UNIVERSITI PUTRA MALAYSIA

RUNGE-KUTTA TYPE METHODS FOR SOLVING THIRD-ORDER ORDINARY DIFFERENTIAL EQUATIONS AND FIRST-ORDER OSCILLATORY PROBLEMS

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By

FIRAS ADEL FAWZI ALSHAREEDA

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

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DEDICATIONS

To my beloved family and friends

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

RUNGE-KUTTA TYPE METHODS FOR SOLVING THIRD-ORDER ORDINARY DIFFERENTIAL EQUATIONS AND FIRST-ORDER OSCILLATORY PROBLEMS

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April 2017

Chair: Associate Professor Norazak Senu, PhD
Faculty: Science

In this study, new Runge-Kutta type methods (RKTG) are derived for directly solving third-order ordinary differential equations ODEs of the form $y''' = f(x,y,y')$. The derivation of third-, fourth- and fifth-order explicit RKTG methods using constant step length and an embedded explicit RKTG denoted by RKTGD methods of 4(3) and 5(4) pairs for variable step size have been derived. Numerical results obtained show that the new RKTG and RKTGD methods are more accurate and efficient than several existing methods in the literature.

In the second part, a Runge-Kutta type methods are derived for directly solving general third-order differential equations of the form $y''' = f(x,y,y',y'')$ denoted as (RKTGG). The derivation of third- and fourth-order explicit RKTGG methods using constant step size have been derived. Numerical results obtained for the new methods have shown efficiency and robustness in terms of accuracy and number of function evaluations.

Next, an explicit Runge-Kutta (RK) and modified Runge-Kutta (MRK) with dispersion and dissipation properties are studied for the integration of initial value problems (IVPs) of first-order ordinary differential equations (ODEs) possessing oscillating solutions. The constructions of RK and MRK methods for constant step size and embedded MRK pair for variable step length have been derived. The strategies in choosing the free parameters are also discussed. The impacts of dispersion and dissipation relations are tested on homogeneous and non-homogeneous test problems which have oscillating solutions.

Meanwhile, trigonometrically-fitted RK and MRK methods are constructed for integration of IVPs of first-order ODEs with periodic behavior. The derivation of fourth-order trigonometrically-fitted explicit RK and MRK methods using constant step size and embedded 6(5) pair trigonometrically-fitted explicit Runge-Kutta (ETFRK) method for variable step size have been derived. We analyzed the numerical results of RK, MRK and ETFRK methods and found that our new methods are more efficient than the existing methods.

In conclusion, the new codes developed are suitable for solving system of first-order ODEs in which the solutions are in the oscillatory form and third-order ODEs.

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

KAEDAH JENIS RUNGE-KUTTA UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA PERINGKAT KETIGA DAN MASALAH AYUNAN PERINGKAT PERTAMA

Oleh

FIRAS ADEL FAWZI ALSHAREEDA

April 2017

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Di dalam kajian ini, kaedah jenis Runge-Kutta (JRKA) yang baharu diterbitkan untuk menyelesaikan secara langsung persamaan pembezaan biasa (PPB) peringkat ketiga berbentuk $y''' = f(x,y,y')$. Terbitan kaedah tak tersirat JRKA peringkat-ketiga, -keempat dan -kelima yang menggunakan panjang langkah malar dan kaedah benaman tak tersirat JRKA ditandakan dengan BJRKA untuk pasangan 4(3) dan 5(4) untuk panjang langkah berubah telah diterbitkan. Keputusan berangka yang diperoleh menunjukkan bahawa kaedah yang baharu JRKA dan BJRKA adalah lebih jitu dan cekap berbanding dengan beberapa kaedah sedia ada di dalam sorotan litratur.

Di dalam bahagian yang kedua, kaedah jenis Runge-Kutta (JRKAA) diterbitkan untuk menyelesaikan secara langsung persamaan pembezaan peringkat-ketiga am berbentuk $y''' = f(x,y,y',y'')$. Terbitan kaedah tak tersirat JRKAA peringkat-ketiga dan -keempat yang menggunakan saiz langkah malar telah diterbitkan. Keputusan berangka yang dapati untuk kaedah baharu ini menunjukkan kecekapan dan keteguhan dari segi kejituan dan bilangan penilaian fungsi.

Seterusnya, kaedah tak tersirat Runge-Kutta (RK) dan Runge-Kutta terubahsuai (RKT) dengan ciri-ciri serakan dan lesapan dikaji untuk mengamir masalah nilai awal (MNA) PPB peringkat pertama yang mempunyai penyelesaian berayun. Pembinaan kaedah RK dan RKT untuk panjang langkah malar dan pasangan benaman RKT untuk panjang langkah berubah telah diterbitkan. Strategi pemilihan parameter bebas juga dibincangkan. Impak dari hubungan serakan dan lesapan diuji ke atas masalah ujian homogen dan bukan homogen yang mempunyai penyelesaian berayun.

