNDARY VALUE PROBLEMS FOR ORDINARY DIFFERENTIAL EQUATIONS USING DIRECT INTEGRATION AND SHOOTING TECHNIQUES

V. MALATHI

FSAS 1999 44

SOLVING BOUNDARY VALUE PROBLEMS FOR ORDINARY DIFFERENTIAL EQUATIONS USING DIRECT INTEGRATION AND SHOOTING TECHNIQUES

By

V. MALATHI

Thesis Submitted in Fulfilment of the Requirements for The Degree of Doctor of Philosophy in the Faculty of Science and Environmental Studies Universiti Putra Malaysia

October 1999

ACKNOWLEDGEMENTS

I wish to express my deep sense of gratitude to the Chairman of my Supervisory Committee, Professor Dr. Mohamed Sulieman for providing financial support in the form of Graduate Assistantship throughout the duration of my research work in the University. He has been an outstanding advisor to the Graduate Students and his guidance, assistance and high standards are the main reason for my success in completing this work. Despite his heavy administrative responsibility as a Chairman of National Accreditation Board, he always found time to go through our work and gave us critical suggestions and guidance.

A significant acknowledgement is also due to Dr. Bachok Taib, Member of my Supervisory Committee for providing Personal Computer and necessary software throughout my study in the University. My sincere thanks are also due to Dr. Saiman for consenting to be a Member of Supervisory Committee and for giving suggestions and guidance.

To carry out a research like this, one must work in a stimulating and friendly atmosphere and enjoy support in the form of facilities, tools, finances and efficient organisations. I have been very fortunate to have all of the above and it has been made possible by the Department of Mathematics led by Dr. Isa.

My sincere thanks are to my friends who helped me in various ways to carry out my research. My thanks are also due to my little son J.Pradeep for his endurance during early days of his childhood when he did not receive as much attention as he deserves from me. He has been a very understanding child and gave me a much-needed break from the monotony of my day to day academic life. Last but not the least, my special thanks are due to my husband Mr. S.Janakiraman for his constant encouragement and consistent support for my doing Ph.D.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

BDF	:	Backward Differentiation Formulae/method
BVP	:	Boundary Value Problem
DI	:	Direct Integration Method
FDE	:	Functional Differential Equation
IVP	:	Initial Value Problem
ODE	:	Ordinary Differential Equation
SL	:	Sturm-Liouville

Abstract of thesis submitted to the Senate of Universiti Putra Malaysia in fulfilment of the requirements for the degree of Doctor of Philosophy.

SOLVING BOUNDARY VALUE PROBLEMS FOR ORDINARY DIFFERENTIAL EQUATIONS USING DIRECT INTEGRATION AND SHOOTING TECHNIQUES

By

Malathi. V

October 1999

Chairman: Professor Mohamed bin Suleiman, Ph. D

Faculty: Science and Environmental Studies

In this thesis, an efficient algorithm and a code BVPDI is developed for solving Boundary Value Problems (BVPs) for Ordinary Differential Equations (ODEs). A generalised variable order variable stepsize Direct Integration (DI) method, a generalised Backward Differentiation method (BDF) and shooting techniques are used to solve the given BVP. When using simple shooting technique, sometimes stability difficulties arise when the differential operator of the given ODE contains rapidly growing and decaying fundamental solution modes. Then the initial value solution is very sensitive to small changes in the initial condition. In order to decrease the bound of this error, the size of domains over which the Initial Value Problems (IVPs) are integrated has to be restricted. This leads to the multiple shooting technique, which is generalisation of the simple shooting technique. Multiple shooting technique for higher order ODEs with automatic partitioning is designed and successfully implemented in the code BVPDI, to solve the underlying IVP.

The well conditioning of a higher order BVP is shown to be related to bounding quantities, one involving the boundary conditions and the other involving the Green's function. It is also shown that the conditioning of the multiple shooting matrix is related to the given BVP. The numerical results are then compared with the only existing direct method code COLNEW. The advantages in computational time and the accuracy of the computed solution, especially, when the range of interval is large, are pointed out. Also the advantages of BVPDI are clearer when the results are compared with the NAG subroutine D02SAF (reduction method).

Stiffness tests for the system of first order ODEs and the techniques of identifying the equations causing stiffness in a system are discussed. The analysis is extended for the higher order ODEs. Numerical results are discussed indicating the advantages of BVPDI code over COLNEW.

