UNIVERSITI PUTRA MALAYSIA

RUNGE-KUTTA TYPE METHODS FOR SOLVING SPECIAL THIRD AND FOURTH ORDER ORDINARY DIFFERENTIAL EQUATIONS

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By

KASIM ABBAS HUSSAIN

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

March 2017

DEDICATIONS

I dedicate this work to

My parents Abbas and Amal as well as my brothers and sisters

for their support and encouragement

and

My wife Zainab for her great patience, support in all my life

and

My beloved daughters Maryam, Daniah and Zahraa

and

My respected Teachers.

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 SPECIAL THIRD AND FOURTH ORDER ORDINARY DIFFERENTIAL EQUATIONS

By

KASIM ABBAS HUSSAIN

March 2017

Chair: Professor Fudziah Ismail, PhD
Faculty: Science

This thesis is focused on developing Runge-Kutta type methods for solving two types of ordinary differential equations (ODEs). The first type is the special third-order ODEs which do not depend on the first derivative $y'(x)$ and the second derivative $y''(x)$ explicitly. The second is the special fourth-order ODEs which are not dependent on the first derivative $y'(x)$, the second derivative $y''(x)$ and third derivative $y'''(x)$ explicitly. These types of ODE often used to describe the mathematical models for problems arises in several fields of applied sciences and engineering.

Traditionally, these ODEs are solved by reducing them to an equivalent system of first-order ordinary differential equations. However, it is more efficient in terms of accuracy, the number of function evaluations as well as computational time, if they can be solved directly by using numerical methods.

The first part of the thesis described the construction of the Improved Runge-Kutta type method for directly solving the special third-order ODEs where the method is denoted as IRKD method. Taylor series expansion is used to derive the order conditions of the IRKD method. Based on these order conditions, three-stage fourth-order and four-stage fifth-order IRKD methods are derived. Codes based on these methods are developed and then used to solve the special third-order ODEs. The IRKD methods are also used to solve physical problem in thin film flow.

The second part of the thesis is focused on the derivation of the direct Runge-Kutta type method denoted as RKFD method for solving the special fourth-order ODEs. The order conditions of the RKFD methods are derived by using two approaches; the

first approach is using the Taylor series expansion and the second approach is using the B-series and the associated relevant-colored trees. Based on the order conditions, three-stage fourth-order, three-stage fifth-order and four-stage sixth-order RKFD methods are derived. Codes based on the RKFD methods are developed and used for solving the special fourth-order ODEs. The RKFD methods are also applied to solve engineering problem which is the ill-posed problem in a beam on elastic foundation. Then two embedded RFKD pairs of order four in five and order five in six are derived. Based on the embedded RKFD methods, the variable step-size codes are developed and used to solve the special fourth-order ODEs.

In conclusion, the new IRKD and RKFD methods developed in this thesis are suitable for directly solving special third-order and fourth-order ODEs respectively. The methods are also more efficient than the existing Runge-Kutta type methods in terms of accuracy, computational time and number of function evaluations.

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

JENIS KAEDAH RUNGE-KUTTA UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA KHAS PERINGKAT TIGA DAN EMPAT

Oleh

KASIM ABBAS HUSSAIN

Mac 2017

Pengerusi: Profesor Fudziah Ismail, PhD
Fakulti: Sains

Tesis ini tertumpu kepada membangunkan kaedah Runge-Kutta untuk menyelesaikan dua jenis persamaan pembezaan biasa (PPB). Jenis yang pertama adalah persamaan pembezaan khas peringkat ketiga yang tidak bersandar kepada pembezaan pertamanya $y'(x)$ dan pembezaan keduanya $y''(x)$ secara tak tersirat. Yang kedua ialah persamaan pembezaan biasa khas peringkat keempat yang juga tidak bersandar kepada pembezaan pertamanya $y'(x)$, pembezaan keduanya $y''(x)$ dan pembezaan yang ketiganya $y'''(x)$ secara tak tersirat. Persamaan pembezaan jenis ini biasa digunakan untuk menerangkan model bermatematik untuk masalah yang timbul dalam beberapa bidang sains gunaan dan kejuruteraan.