Sementara itu, kaedah suai-trigonometri RK dan RKT dibina untuk mengamir MNA bagi PPB peringkat pertama khas yang mempunyai tingkah laku berkala. Terbitan kaedah suai-trigonometri tak tersirat RK dan RKT peringkat-keempat yang menggunakan saiz langkah malar dan pasangan 6(5) kaedah benaman suai-trigonometri tak tersirat Runge-Kutta (BSTRK) untuk saiz langkah berubah telah diterbitkan. Kami menganalisis keputusan berangka terhadap kaedah-kaedah RK, RKT dan BSTRK dan didapati kaedah baharu kami lebih cekap berbanding kaedah sedia ada.

Sebagai kesimpulan, kod baharu yang dibangunkan adalah sesuai untuk menyelesaikan sistem PPB peringkat pertama yang mempunyai penyelesaian bentuk berayun dan PPB peringkat tiga.

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I certify that a Thesis Examination Committee has met on 28 April 2017 to conduct the final examination of Firas Adel Fawzi Alshareeda on his thesis entitled "Runge-Kutta Type Methods for Solving Third-Order Ordinary Differential Equations and First-Order Oscillatory 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 Doctor of Philosophy.

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LIST OF ABBREVIATIONS

ODEs	Ordinary Differential Equations
IVPs	Initial Value Problems
LTE	Local Truncation Error
MAXE	Maximum Error
RK	Runge-Kutta method
RK4	Fourth-order Runge-Kutta Method
MRK	Modified Runge-Kutta Method
RKTG3	The newly derived two-stage third-order RKTG method
RK3	The three-stage third-order RK method derived by Dormand (1996)
RKD3	The five-stage third-order RK method given in Dormand (1996)
RKZ3	The five-stage third-order RK method given in Hairer et al. (2010)
RKTG4	The new four-order three-stage RKTG method
RKS4	The four-stage fourth-order RK method derived by Butcher (2008)
RKZ4	The five-stage fourth-order RK method given in Hairer et al. (2010)
RKE4	The six-stage fourth-order RK method given in Lambert (1991)
RKTG5	The new four-stage fifth-order RKTG method
RK5B	The six-stage fifth-order RK method derived by Butcher (2008)
RK5F	The six-stage fifth-order RK method derived by Lambert (1991)
DOPRI5	The four-stage fourth-order RK method given in Dormand (1996)
TFRKF6(5)	The new embedded 6(5) explicit RK method with trigonometrically-fitted
RKTG4(3)	The new 4(3) pair of embedded method
RKTG5(4)	The new 5(4) pair of embedded method

CHAPTER 1

INTRODUCTION

1.1 Ordinary Differential Equations (ODEs)

The ordinary differential equation is a differential equation that contains only ordinary derivatives of one or more unknown functions with respect to a single independent variable. In practice, however, few of the problems originating from the study of physical phenomena can be solved exactly.

The n-th order ODEs can be written as:

$$y^{(n)} = f\big(x, y, ..., y^{(n-1)}\big), n = 2, 3, 4, \dots \tag{1.1}$$

with initial conditions:

$$y(a) = y_0$$

and

$$y^{(i)}(a) = \eta_i,\ 0 < i \leq n-1,\ x \in [a,b]$$

while the first order ODEs can be written as:

$$\frac{dy}{dx} = f\big(x, y(x)\big), y(a) = y_0 \tag{1.2}$$

for $x \in [a,b]$.
In (1.2), the quantity being differentiated, y is named as the dependent variable, while the quantity with respect to which y is differentiated, x is named as independent variable.

1.2 The Initial Value Problems (IVPs)

Ordinary differential equations (ODEs) are equations that involve an unknown function with independent variable and one or more of its derivatives. ODEs arise in many contexts of engineering and science such as fluid dynamics, radioactive decay and population growth. Many theoretical and numerical studies for such equations have appeared in the literature. The analytical way to solve ODEs is via application of integration technique. However, the anti-derivatives for most realistic systems of ODEs are difficult or impossible to find. Thus, numerical methods for ODEs have attracted considerable attention.

Definition 1.1 *The initial value problems (IVPs) of third order is defined as:*

$$y'''(x) = f(x, y, y'), \tag{1.3}$$

with initial conditions

$$y(x_0) = y_0, \quad y'(x_0) = y'_0, \quad y''(x_0) = y''_0$$

where $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ *, and* $y_0, y'_0, y''_0 \in \mathbb{R}^n$.

