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Kuppalapalle Vajravelu
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Keller-Box Method and Its Application

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Preface

During the past decades there has been an increased interest in solving systems of nonlinear differential equations associated with physical problems. Throughout engineering and technological industries, we are confronted with nonlinear boundary-value problems that cannot be solved by analytical methods. Although remarkable progress has been made in developing new and powerful techniques for solving the nonlinear differential equations, notably in the fields of fluid mechanics, biology, finance, aerospace engineering, chemical, and control engineering, much remains to be done.

In the present book, we highlight the development, analysis and application of the finite difference technique, the Keller-box method, for the solution of coupled nonlinear boundary-value problems. We have tried to present an account of what has been accomplished in the field to date. Accordingly, we shape this book to those interested in the Keller-box method as a working tool for solving physical and engineering problems.

This book can help the reader develop the toolset needed to apply the method, without sifting through the endless literature on the subject. Issues of finite differences, converting a system to first order differential equations, linearization by Newton's method, initial approximations, some basic numerical techniques, and obtaining a tridiagonal system by the Thomas algorithm, are discussed heuristically. As mentioned above, there are plenty of applications of the Keller-box method in the literature. In selecting applications and specific problems to work through, we have restricted our attention to fluid flow and heat transfer phenomena. Hence, in order to illustrate various properties and tools useful when applying the Keller-box method, we have selected recent research results in this area.

We appreciate the support and motivation of the editor A.C.J. Luo. We also acknowledge the role of Higher Education Press (China) and de Gruyter for making this book a reality. Last but not the least, we thank Prof. Mike Taylor for reading the manuscript and suggesting some needed changes.

Orlando, Florida

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Chapter 0

Introduction

Nature is in essence nonlinear. Many fundamental laws in science and engineering are modeled by nonlinear differential equations. The origin of nonlinear differential equations is very old, but it has been undergone remarkable new developments in the field of nonlinear equations for last few decades. One of the main impulses, among others for developing nonlinear differential equations has been the study of boundary layer equations. At high Reynolds number, the effect of viscosity is confined to a layer near the wall where the velocity changes are very large. Prandtl was the pioneer in developing a theory by employing what are now called the boundary layer assumptions. Mathematical analyses based on these assumptions of many physical problems in fluid mechanics agree well with the experimental observations. These equations are derived from the Navier-Stokes equations which describe the behavior of the fluid using boundary layer approximation. Using similarity transformations, these equations can be converted into nonlinear coupled ordinary differential equations (ODEs) or partial differential equations (PDEs). Their solution structure demands sophisticated analytical or numerical schemes. The analysis of flow and heat transfer over an infinite range occurs in many branches of science and technology. The fluid velocity satisfies higher order nonlinear differential equations depending on the stress-strain relation. In some instances one is able to obtain exact analytical solutions. When exact or analytical solutions are obtained, one is often faced with difficulty generalizing such results to other nonlinear differential equations. In many situations one is compelled to develop a good numerical scheme, fast as well as accurate, in order to obtain approximate solution to these coupled equations. Obtaining such numerical schemes to solve these coupled ODEs/PDEs for all prevailing physical parameters is the key point of this book.

Due to the difficulties of the problems, we frequently seek to obtain numerical solutions to a nonlinear problem, valid over some restricted region in the domain of the original problem. One such technique, which has shown a great promise over the past few years, is the Keller-box method. By use of the box method, numerous nonlinear differential equations have been studied in great detail. Like many other finite difference methods, the box method is very useful as it allows us to obtain numerical solutions to systems of nonlinear differential equations. The finite difference method is unique among other numerical techniques as it allows us to effectively control the rate of convergence via an initial approximation and then proceeds as follows:

- reducing them to a system of first order equations;
- writing the difference equations using central differences;
- linearization of the algebraic equations by Newton's method;
- writing them in matrix form; and
- finally solving the system by block tridiagonal elimination technique.

