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COMPUTATIONAL TECHNIQUES FOR DIFFERENTIAL EQUATIONS

Edited by

JOHN NOYE

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PREFACE

Six invited papers on computational methods of solving partial differential equations were presented at the 1981 Conference on Numerical Solutions of Partial Differential Equations held at the University of Melbourne, Australia. They were also printed as part of the Conference Proceedings titled *Numerical Solutions of Partial Differential Equations*, edited by J. Noye and published by the North-Holland Publishing Company. The articles were so well received that it was decided to expand them and print them in a separate book so that the material they contained would be more readily available to postgraduate students and research workers in Universities and Institutes of Technology and to scientists and engineers in other establishments.

Because of the importance of ordinary differential equations and their use in the solution of partial differential equations, it was decided to include an additional article on this topic. Consequently, the first contribution, written by Robert May and John Noye, reviews the methods of solving initial value problems in ordinary differential equations. The next four articles are concerned with alternative techniques which may be used to solve problems involving partial differential equations: finite difference methods are described by John Noye of the University of Adelaide, Galerkin techniques by Clive Fletcher of the University of Sydney, finite element methods by Josef Tomas of the Royal Melbourne Institute of Technology, and boundary integral equation techniques by Leigh Wardle of the CSIRO Division of Applied Geomechanics. The first three of these are updated and extended revisions of the corresponding papers presented at the Melbourne conference; because the last mentioned author was unable to find time to revise his article, it has been reprinted in its original form from the 1981 Proceedings. The last two articles in this book describe the two basic methods of solving large sets of sparse linear algebraic equations: direct methods are presented by Ken Mann of the Chisholm Institute of Technology and iterative techniques by Len Colgan of the South Australian Institute of Technology. These methods are often incooperated in techniques for solving ordinary and partial differential equations.

My personal thanks go to the above-mentioned contributors for their cooperation in this venture, and to Drs. Arjen Sevenster (Mathematics Editor) and John Butterfield

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John Noye
The University of Adelaide
April, 1983

CONTENTS

Computational Techniques for Differential Equations
J. Noye (Editor)

THE NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS: INITIAL VALUE PROBLEMS

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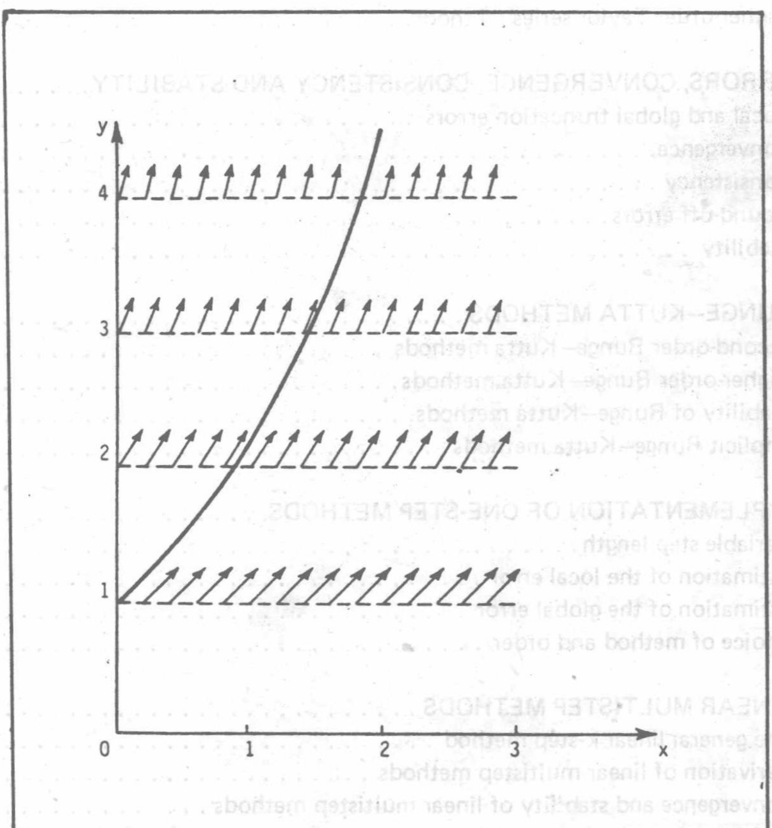

CONTENTS

1. INTRODUCTION

Mathematical models of problems in science and engineering often involve one or more ordinary differential equations. For instance, problems in mechanics such as the motion of projectiles or orbiting bodies, in population dynamics and in chemical kinetics may be modelled by ordinary differential equations.