Definition 1.2 *The initial value problems (IVPs) of general third order is defined as:*

$$y'''(x) = f(x, y, y', y''), \tag{1.4}$$

with initial conditions

$$y(x_0) = y_0, \quad y'(x_0) = y'_0, \quad y''(x_0) = y''_0$$

where $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ *, and* $y_0, y'_0, y''_0 \in \mathbb{R}^n$.

Definition 1.3 *The initial value problems (IVPs) of system first order differential equation is defined as:*

$$y'(x) = f(x, y), \tag{1.5}$$

with initial conditions

$$y(x_0) = y_0, \quad y'(x_0) = y'_0, \quad x \in [a, b]$$

where

$$y(x) = [y_1(x), y_2(x), ..., y_s(x)]^T$$
$$f(x, y) = [f_1(x, y), f_2(x, y), ..., f_s(x, y)]^T ,$$

and y_0 *is a given vector of initial conditions and their solution is oscillatory.*

One way to solve (1.3)–(1.5) is by Runge-Kutta (RK) method. RK method can be divided into two groups which are explicit and implicit methods. An easy and quick way to distinguish the type of these methods is that the implicit methods need an iteration scheme, usually Newton type iteration during the integration, whereas the explicit methods do not. Therefore, the computations for implicit methods are more expensive than explicit methods. In addition to the implementation of the methods, accuracy and stability are to further factors for judging the efficacy of a method. In this study, we are focusing on solving problem (1.3)–(1.4) by using explicit Runge-Kutta type methods for directly solving third-order differential equations and solving problem (1.5) by using RK methods for oscillating problems.

1.3 Existence and Uniqueness of Solution

Initial value problems describe a problem together with the behavior of it's path taken at some initial points of the independent variable x. Some of the characteristic of initial value problems that answer this question, as given by Butcher (2008), are existence of solution, uniqueness of the solution if it exists and the sensitivity of the solution to a small perturbation to the initial information. One of the well known conditions that guarantees these characteristics is the Lipschitz condition.

Definition 1.4 *A function $f : R \times R^d \to R^d$ is said to satisfy Lipschitz condition in its second variable if there exist a constant L such that for any $x \in [a,b]$ and $y_1, y_2 \in R^d$,*

$$\| f(x, y_1 - f(x, y_2) \| \leq L \| y_1 - y_2 \|, \tag{1.6}$$

where L is called Lipschitz constant.

Theorem 1.1 : (Existence and Uniqueness)
Let $f(x, y(x))$ be defined and continuous $\forall$ points $\big(x, y(x)\big)$ in a domain D defined by $x \in [a,b], y \in (-\infty, \infty)$, a and b are finite, and that $f(x, y(x))$ satisfies Lipschitz condition. Then for any given number ζ, $\exists$ a unique solution $y(x)$ of the IVP (1.3)*, where $\forall$ $\big(x, y(x)\big) \in D$, $y(x)$ is continuous and differentiable.*

The proof is given by Henrici (1962).

1.4 Runge-Kutta (RK) Methods

In the fact, Runge-Kutta method is a most common one step method for solving IVPs of first-order ODEs. The general formulation of explicit RK method is given by,

$$y_{n+1} = y_n + h \sum_{i=1}^{m} b_i k_i \tag{1.7}$$

where

$$k_i = f\left(x_n + c_i h,\, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j \right), \quad i = 1, ..., m, \tag{1.8}$$

and the following the row-sum assumption holds

$$c_i = \sum_{j=1}^{m} a_{ij}.$$

The m-stage explicit RK method in the matrix form for first-order equations or system of equations can be written using Butcher Tableau as given in (Table 1.1)

Table 1.1: m-stage explicit Runge-Kutta method

$$
\begin{array}{c|ccccc}
0 & & & & & \\
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
. & . & . & & & \\
. & . & . & & & \\
. & . & . & & & \\
c_m & a_{m1} & a_{m2} & \dots & a_{m,m-1} & \\
\hline
 & b_1 & b_2 & \dots & b_{m-1} & b_m
\end{array}
$$

The method is said to be explicit when $a_{ij} = 0$ for $i \leq j$ and implicit otherwise.

1.4.1 Algebraic Order Conditions for RK method

The order conditions for RK method may be obtained from direct expansion of Taylor series using the Local Truncation Error (LTE). The m-stage up to order six, RK methods are given as follows:

Order 1

$$\sum b_i = 1 \tag{1.9}$$

Order 2

$$\sum b_i c_i = \frac{1}{2} \tag{1.10}$$

Order 3

$$\frac{1}{2}\sum b_i {c_i}^2 = \frac{1}{6} \tag{1.11}$$

Order 4

$$\frac{1}{6}\sum b_i {c_i}^3 = \frac{1}{24}, \sum b_i a_{ij} c_j = \frac{1}{24} \tag{1.12}$$