However, such great freedom comes with the dilemma of deciding just how to proceed. There have been a number of nonlinear differential equations to which the box method has been applied. However the selection of initial approximation varies greatly for different values of the non-dimensional parameters. That said, there are some underlying themes that become apparent when one examines the literature on the topic. Building on such themes, we hope to add some structure and formality to the application of nonlinear flow phenomena. In particular, we discuss several features of the method and the choices one can make in the initial approximation, far field conditions, and the convergence criteria.

We hope that the book helps in achieving this long range goal. We present a number of ways in which one may select the initial conditions, far field boundary conditions, and the convergence criteria while solving a nonlinear differential equation by the finite difference method. We also focus our attention on the properties of solutions resulting from such a choice of the initial approximation, far field conditions, and the convergence criteria. These choices play a large role in the computational efficiency.

We primarily discuss nonlinear ordinary differential equations associated with finite differences. However, such discussion is usually general enough to use for solving nonlinear partial differential equations as well as ordinary differential equations. We discuss many cases in general while still maintaining applicability of the results to actually computing solutions via the finite difference method. As frequent users of the method, we understand the importance of implementing the presented method.

We note that a good companion to this book will be that of Cebeci and Bradshaw [1] which gives physical and computational aspects of convective heat transfer, and some guidelines to solve the boundary value problems. The first half of the book presents the finite difference method and how to implement the box method [2]–[4].

The outline of the book will be as follows:

In Chapters 1–3, which comprise Part I of the book, we sketch the Keller-box method. This first set of chapters serves as a summary to the method which can be directly employed by researchers in engineering, applied physics, and other applied sciences. We keep the discussion general enough so as to provide a framework for researchers. In order to give the reader the best preparation for using the method, we realize that often the best way to convey information is through worked out examples.

In Part II of the book, Chapters 4–6, we shift to examples by considering problems in fluid mechanics and heat transfer governed by nonlinear differential equations [5]–[10]. Such examples will benefit the reader in applying the methods to actual problems of physical relevance. We group such problem into three categories: general fluid flow and heat transfer problems (Chapter 4), coupled nonlinear problems (Chapter 5), and more advanced problems (Chapter 6).

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Chapter 1

Basics of the Finite Difference Approximations

In this chapter we introduce the essentials of finite difference approximations for solving linear/nonlinear differential equations. In Section 1.2, we study the time-dependent differential equations beginning with the initial value problem and then present some theoretical issues pertaining to the equations. Oftentimes when dealing with nonlinear differential equations, the questions of the existence and uniqueness of a solution are of importance, and inveterate. Section 1.3, deals with the discretization of the differential equations and the solution processes for the coupled boundary value problems (BVPs). Further, it also explains the differences between the single-step and multi-step methods of solving BVPs. In Section 1.4, we extend the ideas of the prior section to obtain the numerical solutions for partial differential equations (PDEs). Finally, in Section 1.5 we present the numerical solutions to the PDEs, viz., elliptic, parabolic and hyperbolic differential equations.

1.1 Finite difference approximations

Our goal is to find approximate solutions to differential equations, i.e., to find a function (or some discrete approximation to this function) which satisfies a given relationship between its derivatives on some given region of space and/or time, along with some boundary conditions at the edges of the domain. In general this is a difficult problem and only rarely can an analytic formula be found for the solution. A finite difference method proceeds by replacing the derivatives in the differential equations by finite difference approximations. This gives a large algebraic system of equations to be solved in place of the differential equation, something that is easily solvable on a computer. Before tackling this problem, we first consider the more basic question of how we can approximate the derivatives of a known function by finite difference formulas based only on values of the function itself at discrete points.

Besides providing a basis for the later development of finite difference methods for solving differential equations, this allows us to investigate several key concepts such as the order of accuracy of an approximation in the simplest possible setting.