Secara tradisinya, PPB ini diselesaikan dengan menurunkannya kepada sistem perasamaan pembezaan peringkat pertama yang setara. Walau bagaimanapun, adalah lebih cekap dari segi kejituan, bilangan penilaian fungsi dan masa pengiraan, jika ia boleh diselesaikan secara terus menggunakan kaedah berangka.

Bahagian pertama tesis menerangkan tentang membangunkan kaedah Runge-Kutta Penambaikan yang disebut IRKD untuk menyelesaikan secara terus PPB khas peringkat ketiga. Kembangan siri Taylor digunakan untuk menerbitkan syarat peringkat kaedah IRKD tersebut. Berdasarkan syarat peringkat ini, kaedah IRKD tahap-tiga, peringkat-keempat dan kaedah tahap-empat, peringkat-kelima diterbitkan. Kod berdasarkan kaedah IRKD ini dibangunkan dan digunakan untuk menyelesaikan PPB khas peringkat ketiga. Kaedah IRKD ini juga digunakan untuk menyelesaikan masalah fizikal dalam aliran filem nipis.

Bahagian kedua tesis ini tertumpu kepada menerbitkan kaedah Rung-Kutta yang dikenali sebagai RKFD untuk menyelesaikan secara terus PPB khas peringkat keempat. Syarat peringkat bagi kaedah RKFD ini diterbitkan menggunakan dua pendekatan; yang pertama menggunakan kembangan siri Taylor dan yang kedua menggunakan Siri-B dan pokok berwarna yang bersesuaian dan berkaitan dengannya. Berdasarkan syarat peringkat tersebut, kaedah RKFD tahap-tiga peringkat-keempat, tahap-tiga peringkat-kelima dan tahap-empat peringkat-keenam diterbitkan. Kod berdasarkan kaedah RKFD tersebut dibangunkan dan digunakan untuk menyelesaikan PPB khas peringkat keempat. Kaedah RKFD itu juga digunakan untuk menyelesaikan masalah kejuruteraan, iaitu masalah tak teraju rapi dalam rasuk yang mempunyai asas elastik. Seterusnya dua pasang kaedah RKFD terbenam peringkat-empat dalam peringkat-lima dan peringkat-lima dalam peringkat-enam diterbitkan. Berdasarkan kaedah tersebut kod dengan panjang langkah berubah dibangunkan untuk menyelesaikan PPB khas peringkat keempat.

Kesimpulannya, kaedah baharu IRKD dan RKFD yang dibangunkan dalam tesis ini adalah sesuai untuk menyelesaikan secara terus PPB khas peringkat ketiga dan keempat masing-masingnya. Kaedah ini juga lebih cekap daripada jenis kaedah Runge-Kutta sedia ada dari segi kejituan, masa pengiraan dan bilangan penilaian fungsi.

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I certify that a Thesis Examination Committee has met on 6 March 2017 to conduct the final examination of Kasim Abbas Hussain on his thesis entitled "Runge-Kutta Type Methods for Solving Special Third and Fourth Order Ordinary Differential Equations" 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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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy.

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Declaration by graduate student

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This is to confirm that:

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LIST OF ABBREVIATIONS

RK	Runge-Kutta method
RK4	Fourth-order Runge-Kutta method
RK3/8	3/8 Rule Runge-Kutta method
RK5	Fifth-order Runge-Kutta method
RK5B	Fifth-order Runge-Kutta method given in Butcher (2008)
RK5N	Fifth-order Runge-Kutta method given in Hairer et al. (1993)
RK6B	Sixth-order Runge-Kutta method derived by Butcher (2008)
RK6N	Sixth-order Runge-Kutta method given in Hairer et al. (1987)
ODEs	Ordinary Differential Equations
h	Step size
IVPs	Initial Value Problems
RKN	Runge-Kutta-Nyström method
IRK	Improved Runge-Kutta method
IRKN	Improved Runge-Kutta-Nyström method
IRKD	The new direct improved Runge-Kutta type method
IRKD4	The new direct three-stage fourth-order improved Runge-Kutta type method
IRKD5	The new direct four-stage fifth-order improved Runge-Kutta type method
RKD4	The direct three-stage fourth-order RKD method derived by Mechee (2014)
RKD5	The direct three-stage fifth-order RKD method derived by Mechee et al. (2013)
RKFD	The new direct Runge-Kutta type method for solving fourth-order ODEs
RKFD4	The new direct three-stage fourth-order Runge-Kutta type method for solving fourth-order ODEs
RKFD5	The new direct three-stage fifth-order Runge-Kutta type method for solving fourth-order ODEs
RKFD6	The new direct four-stage sixth-order Runge-Kutta type method for solving fourth-order ODEs
RKFD5(4)	The new direct embedded Runge-Kutta type method of order four embedded in order five for solving fourth-order ODEs
RKFD6(5)	The new direct embedded Runge-Kutta type method of order five embedded in order six for solving fourth-order ODEs
RK5(4)D	The embedded Runge-Kutta method of orders 5(4) with FSAL property derived by Dormand and Prince (1980)
RK5(4)F	The embedded Runge-Kutta method of orders 5(4) derived by Fehlberg (1969)
RK6(5)V	The embedded Runge-Kutta method of orders 6(5) derived by Verner (2014)
RK6(5)F	The embedded Runge-Kutta method of orders 6(5) derived by Fehlberg (1968)