Many clever methods of finding analytical solutions of ordinary differential equations are presented in elementary courses, but the majority of differential equations are not amenable to these methods, and unfortunately most of the differential equations which model practical problems fall into this category. For this reason many texts on mechanics, population dynamics and chemical kinetics develop elegant systems of ordinary differential equations, but give solutions to only very simple idealised problems.

Over the years various numerical methods have been devised, in general not by mathematicians but by people working in other fields for whom the method of solution was only incidental to the problem they were trying to solve. For instance, the technique now referred to as Adams method first appeared in an article on capillary action published by Bashforth and Adams (1883).

However, in the last thirty or so years mathematicians have put the subject on a much sounder theoretical basis, particularly in areas such as stability and the propagation of errors. Much work has been done on the implementation of methods and on their comparative testing. This has produced some agreement on what is the "best" method for a given non-stiff ordinary differential equation. Recently the problem of stiffness has received a lot of attention.

The aim of this article is to provide a practically oriented guide to help people with little or no previous knowledge to solve ordinary differential equations by numerical means. For this reason most of the theoretical results are merely described but not proved. For their proof, the interested reader is referred to the classical work of Henrici (1962) or the book by Stetter (1973). Section 11, on the choice of method and available software, is directed particularly to the beginner who must select a method to solve a particular problem and who wishes to find a suitable program to implement the method.

As the title of this article implies, only initial value problems have been considered. Boundary value problems for ordinary differential equations are also very important. A knowledge of the solution of initial value problems is useful when it comes to boundary value problems, which require more sophisticated numerical techniques for their solution. Keller (1968 and 1976) describes methods for solving the two-point boundary value problem, and Keller (1975) gives a general survey of boundary value problems in general. Unlike initial value problems, for which some well tried automatic computer codes are now readily available, the development of computer programs for boundary value problems is only in its infancy.

The main techniques considered in this article are those based on Taylor series (Section 3), the Runge-Kutta methods (Section 5), linear multi-step methods (Section 7) and extrapolation methods (Section 9).
All calculations made to demonstrate the relative accuracy of these methods were carried out on a CDC-CYBER 170-720, unless otherwise indicated. Besides going to the original articles for information, the

descriptions of these methods given in the books by Gear (1971), Henrici (1962), Ralston (1965), Shampine and Allen (1973), Shampine and Gordon (1975), and Stetter (1973) were used in the preparation of this article. Particular mention must be made of the excellent book by Lambert (1973).

Whenever an initial value problem in ordinary differential equations arises, a quick check to determine whether analytical techniques will give a general solution may be worthwhile. In this regard, books like Murphy (1960) are useful: they contain methods for solution of ordinary differential equations with a list of equations with known solutions. However, if a rapid search of this kind is not successful, the methods described here must be used.

Exact solutions for particular initial value problems are also useful for another reason. They can be used to check the accuracy of a numerical technique, and they are good indicators of possible coding errors.

2. PRELIMINARIES

2.1 Definitions

An equation of the form

$$F(x,y,y',y'',\ldots,y^{(m)}) = 0 \tag{2.1.1}$$

is called an *ordinary differential equation of order* m. A function $y(x)$ defined and m times differentiable on some interval I which satisfies (2.1.1) for all $x \in I$ is called a *solution* of the differential equation. Differential equations generally have many solutions, and extra conditions, known as *boundary conditions*, must be imposed to single out a particular solution. These boundary conditions usually take the form of the solution and/or its derivatives being specified for particular values of x, and it can be shown that a differential equation of order m requires m boundary conditions. If all the boundary conditions apply at one value of x they are called *initial conditions*, and the differential equation together with the initial conditions is termed an *initial value problem* - if more than one value of x is involved in the boundary conditions it is called a *boundary value problem*.