The success of the BVPDI code applied to the general class of BVPs is the motivation to consider the same code for a special class of second order BVPs called Sturm-Liouville (SL) problems. By the application of Floquet theory and shooting algorithm, eigenvalues of SL problems with periodic boundary conditions are determined without reducing to the first order system of equations. Some numerical examples are given to illustrate the success of the method. The results are then compared, when the same problem is reduced to the first order system of equations and the advantages are indicated. The code BVPDI developed in this thesis clearly demonstrates the efficiency of using DI Method and shooting techniques for solving higher order BVP for ODEs.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia bagi memenuhi syarat ijazah Doktor Falsafah

MENYELESAIKAN MASALAH NILAI SEMPADAN BAGI PERSAMAAN PEMBEZAAN BIASA MENGGUNAKAN KAEDAH KAMIRAN TERUS DAN KAEDAH PENEMBAKAN

Oleh

Malathi. V

October 1999

Pengerusi: Professor Mohamed bin Suleiman, Ph. D

Fakulti: Sains dan Pengajian Alam Sekitar

Dalam tesis ini, suatu algoritma dan suatu kod BVPDI yang efisien dibentuk untuk menyelesaikan Masalah Nilai Sempadan (MNS) bagi Persamaan Pembezaan Biasa (PBB). Kaedah umum Kamiran Terus (KT), peringkat berubah dan panjang langkah berubah dan kaedah umum pembezaan kebelakang dan teknik penembakan digunakan untuk menyelesaikan MNS yang diberi. Bila teknik penembakan mudah digunakan, kadangkala timbul masalah kestabilan apabila pengoperasi bagi PBB tersebut mengandungi penyelesaian asas yang menokok dan menyusut secara cepat. Justeru itu, penyelesaian nilai awalnya adalah sangat peka kepada sebarang perubahan kecil dalam syarat awalnya. Untuk mengurangkan batas ralat ini, saiz domain kamiran Masalah

Nilai Awal (MNA) ini hendaklah di bataskan. Ini menjurus kepada teknik penembakan berganda, iaitu pengitlakan teknik penembakan mudah. Teknik penembakan berganda bagi PBB peringkat tinggi dengan pemetakan automatik direkabentuk dan dilaksanakan dengan jayanya dalam kod BVPDI, bagi menyelesaikan MNA yang bersepadanan.

Persuasanaan rapi bagi MNS peringkat tinggi ditunjukkan mempunyai hubungan dengan kuantiti pembatasnya, satu melibatkan syarat pembatasnya dan satu lagi melibatkan fungsi Green. Ditunjukkan juga, bagaimana persuasanaan matriks kaedah penembakan berganda berkait dengan MNS yang diberi. Keputusan berangkanya kemudian dibandingkan dengan keputusan berangka yang diperolehi daripada satu-satunya kaedah terus yang sedia ada iaitu kod COLNEW. Perbandingan juga dibuat bagi menjelaskan kelebihan kaedah ini berdasarkan pengiraan masa dan ketepatan penyelesaiannya terutama bagi julat kamiran yang besar. Kelebihan kaedah BVPDI juga lebih ketara apabila dibandingkan dengan NAG subroutine D02SAF yang menggunakan kaedah penurunan.

Ujian kekakuan bagi sistem PBB peringkat pertama dan teknik mengenalpasti persamaan yang menyebabkan terjadi kekakuan dalam sistem tersebut dibincangkan. Analisis ini diperluaskan kepada PBB peringkat lebih tinggi. Keputusan berangkanya menunjukkan kelebihan kod BVPDI berbanding kod COLNEW.

Kejayaan kod BVPDI apabila digunakan kepada kelas MNS teritlak, menjadi motivasi untuk menggunakan kod tersebut bagi penyelesaian satu kelas khas MNS peringkat dua disebut masalah Sturm-Liouville (SL). Dengan menggunakan teori Floquet dan algoritma penembakan, nilai eigen bagi masalah (SL) bersama dengan syarat sempadan berkala ditentukan tanpa menurunkannya kepada sistem persamaan peringkat pertama. Beberapa contoh berangka diberikan untuk menunjukkan kejayaan kaedah tersebut. Keputusan apabila kaedah ini digunakan menunjukkan kelebihan apabila dibandingkan dengan kaedah penurunan kepada sistem persamaan peringkat pertama. Kod BVPDI yang dibina dalam tesis ini jelas menunjukkan kecekapan kaedah DI dan teknik penembakan apabila digunakan bagi penyelesaian MNS peringkat tinggi bagi PBB.

CHAPTER I

INTRODUCTION

Since the advent of computers, the numerical solution of BVPs for ODEs has been the subject of research by numerical analysts. BVPs manifest themselves in almost all branches of science, engineering and technology. Some examples are boundary layer theory in fluid mechanics, heat power transmission theory, space technology, control and optimisation theory and vibration problems. Considerable amount of work is being done to write general-purpose codes to produce accurate solutions to most of these problems occurring in practice.