CHAPTER 1

INTRODUCTION

Differential equations are the essential tools which are used to model several problems in the applied sciences and engineering in terms of unknown function and their derivatives. For instance, mathematical models of electrical circuits, chemical processes, the problem of determining the motion of a rocket or satellite and mechanical systems. They can be categorized into two types, Ordinary Differential Equations (ODEs) and Partial Differential Equations (PDEs) based on the number of independent variables exist in the differential equations.

Several theoretical and numerical studies for ODEs have appeared in scientific literature. Finding the analytical solutions to these ODEs are too complicated. Thereby, there are several numerical methods which used as an alternative. It is important to obtain the approximate numerical solutions of these ODEs so that, we can understand the behaviour of their solutions.

In the nineteenth century, the early work on numerical solutions of ODEs has begun, through the research paper of Bashforth and Adams in1883 and the research paper of Runge in 1895. They have offered the initial ideas that lead to develop the modern software on numerical methods (Butcher (2000)). Since then, ideas with the proper techniques have been proposed for solving ODEs by several authors.

1.1 Ordinary Differential Equation

If f is a function of x, y, and *nth* derivative of y, therefore the following form of equation

$$f(x,y,y',y'',\ldots,y^{(n)}) = 0. \tag{1.1}$$

is called an Ordinary Differential Equation (ODE) of order n.

In (1.1) the quantity being differentiated, y is called as the dependent variable, while the quantity with respect to which y is differentiated, x is called as the independent variable.

1.1.1 Initial Value Problem of First-Order ODE

The initial value problems (IVPs) for a system of s first order ordinary differential equations (ODEs) is defined by

$$y' = f(x,y), \quad y(a) = \beta. \tag{1.2}$$

where

$$
\begin{aligned}
f &: \Re \times \Re^m \rightarrow \Re^m, \\
y(x) &= [y_1(x), y_2(x), \ldots, y_m(x)]^T, \\
f(x,y) &= [f_1(x,y), f_2(x,y), \ldots, f_m(x,y)]^T, \quad a \leq x \leq b
\end{aligned}
$$

and $\beta = [\beta_1, \beta_2, \ldots, \beta_m]^T$ is a vector of initial conditions.

1.1.2 Initial Value Problem of Special Second-Order ODE

The general form of initial value problem (IVP) of second-order ODE can be written as follows:

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

with initial conditions

$$
y(a) = \beta, \quad y'(a) = \gamma
$$

where $f : \Re \times \Re^m \rightarrow \Re^m$, which is independent on y' explicitly and

$$
\begin{aligned}
y(x) &= [y_1(x), y_2(x), \ldots, y_m(x)]^T, \\
y'(x) &= [y_1'(x), y_2'(x), \ldots, y_m'(x)]^T, \\
f(x,y) &= [f_1(x,y), f_2(x,y), \ldots, f_m(x,y)]^T, \quad a \leq x \leq b
\end{aligned}
$$

with

$$
\begin{aligned}
\beta &= [\beta_1, \beta_2, \ldots, \beta_m]^T, \\
\gamma &= [\gamma_1, \gamma_2, \ldots, \gamma_m]^T.
\end{aligned}
$$

are the vector of initial conditions.