Order 5

$$\frac{1}{24}\sum b_i {c_i}^4 = \frac{1}{120}, \frac{1}{4}\sum b_i c_i a_{ij} c_j = \frac{1}{120},$$

$$\frac{1}{2}\sum b_i a_{ij} {c_j}^2 = \frac{1}{120} \tag{1.13}$$

Order 6

$$\frac{1}{120}\sum b_i {c_i}^5 = \frac{1}{720}, \frac{1}{20}\sum b_i {c_i}^2 a_{ij} c_j = \frac{1}{720},$$

$$\frac{1}{10}\sum b_i c_i a_{ij} {c_j}^2 = \frac{1}{720}, \frac{1}{6}\sum b_i a_{ij} {c_j}^3 = \frac{1}{720}$$

$$\sum b_i a_{i,j} a_{j,k} c_k = \frac{1}{720}. \tag{1.14}$$

Definition 1.5 *A Runge-Kutta method had algebraic order p, when the method's Taylor series expansion agrees with the theoretical solution Taylor series expansion in the p first term:*

$$y^{(n)}(x) = y_n^n(x),\ n = 1, 2, ..., p$$

A Runge-Kutta must satisfy a number of equations, in the order to have a certain algebraic order. These equations are shown during the production of the method.

1.4.2 Local Truncation Error (LTE)

Dormand (1996) mentioned that the Local Truncation Error (LTE) is the amount or value by the exact solution fails to satisfy the numerical solution.
Consider the equations

$$y(x_{n+1}) = y(x_n) + h_n\Delta\left(x_n, y(x_n), h_n\right) \tag{1.15}$$

$$y_{n+1} = y_n + h\Phi\left(x_n, y(x_n), h_n\right) \tag{1.16}$$

$$t_{n+1} = y(x_n) + h\Phi\left(x_n, y(x_n), h_n\right) - y(x_{n+1}) \tag{1.17}$$

From the above equations, the local truncation error for the Taylor series method is

$$t_{n+1} = y(x_n) + h\Phi\left(x_n, y(x_n), h\right) - \left(y(x_n) + h_n\Delta\left(x_n, y(x_n), h\right)\right) \tag{1.18}$$

then yielding

$$t_{n+1} = \left\{h\Phi\left(x_n, y(x_n), h\right) - \Delta\left(x_n, y(x_n), h\right)\right\} \tag{1.19}$$

In terms of derivatives, and using the elementary differentials notation, the pth order method has LTE as

$$\begin{aligned} t_{n+1} &= -\sum_{i=p+1}^{\infty} \frac{h^i}{i!} \sum_{j=1}^{n_!} \alpha_j^{(i)} F_j^{(i)}, \\ &= -\sum_{i=p+1}^{\infty} \frac{h^i}{i!} y^{(i)}(x_n). \end{aligned} \tag{1.20}$$

The Taylor increment can be expressed in finite form as:

$$\begin{aligned} \Delta\left(x_n, y(x_n), h\right) =& y'(x_n)\frac{h}{2}y''(x_n) + \ldots + \frac{h^{p-1}}{p!}y^{(p)}(x_n) \\ &+ \frac{h^p}{(p+1)!}y^{(p+1)}(x_n + \eta h),\ \eta\, \varepsilon\, (0,1) \end{aligned} \tag{1.21}$$

so the LTE derives from the last term of this polynomial. The value of η is not generally. Consequently, there exist a real positive number A independent of the h-step size such that

$$\| t_{n+1} \| \leq Ah^{p+1} \tag{1.22}$$

and for a pth order method it is usual to write

$$t_{n+1} = O(h^{p+1}). \tag{1.23}$$

for any method of type (1.16) the local truncation error may be expressed as

$$t_{n+1} = \sum_{i=p+1}^{\infty} h^i \varphi_{i-1}(x_n, y(x_n)) \tag{1.24}$$

where the φ_i are called error functions. Using (1.20) the Taylor series scheme has error functions

$$\varphi_i = -\frac{y^{(i+1)}}{(i+1)!} \tag{1.25}$$

where the principal error function is φ_p and will be dominant influence on the local truncation error if h is sufficiently small Dormand (1996).

The general formula for the components of the local truncation error RK processes are

$$\begin{aligned} t_{n+1} &= \sum_{i=1}^{\infty} h^i \left[\sum_{j=1}^{n_i} \left(\beta_j^{(i)} - \frac{a_j^{(i)}}{i!} \right) F_j^{(i)} \right] \\ t_{n+1} &= \sum_{i=1}^{\infty} h^i \left[\sum_{j=1}^{n_i} \tau_i^{(i)} F_j^{(i)} \right] \end{aligned} \tag{1.26}$$

where

$$\tau_i^{(i)} = \frac{\beta_i^{(i)} - a_i^{(i)}}{i!}, \ i = 1, 2, \ldots, n_i$$

are called error coefficients.