Let $u(x)$ represent a function of one variable that, unless otherwise stated, will always be assumed to be smooth, meaning that we can differentiate the function several times and each derivative is a well-defined bounded function over an interval containing a particular point of interest $\bar{x}$. Suppose we want to approximate $u'(\bar{x})$ by a finite difference approximation based only on values of u at a finite number of points near $\bar{x}$. One obvious choice would be to use

$$D_+u(\bar{x}) \equiv \frac{u(\bar{x}+h)-u(\bar{x})}{h} \tag{1.1}$$

for some small value of h. This is motivated by the standard definition of the derivative as the limiting value of this expression as $h \to 0$. Note that $D_+u(\bar{x})$ is the slope of the line interpolating u at the points $\bar{x}$ and $\bar{x}+h$. The expression in (1.1) is a one-sided approximation to u' since u is evaluated only at values of $x \geqslant \bar{x}$. Another one-sided approximation would be

$$D_-u(\bar{x}) \equiv \frac{u(\bar{x}-h)-u(\bar{x})}{h}. \tag{1.2}$$

Each of these formulas gives a first order accurate approximation to $u'(\bar{x})$, meaning that the size of the error is roughly proportional to h itself. Another possibility is to use the centered approximation

$$D_0u(\bar{x}) \equiv \frac{u(\bar{x}+h)-u(\bar{x}-h)}{2h} = \frac{1}{2}(D_+u(\bar{x})+D_-u(\bar{x})). \tag{1.3}$$

This is the slope of the line interpolating u at $\bar{x}-h$ and $\bar{x}+h$ and is simply the average of the two one-sided approximations defined above. From Figure 1.1 it should be clear that we would expect $D_0u(\bar{x})$ to give a better approximation than either of the one-sided approximations. In fact this gives a second order accurate approximation, the error is proportional to h^2 and

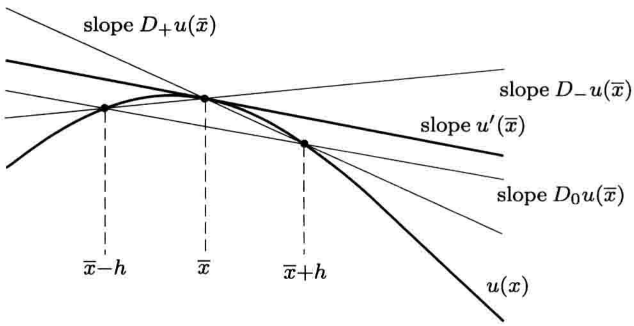

Fig. 1.1 Various approximations to $u'(\bar{x})$, interpreted as slopes of secant lines

hence is much smaller than the error in a first order approximation when h is small. Other approximations are also possible, for example

$$D_3u(\bar{x}) \equiv \frac{1}{6h}(2u(\bar{x}+h) + 3u(\bar{x}) - 6u(\bar{x}-h) + u(\bar{x}-2h)). \tag{1.4}$$

It may not be clear where this came from or why it should approximate u' at all, but in fact it turns out to be a third order accurate approximation, the error is proportional to h^3 when h is small. Our first goal is to develop systematic ways to derive such formulas and to analyze their accuracy and relative worth. First we will look at a typical example of how the errors in these formulas compare.

Example 1.1. Let $u(x) = \sin x, \bar{x} = 1$, so we are trying to approximate $u'(1) = \cos 1 = 0.5403023$. Table 1.1 shows the error $Du(\bar{x}) - u'(\bar{x})$ for various values of h for each of the formulas above.

Table 1.1 Errors in various finite difference approximations to $u'(\bar{x})$

h	D_+	D_-	D_0	D_3
1.0000e–01	–4.2939e–02	4.1138e–02	–9.0005e–04	6.8207e–05
5.0000e–02	–2.1257e–02	2.0807e–02	–2.2510e–04	8.6491e–06
1.0000e–02	–4.2163e–03	4.1983e–03	–9.0050e–06	6.9941e–08
5.0000e–03	–2.1059e–03	2.1014e–03	–2.2513e–06	8.7540e–09
1.0000e–03	–4.2083e–04	4.2065e–04	–9.0050e–08	6.9979e–11