In this thesis, we will focus on the following initial value problems

1. Initial value problems of special third-order ODE.
2. Initial value problems of special fourth-order ODE

1.1.3 Initial Value Problem of Special Third-Order ODE

The general form of initial value problem (IVP) of special third-order ODEs is defined as follows:

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

with initial conditions

$$y(a) = \beta, \quad y'(a) = \gamma, \quad y''(a) = \alpha,$$

where $f : \Re \times \Re^m \to \Re^m$, which is independent on y' and y'' explicitly and

$$\begin{aligned}
y(x) &= [y_1(x), y_2(x), \ldots, y_m(x)]^T, \\
y'(x) &= [y_1'(x), y_2'(x), \ldots, y_m'(x)]^T, \\
y''(x) &= [y_1''(x), y_2''(x), \ldots, y_m''(x)]^T, \\
f(x,y) &= [f_1(x,y), f_2(x,y), \ldots, f_m(x,y)]^T, \quad a \leq x \leq b
\end{aligned}$$

with

$$\begin{aligned}
\beta &= [\beta_1, \beta_2, \ldots, \beta_m]^T, \\
\gamma &= [\gamma_1, \gamma_2, \ldots, \gamma_m]^T, \\
\alpha &= [\alpha_1, \alpha_2, \ldots, \alpha_m]^T.
\end{aligned}$$

are the vector of initial conditions. If the initial value problem (1.4) is in m dimensional space, it can be simplified to

$$u'''(x) = g(u(x)),$$

with initial conditions

$$u(a) = \tilde{\beta}, \quad u'(a) = \tilde{\gamma}, \quad u''(a) = \tilde{\alpha},$$

where

$$u(x) = \begin{pmatrix} y_1(x) \\ y_2(x) \\ \vdots \\ y_m(x) \\ x \end{pmatrix}, \qquad g(u) = \begin{pmatrix} f_1(u_1, u_2, \ldots, u_m, u_{m+1}) \\ f_2(u_1, u_2, \ldots, u_m, u_{m+1}) \\ \vdots \\ f_n(u_1, u_2, \ldots, u_m, u_{m+1}) \\ 0 \end{pmatrix},$$

$$\begin{aligned}
\tilde{\beta} &= [\beta_1, \beta_2, \ldots, \beta_m, a]^T, \\
\tilde{\gamma} &= [\gamma_1, \gamma_2, \ldots, \gamma_m, 1]^T, \\
\tilde{\alpha} &= [\alpha_1, \alpha_2, \ldots, \alpha_m, 0]^T.
\end{aligned}$$

1.1.4 Initial Value Problem of Special Fourth-Order ODE

The general form of initial value problem (IVP) of special fourth-order ODEs is written as follows:

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

with initial conditions

$$y(a) = \beta, \quad y'(a) = \gamma, \quad y''(a) = \alpha, \quad y'''(a) = \zeta,$$

where $f : \Re \times \Re^m \to \Re^m$, which is independent on y', y'' and y''' explicitly, and

$$\begin{aligned}
y(x) &= [y_1(x), y_2(x), \ldots, y_m(x)]^T, \\
y'(x) &= [y'_1(x), y'_2(x), \ldots, y'_m(x)]^T, \\
y''(x) &= [y''_1(x), y''_2(x), \ldots, y''_m(x)]^T, \\
y'''(x) &= [y'''_1(x), y'''_2(x), \ldots, y'''_m(x)]^T, \\
f(x,y) &= [f_1(x,y), f_2(x,y), \ldots, f_m(x,y)]^T, \quad a \le x \le b
\end{aligned}$$

with

$$\begin{aligned}
\beta &= [\beta_1, \beta_2, \ldots, \beta_m]^T, \\
\gamma &= [\gamma_1, \gamma_2, \ldots, \gamma_m]^T, \\
\alpha &= [\alpha_1, \alpha_2, \ldots, \alpha_m]^T, \\
\zeta &= [\zeta_1, \zeta_2, \ldots, \zeta_m]^T.
\end{aligned}$$

are the vector of initial conditions. If the initial value problem (1.5) is in m dimensional space, it can be simplified to

$$w^{(iv)}(x) = g(w(x)),$$

with initial conditions

$$w(a) = \tilde{\beta}, \quad w'(a) = \tilde{\gamma}, \quad w''(a) = \tilde{\alpha}, \quad w'''(a) = \tilde{\zeta},$$