Below are y error coefficients up to order four for the RK processes,

1^{st} Order:

$$\tau_1^{(1)} = \sum_{i=1} b_i - 1 \tag{1.27}$$

2^{nd} Order:

$$\tau_1^{(2)} = \sum_{i=1} b_i c_i - \frac{1}{2} \tag{1.28}$$

3^{rd} Order:

$$\tau_1^{(3)} = \frac{1}{2} \sum_{i=1} b_i c_i^2 - \frac{1}{6}, \tag{1.29}$$

$$\tau_2^{(3)} = \sum_{i,j=1} b_i a_{ij} c_j - \frac{1}{6}. \tag{1.30}$$

4^{th} Order:

$$\tau_1^{(4)} = \frac{1}{6} \sum_{i=1} b_i c_i^3 - \frac{1}{24}, \tag{1.31}$$

$$\tau_2^{(4)} = \sum_{i,j,k=1} b_i a_{ij} a_{ik} c_k - \frac{1}{8}, \tag{1.32}$$

$$\tau_3^{(4)} = \frac{1}{2} \sum_{i,j=1} b_i a_{ij} c_j^2 - \frac{1}{32}, \tag{1.33}$$

$$\tau_4^{(4)} = \sum_{i,j,k} b_i a_{ij} a_{jk} c_k - \frac{1}{24}. \tag{1.34}$$

1.5 Analysis of Phase-fitted and Amplification-fitted RK Method

We consider the following linear scalar equation:

$$y' = iwy. \tag{1.35}$$

The exact solution of this equation with the initial value $y(x_0) = y_0$ satisfies

$$y(x_0 + h) = R(H)\, y_0, \tag{1.36}$$

where $R(H) = exp(H)$. This means that after a period of time h, the exact solution experiences a phase advance $H = wh$ and the amplification remains constant. When applying the RK method (1.8) to (1.35) yield

$$y_{n+1} = R(H)\, y_0, \tag{1.37}$$

where

$$R(H) = 1 + Hb^T (I - HA)^{-1} e,\ e = (1, ..., 1)^T. \tag{1.38}$$

The numerical solution attain a phase advance arg $R(H)$ and the amplification factor $|R(H)|$ where $R(H)$ is called the stability function of the method (1.8).

Denote the real and imaginary part of $R(H)$ by $U(H)$ and $V(H)$ respectively. Then, for small h we have

$$U(H) = 1 - H^2(b^T Ae) + H^4(b^T A^3 e) - H^6(b^T A^5 e) + \dots , \tag{1.39}$$

$$V(H) = H(b^T e) - H^3(b^T A^2 e) + H^5(b^T A^4 e) - H^7(b^T A^6 e) - \dots . \tag{1.40}$$

For small h, *arg R(H)* $= \tan^{-1}\left(\frac{V(H)}{U(H)}\right)$ and $|R(H)| = \sqrt{U^2(H) + V^2(H)}$.
van der Houwen and Sommeijer (1987) stated, the quantities

$$P(v) = v - arg\ R(H),\ D(v) = 1 - |R(H)| \tag{1.41}$$

which are called the phase-lag (or dispersion) and the error of amplification factor (or dissipation) of the method, respectively. If

$$P(H) = O(H^{q+1}),\ D(H) = O(H^{p+1}), \tag{1.42}$$

then the method is called dispersive of order q and dissipative of order p, respectively. If

$$P(H) = 0,\ D(H) = 0, \tag{1.43}$$

the method is called phase-fitted (or zero-dispersive) and amplification-fitted (or zero-dissipative), respectively. It is interesting to consider the phase properties of the update of the scheme (1.1). Suppose that the internal stages have been exact for the linear equation (1.35), that is, $Y_i = exp(c_i H)\ y_0$, then the update gives

$$R(H) = 1 + H \sum_{i=1}^{s} b_i(H)\ exp(c_i H). \tag{1.44}$$

Denote the real and imaginary part of $R(H)$ by $U(H)$ and $V(H)$, respectively. Then, for small h.

$$U(H) = 1 - H \sum_{i=1}^{s} b_i(H) \sin(c_i H), \tag{1.45}$$

$$V(H) = H \sum_{i=1}^{s} b_i(H) \cos(c_i H). \tag{1.46}$$

Theorem 1.2 *The method* (1.8) *is phase-fitted and amplification-fitted if and only if*

$$U(H) = \cos(H),\ V(H) = \sin(H) \tag{1.47}$$

1.6 Modified Runge-Kutta (MRK) Method

An explicit m-stage MRK formula is given by

$$y_{n+1} = y_n + h \sum_{i=1}^{m} b_i f(x_n + c_i h, Y_i) \tag{1.48}$$

where

$$Y_i = g_i y_n + h \sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j). \tag{1.49}$$