The knowledge and understanding of methods for the numerical solution of BVPs is more recent compared with the numerical solution of IVPs. In fact many considered BVPs as a subclass of IVPs, wherein one tries to modify the initial conditions in order to get the required solution at the other end point. It gradually becomes clear that IVPs are actually a special and a relatively simple subclass of BVPs. The fundamental difference is that for IVPs one has complete information about the solution at one point (the initial point), so one may consider marching algorithm, which is always local in nature.

For BVPs on the other hand, no complete information is available at any point, so the end points have to be connected by the solution algorithm in a global way. Only stepping through the entire domain can the solution at any point be determined, though it has to be pointed out that both the mathematical theory and the numerical methods for solving BVPs are closely related to the corresponding techniques of IVPs in ODEs.

Other classes of BVPs like stiff BVPs and SL eigenvalue problems have become much more important in the past few years. Many methods have been proposed and the research continues extensively in these fields. In the next section we review some of these work.

Literature Review

The recent theoretical and practical development of techniques to solve BVPs for ODEs has made it possible to write general purpose computer codes. They efficiently produce accurate solution to most of the problems occurring in practice and there exist a large number of methods to compute solutions of BVPs. See Aziz (1965), Childs (1978), Keller (1976), Reddien (1980), Roberts (1972), Wong and Ji (1992), Lentini, Osborne, and Russell (1985), Kramer and Mattheij (1993), for some good references.

Historically and conceptually, methods have had many different backgrounds. They can be divided into the following groups.

First the initial value methods, namely, the shooting and multiple shooting method (Deuflhard, 1980; Deuflhard and Bader, 1983; Osborne 1969). In particular multiple shooting codes have been developed by Bulirsch et al. (1980) and England et al. (1973) to improve the poor stability of simple shooting.

Scott and Watts (1977) have produced a superposition code with orthonormalization. Another approach has been implemented by Lentini and Pereyra (1974, 1977) where a finite difference method with deferred corrections is used.

Collocation was long considered too expensive and hence not competitive, until a more rigorous investigation showed its usefulness (Ascher et al., 1979; Ascher and Weiss, 1984; Russell, 1977). Based on finite element method, a collocation solver *COLSYS* (Ascher et al., 1979) and later *COLNEW* were developed by Bader et al. (1987), where they first impose the collocation equations, followed by local parameter elimination and then connecting them to the computation in adjacent subintervals. This is a multiple shooting type approach, which allows to capitalise on previous theoretical results and to avoid introducing heavier functional analysis implementation. Collocation method may also be compared to some finite difference methods cf., Russell (1977).

An important and detailed analysis of singular perturbation problems was given by Vasileeva and Butuzov (1980). Aiken (1985) gave examples of how stiff problems arise, the theory of numerical methods for solving stiff problems, and a survey of computer codes for their solution. Ascher and Mattheij (1987) address various issues concerning the stability of stiff BVPs. The shooting codes, which use *prüfer* transformations for SL eigenvalue problems, are discussed by Bailey et al. (1978) and Pryce (1979).

Among the general purpose BVP software available to date, codes based on initial value techniques perform, by and large, poorly for stiff problems, while those based on symmetric difference schemes do much better, even if the theory on which they are based does not strictly hold for stiff BVPs. Also most of the existing codes for stiff and nonstiff BVPs using initial value techniques reduce the higher order system to first order system of equations. The BVP code COLNEW achieves some efficiency by applying the collocation method directly to higher order equations. This is the main motivation of this research work.

Objective of the Thesis

We first introduce some notation and an important theorem concerning BVPs.

A BVP consists of a differential equation (or equations) on a given interval and an explicit condition (or conditions) that a solution must satisfy at one or several points. Often there are two points, which correspond physically to the boundaries of some region, so that it is a two point BVP. A simple and common form of BVP is

$$y'' = f(x, y, y'), \qquad a \le x \le b$$
$$y(a) = \alpha, \quad y(b) = \beta, \qquad [1.1]$$

where α and β are known end points. In many applications ODEs appear in the form of mixed order systems. The general form of BVP considered here is

$$y^{(m)} = f\left(x, y, y', \ldots, y^{(m-1)}\right). \qquad [1.2]$$

Denoting, $\bar{y}(x) = \left(y(x), y'(x), \ldots, y^{(m-1)}(x)\right)^T$,

the form of boundary condition is,

$$g(\bar{y}(a), \bar{y}(b)) = 0 .$$

The following theorem gives the general conditions that ensure that the solution to a second BVP exists and is unique.