where

$$w(x) = \begin{pmatrix} y_1(x) \\ y_2(x) \\ \vdots \\ y_m(x) \\ x \end{pmatrix}, \qquad g(w) = \begin{pmatrix} f_1(w_1, w_2, \ldots, w_m, w_{m+1}) \\ f_2(w_1, w_2, \ldots, w_m, w_{m+1}) \\ \vdots \\ f_n(w_1, w_2, \ldots, w_m, w_{m+1}) \\ 0 \end{pmatrix},$$

$$\tilde{\beta} = [\beta_1, \beta_2, \ldots, \beta_m, a]^T,$$
$$\tilde{\gamma} = [\gamma_1, \gamma_2, \ldots, \gamma_m, 1]^T,$$
$$\tilde{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_m, 0]^T,$$
$$\tilde{\zeta} = [\zeta_1, \zeta_2, \ldots, \zeta_m, 0]^T.$$

In this thesis, we suppose that the unique solution of the problems always exists. Therefore the hypothesis of the following theorem of existence and uniqueness is satisfied by each component of the system.

Theorem 1.1 :(Existence and Uniqueness)
Let $f(x,y)$ be defined and continuous for all points (x,y) in the region D defined by $a \le x \le b, -\infty < y < \infty$, a and b finite, and let there exists a constant L such that

$$|f(x,y) - f(x,y^*)| \le L|y - y^*|. \tag{1.6}$$

satisfies for all $(x,y),(x,y^*) \in D$. Then if $y_0 \in R$ is any number, there exists a unique solution $y(x)$ of initial value problem (1.2)*, where $y(x)$ is continuous and differentiable for all $(x,y) \in D$. The requirement* (1.6) *is known as a Lipschitz condition and the constant L as a Lipschitz constant.*

The proof of Theorem 1.1 can be found in Henrici (1962).

Definition 1.1 :*(see Burden and Faires (2011))*
The initial-value problem (1.2)*, is said to be an ill-posed problem if it is not satisfied any one of the following conditions:*

1. *the solution $y(x)$, to the problem* (1.2) *exists,*
2. *the solution $y(x)$, is unique,*
3. *for any ε, there exist constants ε_0, and κ, such that $\varepsilon_0 > \varepsilon > 0$, whenever $\beta(x)$ is continuous with $|\beta(x)| < \varepsilon$, for all x in $[a,b]$, and when $|\beta_0| < \varepsilon$,, the initial value problem*

$$z' = f(x,z) + \beta(x), \quad a \le x \le b, \quad z(a) = \alpha + \beta_0,$$

has a unique solution $z(x)$ that satisfies
$$|z(x) - y(x)| < \kappa\varepsilon, \text{ for all } x \text{ in } [a,b].$$

1.2 Numerical Methods for Solving Initial Value Problem

Numerical methods for solving initial value problems of ODEs are commonly classified into one-step methods or two-step methods. In one-step methods, the approximation of the solution is computed using the information of only one previous point. On the other hand, multistep methods, the approximation of the solution is computed using the information of n previous points. These techniques have their advantages and drawbacks.

1.2.1 Runge-Kutta Method

The general s-stage Runge-Kutta method for solving first-order ODEs (1.2) can be defined as follows:

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

where

$$k_1 = f(x_n, y_n), \tag{1.8}$$

$$k_i = f\left(x_n + c_i h, y_n + h\sum_{j=1}^{s} a_{ij}k_j\right), \quad i = 1,2,\ldots,s, \tag{1.9}$$

and the following row-sum assumption holds

$$c_i = \sum_{j=1}^{s} a_{ij}, \quad i = 1,2,\ldots,s. \tag{1.10}$$

It is appropriate to display the coefficients of RK method (1.7)–(1.9) as in Butcher notation or Butcher tableau as shown in Table 1.1.

Table 1.1: Butcher tableau for RK method

$$\begin{array}{c|c} \mathrm{c} & \mathrm{A} \\ \hline & b^T \end{array} = \begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

The s-dimension vectors b and c and the $s \times s$ matrix A can be defined as follows

$$b = [b_1, b_2, \ldots, b_s]^T,$$
$$c = [c_1, c_2, \ldots, c_s]^T,$$
$$A = [a_{ij}].$$

The RK method is said to be explicit if $a_{ij} = 0$ for $i \leq j, i = 1, 2, \ldots, s$, and semi implicit if $a_{ij} \neq 0$ for $i \leq j, i = 1, 2, \ldots, s$ and fully implicit otherwise.