The method is said to be explicit when $a_{ij} = 0$ for $i \leq j$ and implicit otherwise. The method in (1.48) and (1.49) can be reduced into Butcher tableau form $\big($see Table 1.2$\big)$

Table 1.2: *m*-stage modified explicit Runge-Kutta method

$$\begin{array}{c|c|cccccc}
0 & & & & & & \\
c_2 & g_2 & a_{21} & & & & \\
c_3 & g_3 & a_{31} & a_{32} & & & \\
. & . & . & . & & & \\
. & . & . & . & & & \\
. & . & . & . & & & \\
c_m & g_m & a_{m1} & a_{m2} & ... & a_{m,m-1} & \\
\hline
 & & b_1 & b_2 & ... & b_{m-1} & b_m
\end{array}$$

1.7 Analysis of Phase-Lag of the MRK Method

To develop the MRK method, we utilize the test equation (1.35) based on van der Houwen and Sommeijer (1987). Then, we compare the theoretical solution and the numerical solution for this equation. By requiring that the solutions are in phase with maximal order in the step-size h, we derive the so-called dispersion relation. Applying the method (1.48) and (1.49) to the test equation (1.35) we obtain

$$y_n = a_*^n y_0$$

with

$$a_* = A_m(H^2) + iHB_m(H^2), H = wh \tag{1.50}$$

The amplification factor is $a_* = a_*(H)$, and y_n denotes the approximation to $y(x_n)$. A comparison of (1.50) with the solution of (1.35) leads to the following definition of the dispersion or phase error or phase-lag and the amplification error.

Definition 1.6 *An explicit* m*-stage MRK, presented in Table* (1.2) *where the quantities:*

$$t(H) = H - arg[a_*(H)],\ a(H) = 1 - \mid a_*(H) \mid \tag{1.51}$$

are called the dispersion or phase error or phase-lag and the amplification error respectively. If $t(H) = O(H^{r+1})$, and $a(H) = O(H^{s+1})$ then the method is said to be phase-lag of order r and dissipative of order s.

From the (1.51) it follows that,

$$a(H) = 1 - \sqrt{[A_m^2(H^2) + H^2 B_m^2(H^2)]}. \tag{1.52}$$

Meanwhile, for the modified Runge-Kutta method given in Table 1.2, the following formula is used for the direct calculation of the phase-lag order r and the phase-lag constant q

$$\tan(H) - H\left[\frac{B_m(H^2)}{A_m(H^2)}\right] = qH^{r+1} + O(H^{s+3}). \tag{1.53}$$

The analysis of phase-fitted (dispersion of order infinity) and amplification-fitted (dissipation of order infinity) are based on dispersion and dissipation quantities that have discussed above. The modified RK method is phase-fitted and amplification-fitted if the following conditions hold:

$$t(H) = 0 \qquad \text{and} \qquad a(H) = 0.$$

1.8 Absolute Stability Analysis for MRK

Consider the test problem of differential equation (1.35) and applying to MRK (1.48) and (1.49) form, then we have

$$Y_i = g_i y_n + \widehat{h}\sum_{j=1}^{s} a_{ij} Y_j \tag{1.54}$$

$$y_{n+1} = y_n + \widehat{h}\sum_{i=1}^{s} b_i Y_i \tag{1.55}$$

$$\mathbf{Y} = [Y_1, Y_2, ..., Y_s]^T, \mathbf{g} = [g_1, g_2, ..., g_s]^T$$

Substitute in (1.55) gives

$$y_{n+1} = y_n + \widehat{h}[b_1 Y_1 + b_2 Y_2 + ... + b_s Y_s]$$

or

$$y_{n+1} = y_n + \widehat{h}[\, b_1 \; b_2 \; ... \; b_s] \begin{bmatrix} Y_1 \\ Y_2 \\ . \\ . \\ . \\ Y_s \end{bmatrix}$$

Substitute in (1.54) then

$$Y_1 = g_1 y_n + \widehat{h}[a_{11} Y_1 + a_{12} Y_2 + ... + a_{1s} Y_s]$$

$$Y_2 = g_2 y_n + \widehat{h}[a_{21} Y_1 + a_{22} Y_2 + ... + a_{2s} Y_s]$$

$$.$$
$$.$$
$$.$$
$$Y_s = g_s y_n + \widehat{h}[a_{s1}Y_1 + a_{s2}Y_2 + ... + a_{ss}Y_s]$$

$$\begin{bmatrix} Y_1 \\ Y_2 \\ . \\ . \\ . \\ Y_s \end{bmatrix} = y_n \begin{bmatrix} g_1 \\ g_2 \\ . \\ . \\ . \\ g_s \end{bmatrix} + \widehat{h} \begin{bmatrix} a_{11} & ... & a_{1s} \\ . & ... & . \\ . & ... & . \\ . & ... & . \\ a_{s1} & ... & a_{ss} \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ . \\ . \\ . \\ Y_s \end{bmatrix}$$