Theorem: Suppose the function *f* in the BVP [1.1] is continuous on the set,

$$D = \{(x, y, y' / a \le x \le b, -\infty < y < \infty, -\infty < y' < \infty\},$$

and that $\frac{\partial f}{\partial y}$ and $\frac{\partial f}{\partial y'}$ are continuous on D. Also assume that *f* satisfies the Lipschitz condition on D. (i.e.)

$$|f(x, y_1, y') - f(x, y_2, y')| \le k|y_1 - y_2|$$

$$|f(x, y, y_1') - f(x, y, y_2')| \le k|y_1' - y_2'|$$

for all points $(x, y_i, y'), (x, y, y_i'),\ i = 1,2$ in the region D, and if

(i) $\frac{\partial f(x, y, y')}{\partial y} > 0$ for all $(x, y, y') \in D$, and

(ii) a constant M exists, with

$$\left|\frac{\partial f(x, y, y')}{\partial y'}\right| \le M \quad \text{for all} \quad (x, y, y') \in D.$$

then the BVP has a unique solution.

As there is a close relationship between BVPs and IVPs, it makes sense then, to construct a numerical method for a given BVP by relating the problem to corresponding IVPs and solving the latter numerically.

In this thesis we discuss an implementation of initial value methods for solving BVPs for ordinary differential equations using direct integration method.

The code BVPDI is designed to solve mixed order systems of linear and nonlinear BVPs. This is in contrast to the other codes mentioned above in the previous section, which require conversion of the given problem to first order system, thereby increasing the number of equations and changing the algebraic structure of the discretized problem. This is with the exception of COLNEW, which solves the higher order equations directly.

Numerous numerical experiments have demonstrated the stability and efficiency of the direct integration methods. Further, the advantage of the initial value method is that it can deal with subintervals separately and so needs less memory space. In fact it may even lead to parallel implementation. Therefore it is an attractive idea to combine the virtue of classes, the DI methods and the initial value methods. For these reasons we feel that a robust, efficient, initial value direct method can be developed to reliably solve a large class of BVPs.

The concept of stiff BVP in numerical analysis relates to the concept of singularly perturbed BVP in applied mathematics. When the system is stiff, implicit methods are used on the full system, whereas in practice only a few of the equations may be the cause of the stiffness. Therefore in our algorithm we deal differently in the case of stiff BVPs.

Initially the system is solved by the DI method using the Adams variable order variable stepsize formulation. If difficulties arise, tests for stiffness are made. Equations which cause the stiffness are then identified and solved with the implicit backward differentiation methods.

The underlying problem in the study of many physical phenomena, such as the vibration of strings, the interaction of atomic particles, or the earth's free oscillations, yields a SL eigenvalue problems. A homogeneous ODE and homogeneous boundary conditions, one or both of which depends upon a parameter, say λ, is given. Then λ is desired such that the BVP has nontrivial solution. The real difference between the treatment for BVPs and the SL eigenvalue problem is that, instead of changing an initial condition and keeping the ODE fixed each step, we keep the initial conditions fixed and change the ODE, by adjusting the eigenvalue λ , and by effectively employing the Floquet theory.

Briefly, in this thesis we discuss about the solution of second order and higher order nonstiff and stiff BVPs, and the solution of linear SL eigenvalue problems using a general class of multistep methods using shooting and multiple shooting techniques.

Outline of the Thesis

In Chapter II the well conditioning of a BVP is shown to be related to some bounding quantities, one involving the boundary conditions and the other involving Green's function. In the case of a solution dichotomy, they are related to known stability results. It is shown how multiple shooting overcomes some of the difficulties by relating its matrix conditioning to the underlying BVP. Discussion on how the multiple shooting derive their stability from the fact that it transforms the given interval to a much smaller interval at some desirable point is also given.

A most popular initial value method for BVPs, the simple shooting, is briefly explained in Chapter III. Also, how the stability drawbacks arise in simple shooting can be overcome by multiple shooting technique is discussed. The multiple shooting method for higher order ODE is derived. The k-step Adams method that is used to solve a higher order nonstiff ODE directly is explained in detail.

A general algorithm for the code BVPDI to solve nonstiff BVPs along with the numerical results and comparison of the performance of BVPDI with the collocation code COLNEW are given in Chapter IV.

Chapter V provides a general framework within which various numerical methods for stiff BVP can be analysed. The algorithm which would solve either stiff or nonstiff equations for first order system is developed, giving a detailed discussion of the test for stiffness. The work is further extended for higher order ODEs. The strategies adopted in order to get the required accurate solution are discussed in detail. Finally numerical results are presented and compared with the code COLNEW.

Chapter VI is concerned with the solution of SL eigenvalue problems. The boundary conditions are periodic and the shooting algorithm employed is explained. The proposed technique is based on the application of Floquet theory. Convergent analysis and general guidelines to provide the starting values for the computed eigenvalues are presented. Some numerical results are also reported.

Summary of the whole thesis, conclusions and future work are further presented in Chapter VII.