1.2.2 Runge-Kutta-Nyström Method

A numerical method for solving second-order ODEs (1.3) was introduced in 1925 by E.J. Nyström denoted as Runge-Kutta-Nyström (RKN) method.

The general s-stage RKN method can be expressed as follows:

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{i=1}^{s} b_i k_i, \tag{1.11}$$

$$y'_{n+1} = y'_n + h \sum_{i=1}^{s} b'_i k_i, \tag{1.12}$$

where

$$k_i = f\left(x_n + c_i h, y_n + hc_i y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} k_j\right), \quad i = 1, 2, \ldots, s, \tag{1.13}$$

All the coefficients c_i, b_i, b'_i and a_{ij} of RKN method are supposed to be real. The s-dimension vectors b, b' and c and the $s \times s$ matrix A can be defined as follows

$$\begin{aligned} b &= [b_1, b_2, \ldots, b_s]^T, \\ b' &= [b'_1, b'_2, \ldots, b'_s]^T, \\ c &= [c_1, c_2, \ldots, c_s]^T, \\ A &= [a_{ij}]. \end{aligned}$$

and the following Nyström row condition holds

$$\frac{1}{2} c_i = \sum_{j=1}^{s} a_{ij}, \quad i = 1, 2, \ldots, s. \tag{1.14}$$

The RKN method (1.11)–(1.13) can be represented in Butcher tableau as illustrated in Table 1.2.

Table 1.2: Butcher tableau for RKN method

$$\begin{array}{c|c} \mathrm{c} & \mathrm{A} \\ \hline & b^T \\ & b'^T \end{array} = \begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \ldots & a_{1s} \\ c_2 & a_{21} & a_{22} & \ldots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \ldots & a_{ss} \\ \hline & b_1 & b_2 & \ldots & b_s \\ & b'_1 & b'_2 & \ldots & b'_s \end{array}$$

1.2.3 Improved Runge-Kutta Method

Rabiei (2012) derived explicit Improved Runge-Kutta (IRK) method for solving first order ordinary differential equation (1.2). The general s-stage of explicit IRK method is given by

$$y_{n+1} = y_n + h\Big(b_1 k_1 - b_{-1} k_{-1} + \sum_{i=2}^{s} b_i (k_i - k_{-i})\Big), \quad 1 \le n \le N-1, \tag{1.15}$$

where

$$k_1 = f(x_n, y_n), \tag{1.16}$$

$$k_{-1} = f(x_{n-1}, y_{n-1}), \tag{1.17}$$

$$k_i = f\Big(x_n + c_i h, y_n + h\sum_{j=1}^{i-1} a_{ij} k_j\Big), \tag{1.18}$$

$$k_{-i} = f\Big(x_{n-1} + c_i h, y_{n-1} + h\sum_{j=1}^{i-1} a_{ij} k_{-j}\Big), \quad i = 2, 3, \ldots, s. \tag{1.19}$$

and the row-sum condition (1.10) must be satisfied. The values of k_i and k_{-i} are based on the values of k_j and k_{-j} respectively. In every step we only require to evaluate the values of $k_j, i = 1, 2, \ldots, i-1$, while k_{-j} is computed from the previous step. The extra k values aimed to make the method more precise. The IRK method (1.15)–(1.19) are written in Butcher tableau as depicted in Table 1.3.

Table 1.3: Butcher tableau for IRK method

$$\begin{array}{c|ccccc}
0 & 0 & & & & \\
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
\vdots & \vdots & \vdots & \ddots & & \\
c_s & a_{s1} & a_{s2} & \cdots & a_{ss-1} & \\
\hline
b_{-1} & b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}$$

The idea of the IRK method can be described in Figure 1.1.