$$Y = y_n G + \widehat{h}AY, \tag{1.56}$$

$$Y = [Y_1, Y_2, ..., Y_s], \quad G = [g_1, g_2, ..., g_s],$$

$$y_{n+1} = y_n + \widehat{h}BY, \tag{1.57}$$

where

$$B = [b_1 b_2 ... b_s].$$

From (1.56)

$$Y - \widehat{h}AY = y_n G,$$
$$\left(I - \widehat{h}A\right) Y = y_n G,$$
$$Y = \left(1 - \widehat{h}A\right)^{-1} y_n G. \tag{1.58}$$

Substitute (1.58) in (1.57), we have

$$y_{n+1} = y_n + \widehat{h}B\left(I - \widehat{h}A\right)^{-1} Y_n G,$$

$$Y_{n+1} = \left[1 + \widehat{h}B\left(1 - \widehat{h}A\right)^{-1} G\right] Y_n. \tag{1.59}$$

1.9 Trigonometrically-fitting Explicit MRK Method

A generalized explicit modified Runge-Kutta MRK method formula is given in (1.48) and (1.49) led us to the following theorem:

Theorem 1.3 *(see Liu et al. (2013))*
Method (1.49) *is of exponential order p if the following condition is satisfied:*

$$\cos(v) + i\sin(v) = 1 + \sum_{k=1}^{s} (iv)^k bA^{k-1}e \ , \tag{1.60}$$

where $v = w_i h$ *for* $i = 0, 1, ..., p$.

Definition 1.7 *A Runge-Kutta method that integrates exactly the function* e^{iwx} *and* e^{-iwx} *or equivalently* $\sin(wx)$ *and* $\cos(wx)$ *with* $w > 0$ *the principal frequency of the problem when applied to the test equation* $y' = iwy$ *is said to be trigonometrically-fitted.*

Let $y_n = e^{iwx_n}$ be the solution that integrate the ordinary differential equation

$$\begin{aligned} y'(x) &= f(x,y),\ y(x_0) = y_0, \\ y'(x_0) &= y'_0,\ x \in [a,b] \end{aligned} \tag{1.61}$$

Computing the value of $y_{n+1},\ y'_n$ and substitution in (1.49) we have:

$$e^v = 1 + iv \sum_{i=1}^{m} b_i g_i - v^2 \sum_{i=1}^{m} b_i \sum_{j=1}^{i-1} a_{ij}(Y_j e^{-iwx_n}). \tag{1.62}$$

where $v = wh$. Using the formula :

$$e^v = \cos(v) + i\sin(v) \tag{1.63}$$

and by comparing the real and imaginary part we have:

$$\begin{aligned} \cos(v) =& 1 - v^2 \sum_{i=1}^{m} b_i \sum_{j=1}^{i-1} a_{ij}(Y_j e^{-iwx_n}), \\ \sin(v) =& v \sum_{i=1}^{m} b_i g_i \ . \end{aligned} \tag{1.64}$$

1.10 Embedded Runge-Kutta Methods

An explicit m-stage Runge-Kutta formula is given by

$$y_{n+1} = y_n + h \sum_{i=1}^{m} b_i f(x_n + c_i h, Y_i) \tag{1.65}$$

where

$$Y_i = y_n + h\sum_{j=1}^{i-1} a_{ij} f(x_n + c_i h, Y_j),\ i = 1,...,m. \tag{1.66}$$

with the associated Butcher tableau (see Table (1.1)), or in matrix form

$$\begin{array}{c|c} \mathrm{c} & A \\ \hline & b \end{array}$$

where A is matrix $(a_{i,j})_{m\times m}$, $c = (c_1, c_2, ..., c_m)^T$, $b = (b_1, b_2, ..., b_m)$. In RK method the embedded pair $q(p)$ is based on the RK method (c, A, b) of order q and another RK method (c, A, b^*) of order $p < q$. An embedded pair is characterized by Butcher tableau

$$\begin{array}{c|c} \mathrm{c} & A \\ \hline & b \\ \hline & b^* \end{array}$$

An embedded pair of explicit Runge-Kutta method is used in variable step-size algorithm because its provide a cheap error estimation. From embedded method we obtain an estimate

$$EST_{n+1} = \| y_{n+1} - y^*_{n+1} \| . \tag{1.67}$$

For the numerical integration of the equation (**??**) we used step-size control procedure by Raptis and Cash (1985):

- if $EST_{n+1} < \frac{Tol}{100},\ h_{n+1} = 2h_n,$
- if $\frac{Tol}{100} \leq EST_{n+1} < Tol,\ h_{n+1} = h_n,$
- if $EST_{n+1} \geq Tol,\ h_{n+1} = \frac{h_n}{2}$ and repeat the step,

where Tol is the requested local error. It should be noted that the q th-order approximation y_n is used as the initial value for the (n+1) th step, that mean the embedded pair is applied in local extrapolation mode or higher order mode.

