UNIVERSITI PUTRA MALAYSIA

NUMERICAL SOLUTION OF ORDINARY AND DELAY DIFFERENTIAL EQUATIONS BY RUNGE-KUTTA TYPE METHODS

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By

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TO MY FAMILY

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LIST OF ABBREVIATIONS

IVP	Initial Value Problem
IRK	Implicit Runge-Kutta
ODE	Ordinary Differential Equation
ODEs	Ordinary Differential Equations
SDIRK	Singly Diagonally Implicit Runge-Kutta
BDF	Backward Differentiation Formula
ROW	Rosenbrock Wanner Method
DDE	Delay Differential Equation
DDEs	Delay Differential Equations
RDE	Retarded Delay Differential Equation
NDE	Neutral Delay Differential Equation
CRK	Continuous Runge-Kutta
RKF	Runge-Kutta Felhberg

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

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Chairman: **Professor Mohamed bin Suleiman, Ph.D.**

Faculty: **Science and Environmental Studies**

Runge-Kutta methods for the solution of systems of ordinary differential equations (ODEs) are described. To overcome the difficulty in implementing fully implicit Runge-Kutta method and to avoid the limitations of explicit Runge-Kutta method, we resort to Singly Diagonally Implicit Runge-Kutta (SDIRK) method, which is computationally efficient and stiffly stable. Consequently, embedded SDIRK methods of fourth order five stages in fifth order six stages are constructed. Their regions of stability are presented and numerical results of the methods are compared with the existing methods.

Stiff systems of ODEs are solved using implicit formulae and require the use of Newton-like iteration, which needs a lot of computational effort. If the systems

can be partitioned dynamically into stiff and nonstiff subsystems then a more effective code can be developed. Hence, partitioning strategies are discussed in detail and numerical results based on two techniques to detect stiffness using SDIRK methods are compared.

A brief introduction to delay differential equations (DDEs) is given. The stability properties of SDIRK methods, when applied to DDEs, using Lagrange interpolation to evaluate the delay term, are investigated.

Finally, partitioning strategies for ODEs are adapted to DDEs and numerical results based on two partitioning techniques, intervalwise partitioning and componentwise partitioning are tabulated and compared.

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

PENYELESAIAN BERANGKA BAGI PERSAMAAN PEMBEZAAN BIASA DAN LENGAH MENGGUNAKAN KAEDAH RUNGE-KUTTA

Oleh

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Kaedah Runge-Kutta untuk penyelesaian sistem persamaan pembezaan biasa (PPB) diterangkan. Untuk mengatasi kerumitan dalam melaksanakan kaedah Runge-Kutta sepenuh tersirat dan untuk menghindarkan kekurangan yang ada pada kaedah Runge-Kutta tak tersirat, kami menumpukan sepenuh perhatian terhadap kaedah Runge-Kutta pepenjuru tunggal tersirat yang lebih efisien serta stabil kaku. Justeru itu, kaedah terbenam Runge-Kutta pepenjuru tunggal tersirat (RKPTT) peringkat empat tahap lima dalam peringkat lima tahap enam diterbitkan. Rantau kestabilannya diberikan dan keputusan berangka bagi kaedah tersebut dibandingkan dengan keputusan berangka bagi kaedah yang sedia ada.

Sistem persamaan pembezaan biasa kaku biasanya diselesaikan dengan kaedah tersirat dan melibatkan lelaran Newton serta memerlukan pengiraan yang

banyak. Andainya sistem tersebut boleh dipetakkan kepada sistem kaku dan tak kaku, maka suatu kod penyelesaian yang lebih efektif dapat dibentuk. Oleh itu strategi pemetakan dibincangkan secara mendalam dan keputusan berangka kaedah RKPTT berdasarkan dua teknik mengesan kekakuan dibandingkan.

Pengenalan ringkas kepada persamaan pembezaan lengah (PPL) diberikan dan sifat kestabilan kaedah RKPTT bila digunakan keatas PPL menggunakan interpolasi Lagrange untuk mengira sebutan lengahnya dikaji.

Akhir sekali strategi pemetakan bagi PPB diadaptasikan kepada PPL dan keputusan berangka berdasarkan dua teknik pemetakan, iaitu pemetakan berselang dan pemetakan berkomponen, dijadualkan dan dibandingkan.

CHAPTER I

INTRODUCTION AND OBJECTIVES

Introduction

Many important and significant problems in engineering, the physical sciences and the social sciences can be formulated in terms of differential equations. The problems of the bending of a thin beam clamped at both ends, the steady state flow of viscoelastic fluid parallel to an infinite plane surface with uniform sunction and some problems in control theory can be formulated in terms of differential equations. Differential equations also appear naturally in the field of medicine. For example, the blood glucose regulatory system can be modeled into differential equations to obtain a fairly reliable criterion for the diagnosis of diabetes. A system of differential equations also govern the spread of epidemic in a population, this model enables researchers to prove the famous " threshold theorem of epidemiology" which states that an epidemic will occur only if the number of people susceptible to the disease exceeds a certain threshold value.