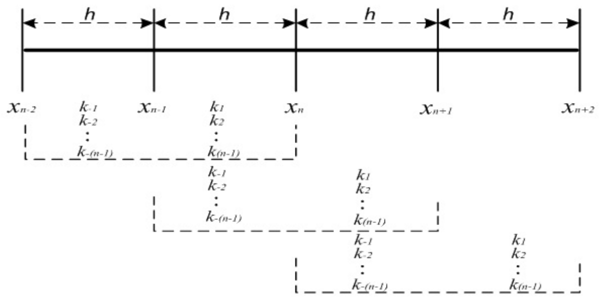

Figure 1.1: General concept for IRK method

1.2.3.1 Algebraic Order Conditions for IRK method

The order conditions of IRK method up to sixth order have been obtained by Rabiei (2012) as follows:

order 1: $$b_1 - b_{-1} = 1 \tag{1.20}$$

order 2: $$b_{-1} + \sum_i b_i = \frac{1}{2} \tag{1.21}$$

order 3: $$\sum_i b_i c_i = \frac{5}{12} \tag{1.22}$$

order 4: $$\sum_i b_i c_i^2 = \frac{1}{3} \tag{1.23}$$

$$\sum_{i,j} b_i a_{ij} c_j = \frac{1}{6} \tag{1.24}$$

order 5: $$\sum_i b_i c_i^3 = \frac{31}{120} \tag{1.25}$$

$$\sum_{i,j} b_i c_i a_{ij} c_j = \frac{31}{240} \tag{1.26}$$

$$\sum_{i,j} b_i a_{ij} c_j^2 = \frac{31}{360} \tag{1.27}$$

$$\sum_{i,j,k} b_i a_{ij} a_{jk} c_k = \frac{31}{720} \tag{1.28}$$

order 6: $$\sum_i b_i c_i^4 = \frac{1}{5} \tag{1.29}$$

$$\sum_{i,j} b_i c_i^2 a_{ij} c_j = \frac{1}{10} \tag{1.30}$$

$$\sum_{i,j,k} b_i a_{ij} c_j a_{ik} c_k = \frac{1}{20} \tag{1.31}$$

$$\sum_{i,j,k} b_i c_i a_{ij} c_j^2 = \frac{1}{15} \tag{1.32}$$

$$\sum_{i,j} b_i a_{ij} c_j^3 = \frac{1}{20} \tag{1.33}$$

$$\sum_{i,j,k} b_i c_i a_{ij} a_{jk} c_k = \frac{1}{30} \tag{1.34}$$

$$\sum_{i,j,k} b_i a_{ij} c_j a_{jk} c_k = \frac{1}{40} \tag{1.35}$$

$$\sum_{i,j,k} b_i a_{ij} a_{jk} c_k^2 = \frac{1}{60} \tag{1.36}$$

$$\sum_{i,j,k} b_i a_{ij} a_{jk} a_{km} c_m = \frac{1}{120} \tag{1.37}$$

1.2.4 Improved Runge-Kutta-Nyström Method

Rabiei and Ismail (2012) constructed an explicit Improved Runge-Kutta-Nyström (IRKN) method for solving second-order ODEs (1.3). The general s-stage explicit IRKN method is defined by

$$y_{n+1} = y_n + \frac{3h}{2} y'_n - \frac{h}{2} y'_{n-1} + h^2 \sum_{i=2}^{s} b'_i (k_i - k_{-i}), \tag{1.38}$$

$$y'_{n+1} = y'_n + h\Big(b_1 k_1 - b_{-1} k_{-1} + \sum_{i=2}^{s} b_i (k_i - k_{-i})\Big), \tag{1.39}$$

where

$$k_1 = f(x_n, y_n), \tag{1.40}$$

$$k_{-1} = f(x_{n-1}, y_{n-1}), \tag{1.41}$$

$$k_i = f\Big(x_n + c_i h, y_n + h c_i y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} k_j\Big), \quad i = 2, 3, \ldots, s, \tag{1.42}$$

$$k_{-i} = f\Big(x_{n-1} + c_i h, y_{n-1} + h c_i y'_{n-1} + h^2 \sum_{j=1}^{i-1} a_{ij} k_{-j}\Big), \quad i = 2, 3, \ldots, s. \tag{1.43}$$

It is appropriate to express of the explicit IRKN (1.38)–(1.43) method in Butcher tableau as shown in Table 1.4.

Table 1.4: Butcher tableau for IRKN method

$$
\begin{array}{c|ccccc}
0 & 0 & & & & \\
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
\vdots & \vdots & \vdots & \ddots & & \\
c_s & a_{s1} & a_{s2} & \dots & a_{ss-1} & \\
\hline
b_{-1} & b_1 & b_2 & \dots & b_{s-1} & b_s \\
 & & b'_2 & \dots & b'_{s-1} & b'_s
\end{array}
$$

also the Nyström row condition (1.14) must be satisfied.