We see that $D_+(u)$ and $D_-(u)$ behave similarly though one exhibits an error that is roughly the negative of the other. This is reasonable from Figure 1.1 and explains why $D_0(u)$ the average of the two, has an error that is much smaller than either. We see that

$$\begin{aligned}
D_+u(\bar{x}) - u'(\bar{x}) &\approx -0.42h, \\
D_0u(\bar{x}) - u'(\bar{x}) &\approx -0.09h^2, \\
D_3u(\bar{x}) - u'(\bar{x}) &\approx 0.007h^3,
\end{aligned}$$

confirming that these methods are first order, second order, and third order, respectively. Figure 1.2 shows these errors plotted against h on a log-log scale. This is a good way to plot errors when we expect them to behave like some power of h, since if the error $E(h)$ behaves like

$$E(h) \approx Ch^p \quad \text{then} \quad \log|E(h)| \approx \log|C| + p\log h.$$

So on a log-log scale the error behaves linearly with a slope that is equal to p, the order of accuracy.

Truncation errors

The standard approach to analyzing the error in a finite difference approximation is to expand each of the function values of u in a Taylor series about

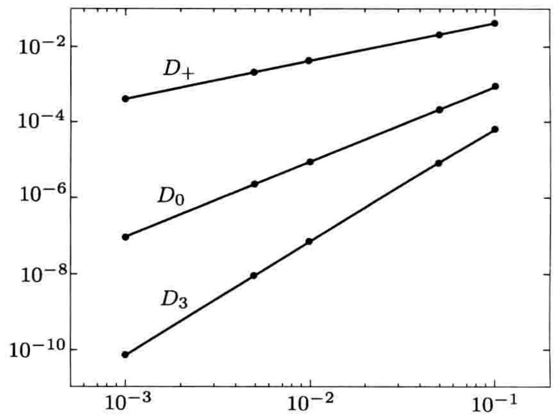

Fig. 1.2 The errors in Table 1.1 are plotted against h on a log-log scale

the point $\bar{x}$, e.g.,

$$u(\bar{x}+h) = u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2!}u''(\bar{x}) + \frac{h^3}{3!}u'''(\bar{x}) + O(h^4), \tag{1.5a}$$

$$u(\bar{x}-h) = u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2!}u''(\bar{x}) - \frac{h^3}{3!}u'''(\bar{x}) + O(h^4). \tag{1.5b}$$

These expansions are valid provided that u is sufficiently smooth. Using (1.5a), we can compute that

$$D_+u(\bar{x}) \equiv \frac{u(\bar{x}+h)-u(\bar{x})}{h} = u'(\bar{x}) + \frac{h}{2!}u''(\bar{x}) + \frac{h^2}{3!}u'''(\bar{x}) + O(h^3).$$

Recall that $\bar{x}$ is a fixed point so that $u''(\bar{x})$, $u'''(\bar{x})$, etc. are fixed constants independent of h. They depend on u of course, but the function is also fixed as we vary h. For h sufficiently small, the error will be dominated by the first term $0.5hu''(\bar{x})$ and all the other terms will be negligible compared to this term; we expect the error to behave roughly like a constant times h, where the constant has the value $0.5u''(\bar{x})$. Note that in Example 1.1, where $u(x) = \sin x$, we have $0.5u''(1) = -0.4207355$ which agrees with the value seen in Table 1.1. Similarly, from (1.5b) we can compute that the error in $D_-u(\bar{x})$ as

$$D_-u(\bar{x}) - u'(\bar{x}) = -\frac{h}{2!}u''(\bar{x}) + \frac{h^2}{3!}u'''(\bar{x}) + O(h^3)$$

which also agrees with our expectations. Combining (1.5a) and (1.5b) we get

$$u(\bar{x}+h) - u(\bar{x}-h) = 2hu'(\bar{x}) + \frac{h^3}{3}u'''(\bar{x}) + O(h^5),$$

so that

$$D_0u(\bar{x}) - u'(\bar{x}) = \frac{h^2}{6}u'''(\bar{x}) + O(h^4). \tag{1.6}$$