Very often, mathematical problems cannot be conveniently solved using exact formulae, hence numerical methods are used as an alternative. This is the technique widely used by scientists and engineers to solve their problems. Analytical methods usually give a result in the form of mathematical functions that can then be evaluated for specific instances, hence the behaviour and properties of the functions are often apparent. However results from numerical methods can be plotted to show some of the behaviour of the solution. Though results from numerical methods are approximations, they can be made as accurate as desired.

In the following sections, we give a brief review on differential equations and also numerical methods to solve them.

The Initial Value Problem

Consider the initial value problem (IVP) for a system of s first order ordinary differential equations (ODEs), defined by

$$y' = f(x, y), \qquad y(a) = \eta, \qquad [1.1]$$

where $y = [y_1(x), y_2(x), \ldots, y_s(x)]^T$

$f(x, y) = [f_1(x, y), \ldots, f_s(x, y)]^T, \qquad x \in [a, b]$

and $\eta = [\eta_1, \ldots, \eta_s]^T$ is a known vector.

Theorem (Existence and Uniqueness)

For (IVP) [1.1], let

(1) $f(x, y)$ be continuous in a domain D, where

$$D = \{(x, y) \mid a < x < b, \|y\| < \infty\}$$

(2) There exists $L>0$ such that

$$\|f(x,y)-f(x,z)\| < L\|y-z\| \quad \text{for all } (x,y)\in D$$

and $(x,z)\in D$.

Then there exists a unique function $y(x)$, which satisfies the (IVP) [1.1].

For proof, see Henrici (1962). In this work, we shall assume the problem in [1.1] satisfies the conditions of the Existence and Uniqueness theorem.

The Discrete Variable Methods

The exact solution of the (IVP) [1.1] can be approximated using a numerical method, that is, the method will yield a sequence of approximations $y_n \cong y(x_n)$ on the set of points $x_{n+1} = x_n$

The simplest way of advancing the solution from the point x_n to x_{n+1} is by Taylor series.

$$y(x_{n+1}) = y(x_n) + h\Delta(x_n, y_n; h),$$

where $\Delta(x,y;h) = y'(x) + \frac{h}{2}y''(x) + \frac{h^3}{3!}y'''(x) + O(h^4)$.

If the series is truncated and $y(x_n)$ is replaced by y_n further approximation can be obtained

$$y_{n+1} = y_n + h\Phi(x_n, y_n; h), \qquad n=0,1,2,\ldots$$

where $\Phi(x, y, h) = f(x, y) + \frac{h}{2} f'(x, y) +, \ldots, + \frac{h^{p-1}}{p!} f^{(p-1)}(x, y)$.

For p=1, we have the formula

$$y_{n+1} = y_n + hf(x_n, y_n)$$

which is the well known Euler method, and if p=2,

$$y_{n+1} = y_n + h[f(x_n, y_n) + \frac{h}{2}(f_x(x_n, y_n) + f_y(x_n, y_n) f(x_n, y_n))].$$

Runge (1895), Heun (1900) and Kutta (1901) introduced an idea which is equivalent to constructing a formula for Φ which agrees with Δ as closely as possible, without involving derivatives of f. This process of "matching" the Taylor series can be illustrated by setting

$$\Phi(x, y, h) = b_1 f(x, y) + b_2 f(x + hc_2, y + a_{21} f(x, y)),$$

where b_1, b_2, c_2 and a_{21} are constants to be determined. Expanding both Φ and Δ in powers of h, we obtained

$$\Phi(x, y, h) = (b_1 + b_2) f(x, y) + hb_2[c_2 f_x(x, y) + a_{21} f_y(x, y) f(x, y)] + O(h^2) \quad [1.2]$$

$$\Delta(x, y, h) = f(x, y) + \frac{1}{2} h[f_x(x, y) + f_y(x, y) f(x, y)] + O(h^2),$$

yielding equation

$$b_1 + b_2 = 1, \qquad b_2 c_2 = \frac{1}{2}, \qquad b_2 a_{21} = \frac{1}{2}$$

The expression [1.2] and the above matching process can be extended to involve m equations of f yielding the general m-stage explicit Runge-Kutta method. Kutta (1901) completely characterized the set of Runge-Kutta methods of order 4 and proposed the first method of order 5.

When y_{n+1} is obtained by the Runge-Kutta method, the approximation y_n is then discarded. The method which makes direct use of some of the previously computed values of y_n is the multistep method. A linear multistep method of stepnumber k or k-step method is a computational method for determining the sequence $\{y_n\}$ which takes the form of a linear relationship between y_{n+j} and f_{n+j}, $j = 0,1,\ldots,k$. The general linear multistep method may be written as

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

The method is explicit if $\beta_k = 0$ and implicit otherwise. Euler method is an explicit linear one-step method.