A differential equation is *linear* if y and its derivatives occur linearly, that is if the equation is of the form

$$a_m(x)y^{(m)} + a_{m-1}(x)y^{(m-1)} + \ldots + a_0(x)y = g(x). \tag{2.1.2}$$

In this paper we consider only *explicit differential equations*, that is differential equations which can be put in the form

$$y^{(m)} = f(x,y,y'',y''',\ldots,y^{(m-1)}). \tag{2.1.3}$$

Clearly all linear differential equations are in this category, as are the majority of non-linear equations. For the numerical solution of implicit differential equations see Fox and Mayers (1981).

2.2 Reduction of Higher-Order Differential Equations to First-Order Systems

Consider the m^{th}-order initial value problem

$$y^{(m)} = f(x,y,y',\ldots,y^{(m-1)}),$$
$$y^{(i-1)}(a) = \eta_i, \quad i=1,2,\ldots,m. \tag{2.2.1}$$

By introducing the variables y_i, $i=1,2,\ldots,m$, where

$$\begin{aligned} y_1 &\equiv y, \\ y_2 &\equiv y', \\ y_3 &\equiv y'', \\ &\vdots \\ y_m &\equiv y^{(m-1)}, \end{aligned} \tag{2.2.2}$$

equation (2.2.1) may be written as an initial value problem for a first-order system, namely

$$\begin{aligned} y_1' &= y_2, & y_1(a) &= \eta_1, \\ y_2' &= y_3, & y_2(a) &= \eta_2, \\ y_3' &= y_4, & y_3(a) &= \eta_3, \\ &\vdots & &\vdots \\ y_m' &= f(x,y_1,y_2,\ldots,y_m), & y_m(a) &= \eta_m. \end{aligned} \tag{2.2.3}$$

Using the matrix notation

$$\begin{aligned} \underset{\sim}{y} &= [y_1,y_2,\ldots,y_m]^T \\ \underset{\sim}{\eta} &= [\eta_1,\eta_2,\ldots,\eta_m]^T \\ \underset{\sim}{f} &= [y_2,y_3,\ldots,y_m,\ f(x,y_1,y_2,\ldots,y_m)]^T, \end{aligned} \tag{2.2.4}$$

the initial value problem becomes

$$\underset{\sim}{y}' = \underset{\sim}{f}(x,\underset{\sim}{y}), \quad \underset{\sim}{y}(a) = \underset{\sim}{\eta} . \tag{2.2.5}$$

In the same way an initial value problem involving a system of higher order equations can be put in the form (2.2.5).

Note that if the vector signs are omitted (2.2.5) defines a first-order initial value problem. This is particularly important because it means that most results which hold for a first-order initial value problem can be generalised to a system of m first-order equations and hence apply to an m^{th}-order initial value problem. Similarly, any method of solution of a first-order initial value problem can be extended to a system of equations and thus may be used to solve an m^{th}-order initial value problem. Throughout the rest of this article only first-order equations will be considered and from time-to-time it will be indicated how the result applies to the more general case.

Boundary value problems can also be reduced to a system of first-order equations, but the boundary conditions do not apply at the same value of x. Methods of solution of initial value problems can also be modified to solve boundary value problems.

2.3 Existence and Uniqueness of Solutions

The solutions of $y' = f(x,y)$ are generally a family of curves, and the initial condition $y(a) = \eta$ usually singles out one of these to give a unique solution. For example $y' = y$ has the solutions $y = ce^x$, and $y(0) = 1$ implies that $c = 1$, giving the unique solution $y = e^x$ (see Figure 2.1). However not all such problems have a unique solution. Consider

$$y' = \sqrt{y} , \quad y(0) = 0 . \tag{2.3.1}$$

Clearly $y \equiv 0$ is a solution, but so is

$$y(x) = \begin{cases} 0 & 0 \le x \le c \\ \frac{1}{4}(x-c)^2 & x > c , \end{cases} \tag{2.3.2}$$

for any constant c. Thus this problem has infinitely many solutions (see Figure 2.2), and would obviously prove difficult to solve numerically.