1.11 Problem Statement

Initial value problem (IVP) of third-order ODEs of the form $y''' = f(x,y,y')$ where the second derivative do not appear explicitly and the general third-order ODEs $y''' = f(x,y,y',y'')$ often arise in many fields of applied sciences such as electromagnetic wave, thin film flow and gravity driven flow. The aim of this research is to develop algebraic order conditions for Runge-Kutta type methods to directly solve third-order ODEs $y''' = f(x,y,y')$ and $y''' = f(x,y,y',y'')$ and then derive a Runge-Kutta method based on the order conditions developed.

1.12 Scope of Study

First of all, the main purpose of this research is to construct Runge-Kutta type methods for directly solving third-order ODEs of the form $y''' = f(x,y,y')$ and general third-order ODEs of the form $y''' = f(x,y,y',y'')$. Then, the secondary aim for this research is to solve first-order ordinary differential equations (1.5) in which the solutions exhibit a pronounced oscillatory character and we are focusing on solving problem (1.5) by using explicit Runge-Kutta and modified Runge-Kutta methods for oscillatory problems with phase-fitted, amplification-fitted and trigonometrically-fitted techniques for constant and variable step size mode.

1.13 Objectives of the Study

This study concerns on the derivation of new and efficient codes that are based on the explicit RK method for solving systems of third-order ODE directly for both constant and variable step size and to develop an improved numerical methods based on RK method that can accurately and efficiently integrate first-order IVPs whose the solution is oscillatory in nature. Specifically, we suggest the following:

- To develop algebraic order conditions and to derive Runge-Kutta type methods for directly solving third-order ordinary differential equations $y''' = f(x,y,y')$.
- To construct embedded explicit Runge-Kutta type methods for directly solving third-order ordinary differential equations $y''' = f(x,y,y')$.
- To develop algebraic order conditions and to derive Runge-Kutta type methods for directly solving general third-order ordinary differential equations $y''' = f(x,y,y',y'')$.
- To derive phase-fitted and amplification-fitted explicit Runge-Kutta and modified Runge-Kutta (MRK) method for solving oscillatory first order ordinary differential equations.
- To construct embedded high order phase-fitted MRK method for solving oscillatory first order ordinary differential equations.

- To derive trigonometrically-fitted explicit Runge-Kutta and modified Runge-Kutta methods for solving oscillatory first-order ordinary differential equations.
- To construct embedded high order trigonometrically-fitted RK method for solving oscillatory first-order ordinary differential equations.

1.14 Outline of Thesis

In Chapter 1, a concise introduction on ordinary differential equations and development of the numerical methods, basic theory on algebraic order of RK method, dispersion order, dissipation order and local truncation error (LTE) for RK are discussed.

In Chapter 2, we are dealing with the review of the numerical methods for solving third-order and general third-order ODEs. Fallowed by with the review of the earlier works on numerical methods for solving first-order ODEs.

In Chapter 3, we derive two-stage third-order, three-stage fourth-order and four-stage fifth-order with algebraic order up to order six for solving directly third-order ODEs. The development of the new RK type method and the construction of order conditions for solving third-order ODEs of the form $y''' = f(x,y,y')$ are discussed. The numerical outcomes of the new methods for solving directly third-order ODEs with form $y''' = f(x,y,y')$ have been compared with methods that reduced the third-order ODEs to the system of first-order ODEs.

In Chapter 4, we construct the embedded pairs for RKTG methods for variable step-size where the higher order of the methods are based on the methods derived in Chapter 3. The methods have been compared with embedded existing RK methods for solving third-order ODEs.

In Chapter 5, the development of derive three-stage third-order and four-stage fourth-order and we discussed the strategies for obtained the new methods. The results have been compared with existing methods for directly solving general third-order ODEs of the form $y''' = f(x,y,y',y'')$.

In Chapter 6, we debated the phase-fitted and amplification-fitted for explicit RK and MRK methods. We also discuss the embedded pair of phase-fitted MRK. The choice of free parameters in getting the optimized pair are also discussed. The numerical results have been obtained and compared with existing methods.

In Chapter 7, we discussed the trigonometrically-fitted RK and MRK. Moreover, we discuss the embedded pair for explicit RK. The numerical outcomes compared with existing methods for solving oscillatory problems.

Lastly, the summary of the entire thesis, conclusions and future studies are given in Chapter 8.

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