Taylor series for $y(x_{n-1}$

$$y(x_n \quad) \qquad (\quad) \quad h \; ' \quad) \quad \frac{h^2}{2!} \; '' \quad) \quad \frac{h^3}{3!} \; ''' \qquad O \; h^4$$

Subracting it from the Taylor series for $y(x_{n+1}$

$$y(x_{n+1} \qquad\qquad \frac{h^3}{3} y'''(x_n) + \ldots$$

replacing $y(x_n)$ by y_n, yielding

$$y_{n+1} = y_{n-1} + 2hf_n$$

or in standard form, it can be written as

$$y_{n+2} = y_n + 2hf_{n+1} .$$

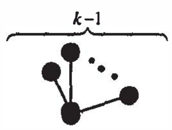
This is the Mid-point rule, which local truncation error is $\pm \frac{1}{3} h^3 y'''(x_n)$ and it is an explicit 2-step method. In order to generate a sequence $\{ y_n \}$ it is necessary to obtain two starting values y_0 and y_1. Other methods used are the block methods and the hybrid methods. Further information on all the methods can be obtained from Lambert (1973) and Hall and Watt (1976). The details of the literature review will be given at the beginning of the relevant chapters namely Chapter II, III, V and VI.

Runge-Kutta Method

A number of different approaches have been used in the analysis of Runge-Kutta methods, but the commonly used is the one developed by Butcher (1963), following on the work of Gill (1951) and Merson (1957), and it is as follows.

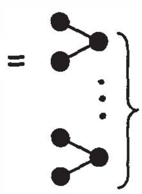
Let t denote the set of all rooted trees (t), where the trees are drawn with the root at the bottom. Refer to certain particular trees whose names are designated as t_k, t^k and $t_{k,l}$, where

t_k =



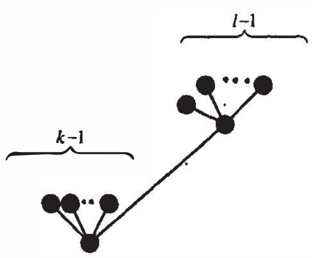
(k vertices)

t^k =



(k vertices)

and $t_{k,l}$ =



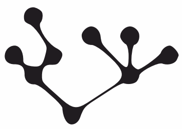
For each $t \in T$ form a quantity $F(t)(y_{n-1})$ which is given by associating each vertex of t, the nth linear operator $f^{(n)}(y_{n-1})$ which is written as $f^{($ the number of upward growing branches from this vertex. Thus

$$F(t_k)(y_{n-1}) = f^{(k-1)}\underbrace{(f,\ldots,f)}_{k-1}$$

$$F(t^k)(y_{n-1}) = (f^{(1)})^k f \, .$$

One further example is for the tree

t =



for which $F(t)(y_{n-1}) = f''(f''(f, f'(f)), f'''(f, f, f))$.

For each of the trees defined three numbers, they are

$r(t)$ ~ the number of vertices in t

$\sigma(t)$ ~ the order of the symmetry group of t

$\gamma(t)$ ~ the product of $r(u)$ over u, where for each vertex t, u is the sub tree formed from that vertex and all vertices can be reached from it following upward growing branch.

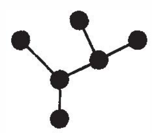
With this terminology, the formal Taylor series for $y(x_n)$ can be written as follows.

$$y(x_{n-1} + h) = y(x_{n-1}) + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)\gamma(t)F(t)(y(x_{n-1}))}$$

$$= y_{n-1} + hf + \frac{h}{2} f'(f) + h^3 (\frac{1}{6} f''(f, f) + \frac{1}{6} f'(f'(f))) + O(h^4)$$

With each tree t associate a polynomial $\Phi(t)$, by attaching labels *i,j,k,..* to each of the vertices of t, where i is the node. Form the product of b_i and of a_{jk} for each upward growing branch from *j* to *k*, and then sum over each label.

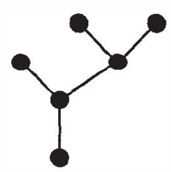
For example for the tree



$\Phi(t) = \sum b_i a_{ij} a_{jl} a_{jk} a_{km} a_{kn}$ but $c_j = \sum_k a_{jk}$

Therefore $\Phi(t) = \sum b_i a_{ij} c_j a_{jk} c_k^2$

To obtain the value of $\gamma(t)$ for a particular *t*, associate a value 1 to all the terminal vertices and a value $i+1$ with all vertices for which i is the sum of the numbers attached to vertices which branch outwards from this one. The value of $\gamma(t)$ is simply the product of the integers associated with each vertex. For the above tree, we have



$\gamma(t) = 90$

The necessary and sufficient condition for the order of the method to be q is that $\Phi(t) = \dfrac{1}{\gamma(t)}$ for all t with no more than q vertices. This approach will be explained further in Chapter II.