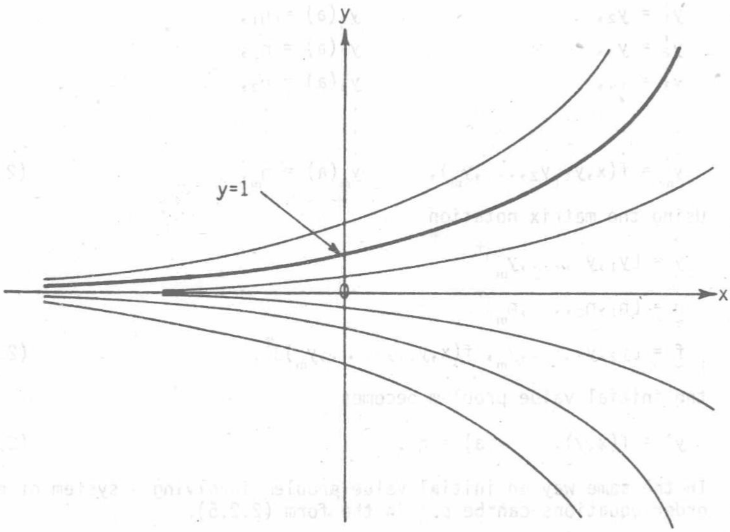

FIGURE 2.1: Solutions of $y'=y$ and the unique solution satisfying $y(0)=1$.

The initial value problem

$$y' = f(x,y), \quad y(a) = \eta, \tag{2.3.3}$$

is guaranteed a unique solution on some interval $[a,b]$ if $f(x,y)$ satisfies certain conditions, as the following theorem proved in Henrici (1962) shows.

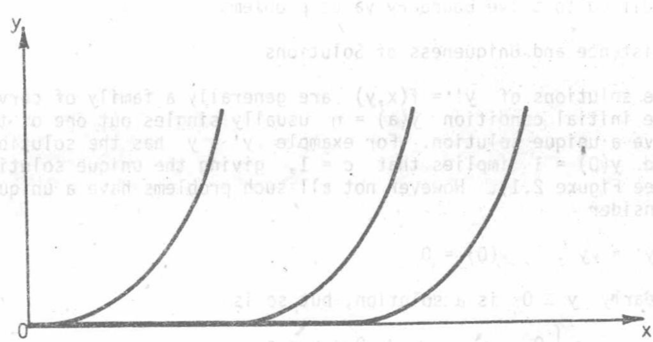

FIGURE 2.2: Some of the solutions of $y'=\sqrt{y}$, $y(0)=0$.

Theorem: *If $f(x,y)$ is defined and continuous for all points in the region*

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

and there exists a constant L such that for all (x,y) and (x,y^*) in D

$$|f(x,y) - f(x,y^*)| \le L\,|y-y^*| , \qquad (2.3.4)$$

then the initial value problem (2.3.3) has a unique solution on $[a,b]$ for any given number η.

The constant L is called a *Lipschitz constant*, and the condition (2.3.4) is called the *Lipschitz condition*. This theorem applies to a system of equations - vector signs must be put under f, y and η and the absolute values in (2.3.4) replaced by vector norms.

In the case that $f(x,y)$ has a continuous partial derivative with respect to y, the mean value theorem gives

$$f(x,y) - f(x,y^*) = \partial f/\partial y\big|_{(x,\bar{y})} (y-y^*) \qquad (2.3.5)$$

where $\bar{y}$ lies between y and y^*. If $\partial f/\partial y$ is bounded by K on D, that is there exists some constant K such that

$$|\partial f/\partial y| < K \quad \text{for all} \quad (x,y) \in D , \qquad (2.3.6)$$

we can take $L = K$. However, if $\partial f/\partial y$ is unbounded on D, then f does not satisfy a Lipschitz condition. For a system of m equations both f and y are m-vectors, and $\partial f/\partial y$ is the *Jacobian* of f with respect to y, that is a $m \times m$ matrix whose i,j element is $\partial f_i/\partial y_j$, so that a matrix norm subordinate to the vector norm used in (2.3.4) must replace the absolute value in (2.3.6).

Many problems do not satisfy the above theorem even though they have a unique solution. In this case it is often possible to modify the problem in such a way that the theorem is satisfied, but the solution is unchanged. Consider for example the initial value problem

$$y' = y^2, \qquad y(0) = 1 . \qquad (2.3.7)$$

On any interval $[0,c]$, where $c < 1$, this has the unique solution

$$y(x) = \frac{1}{1-x} , \qquad (2.3.8)$$

but $f(x,y) = y^2$ giving $\partial f/\partial y = 2y$, and since this is unbounded as $y \to \pm\infty$, f does not satisfy a Lipschitz condition. However $\partial f/\partial y$ is bounded on any finite region, so if we define

$$f^*(x,y) = \begin{cases} y^2 & |y| \le M , \\ M^2 & |y| > M , \end{cases} \qquad (2.3.9)$$

then $f^*(x,y)$ is continuous and satisfies a Lipschitz condition. Thus the initial value problem

$$y' = f^*(x,y), \qquad y(0) = 1, \qquad (2.3.10)$$

is guaranteed a unique solution, and the solution of (2.3.10) is identically equal to that of (2.3.7) for $|y| \le M$.

Another example is

$$y' = \sqrt{y}, \quad y(0) = 1. \tag{2.3.11}$$

Here $\partial f/\partial y = 1/2\sqrt{y}$ is unbounded as $y \to 0$ and f is not defined for $y < 0$. We can define

$$f^*(x,y) = \begin{cases} \sqrt{y} & y \ge 1 , \\ 1 & y < 1 , \end{cases} \tag{2.3.12}$$

which is clearly continuous and satisfies a Lipschitz condition, and since the solution of (2.3.11) is monotone increasing $(y' > 0)$ then $y \ge 1$ for $x > 0$ so the modified problem has the same unique solution. Note that this example is nearly the same as the earlier example (2.3.1) of an initial value problem with more than one solution - only the initial value has been changed. The above modification cannot be carried out for (2.3.1) since the initial value $y(0) = 0$ is that at which f fails to satisfy a Lipschitz condition.

In many practical problems the function $f(x,y)$ is not continuous, but is only piecewise continuous. An example is the equations describing the motion of a multi-stage rocket - when a burnt out stage is detached the mass changes discontinuously. If the problem is split up into several problems, each corresponding to an interval on which f is continuous, then they may individually satisfy the theorem, and the end point of the solution on one interval is used as the initial value for the problem on the next interval.

A more complete and rigorous treatment of the uniqueness of solutions of ordinary differential equations is given by Coddington and Levinson (1955).

2.4 Autonomous Systems of Differential Equations

Some papers consider only the *autonomous system* of differential equations

$$\underset{\sim}{y}' = \underset{\sim}{f}(\underset{\sim}{y}), \quad \underset{\sim}{y}(a) = \underset{\sim}{\eta} , \tag{2.4.1}$$

that is a system where the derivatives are independent of x. Any system of differential equations can be put into the form (2.4.1) with the addition of one equation. Consider the general system of m first-order differential equations

$$\begin{aligned}
y_1' &= f_1(x,y_1,y_2,\dots,y_m), & y_1(a) &= \eta_1, \\
y_2' &= f_2(x,y_1,y_2,\dots,y_m), & y_2(a) &= \eta_2, \\
\vdots &\quad \vdots & \vdots &\quad \vdots \\
y_m' &= f_m(x,y_1,y_2,\dots,y_m), & y_m(a) &= \eta_m.
\end{aligned} \tag{2.4.2}$$

Introducing the variable $y_{m+1} = x$, we have $dy_{m+1}/dx = 1$ and $y_{m+1}(a) = a$ so that

$$
\begin{aligned}
y_1' &= f_1(y_{m+1}, y_1, y_2, \ldots, y_m), & y_1(a) &= \eta_1, \\
y_2' &= f_2(y_{m+1}, y_1, y_2, \ldots, y_m), & y_2(a) &= \eta_2, \\
&\vdots & &\vdots \\
y_m' &= f_m(y_{m+1}, y_1, y_2, \ldots, y_m), & y_m(a) &= \eta_m, \\
y_{m+1}' &= 1, & y_{m+1}(a) &= a, \qquad (2.4.3)
\end{aligned}
$$

which is an autonomous system. Hence any method of solution of an autonomous system of differential equations can be used for a non-autonomous system.

2.5 Graphical Solution

A method of finding an approximate solution, but only to a single first-order equation, is the *graphical method*. If (x,y) is a point on the graph of $y(x)$, the solution of

$$y' = f(x,y), \quad y(a) = \eta, \tag{2.5.1}$$

then the value $f(x,y)$ is the slope of the tangent to the solution curve at the point (x,y). A *direction field* may be drawn by evaluating $f(x,y)$ at various points in the x-y plane and drawing a small arrow of slope $f(x,y)$ from (x,y). The approximate solution is then found by sketching a curve from the point (a,η) such that the arrows are tangential to it. Figure 2.3 shows the approximate solution to (2.3.11) obtained in this way.

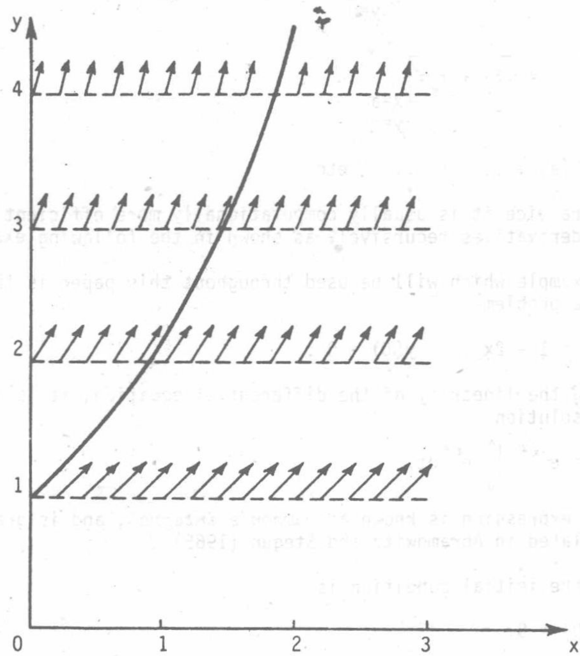

FIGURE 2.3: The graphical solution of $y'=\sqrt{y}$, $y(0)=1$.

3. TAYLOR SERIES METHODS

3.1 The Solution as a Taylor Series

The solution of the initial value problem

$$y' = f(x,y), \quad y(a) = \eta , \tag{3.1.1}$$

may be expressed as the Taylor series

$$y(x) = y(a) + (x-a)y'(a) + \frac{(x-a)^2}{2!}y''(a) + \frac{(x-a)^3}{3!}y'''(a) + \ldots \tag{3.1.2}$$

provided it is infinitely differentiable at $x = a$. The second and higher derivatives in (3.1.2) may be obtained (if they exist) by repeatedly differentiating the differential equation using the chain rule. Thus

$$y(a) = \eta ,$$

$$y'(a) = f(x,y)\Big|_{\substack{x=a\\y=\eta}} ,$$

$$y''(a) = \frac{d}{dx} f(x,y)\Big|_{\substack{x=a\\y=\eta}}$$

$$= \left[\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx}\right]_{\substack{x=a\\y=\eta}}$$

$$= \left[f_x + f_y f\right]_{\substack{x=a\\y=\eta}} ,$$

$$y'''(a) = \ldots\ldots\ldots\ldots \text{ etc.} \tag{3.1.3}$$

In practice it is usually computationally more efficient to calculate the derivatives recursively as shown in the following example.

An example which will be used throughout this paper is the initial value problem

$$y' = 1 - 2xy, \quad y(0) = 0 . \tag{3.1.4}$$

Using the linearity of the differential equation, it is easy to derive the solution

$$y = e^{-x^2} \int_0^x e^{t^2} dt. \tag{3.1.5}$$

This expression is known as *Dawson's integral*, and is graphed and tabulated in Abramowitz and Stegun (1965).

Now the initial condition is

$$y(0) = 0,$$

and substituting $x = 0$ into the differential equation gives