1.3 Taylor Series Expansion

If the function $y(x)$ is sufficiently differentiable, then $y(x+h)$ can be expanded in Taylor series form as follows:

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2}y''(x) + \dots + \frac{h^q}{q!}y^{(q)}(x) + \dots \quad (1.44)$$

where $y^{(q)} = \frac{d^q y}{dx^q}, q = 1, 2, \cdots$.
Similarly, we can write the Taylor series expansion of $y(x_n + h)$ as follows

$$y(x_n+h) = y(x_n) + hy'(x_n) + \frac{h^2}{2}y''(x_n) + \dots + \frac{h^q}{q!}y^{(q)}(x_n) + \dots \quad (1.45)$$

In practice all terms up to involve h^q are included, that is

$$\begin{aligned} y(x_{n+1}) &= y(x_n+h) \\ &= y(x_n) + hy'(x_n) + \frac{h^2}{2}y''(x_n) + \dots + \frac{h^q}{q!}y^{(q)}(x_n) + h^{q+1}E_{q+1}(\varepsilon_n). \end{aligned} \quad (1.46)$$

where $E_{q+1}(\varepsilon_n), x_n \le \varepsilon_n \le x_n + h$, is the residual term. By removing the residual term from (1.46), we obtain the Taylor series expansion of order q as follows

$$y(x_{n+1}) = y(x_n+h) = y(x_n) + hy'(x_n) + \frac{h^2}{2}y''(x_n) + \dots + \frac{h^q}{q!}y^{(q)}(x_n). \quad (1.47)$$

From (1.47) the general form of explicit one-step method can be defined as

$$y_{n+1} = y_n + h\psi(x_n, y(x_n), h). \quad (1.48)$$

where the function $\psi(x,y,h)$ is called the increment function and y_n is the estimation of the exact solution $y(x_n)$.

Definition 1.2 **:***(see Dormand (1996))*
The exact solution $y(x_n)$ will satisfy

$$y(x_{n+1}) = y(x_n) + h\psi(x_n.y(x_n),h) + t_{n+1}. \tag{1.49}$$

where t_{n+1} is called the local truncation error.

Definition 1.3 **:***(see Dormand (1996))*
The one-step method (1.48) *is said to have order q if q is the largest positive integer such that*

$$y(x+h) - y(x) - h\psi(x,y(x),h) = \mathrm{O}(h^{q+1}). \tag{1.50}$$

Definition 1.4 **:***(see Dormand (1996))*
The one-step method (1.48) *is consistent if $\psi(x,y,0) = f(x,y)$.*

1.4 Problem Statement

The common technique for solving higher order ODEs is by transforming the problems into a system of first order ODEs and solving it using a suitable numerical method in the literature. The disadvantage of this technique is that more function evaluations are needed to be evaluated or computed, which leads to a longer execution time and more computational effort. Hence, the direct numerical method for solving higher order ODEs becomes essential in the field of numerical analysis.

Herein, we will derive the Improved Runge-Kutta type method for directly solving special third-order ODEs. In addition, we are going to cover the formulation and consider the implementation in details.

When this research study began, no study had been carried on the Runge-Kutta method for directly solving special fourth-order ODEs. Therefore, the following problems are treated in this thesis to handle the gap in the scientific literature on numerical solutions of special fourth-order ODEs; the construction of Runge-Kutta type method for directly solving special fourth-order ODEs denoted as RKFD methods; the derivation of order conditions for RKFD methods; the derivation of direct numerical RKFD methods of different orders for solving special fourth-order ODEs; and the derivation of different orders of embedded RKFD pairs for solving special fourth-order ODEs.

1.5 Scope of the Thesis

The research focuses on special third and fourth order ODEs because the methods derived in this thesis are nonlinear (Runge-Kutta type methods). Therefore, it is not easy and it is not computationally efficient to solve the general form of the third and fourth order ODEs using these methods. Hence, the methods derived are limited to solve the special form of the third and fourth order ODEs.

1.6 Objectives of the Thesis

The objectives of this thesis are:

1. to derive the order conditions of Improved Runge-Kutta type method for directly solving special third-order ODEs, denoted by IRKD methods. Based on the order conditions, IRKD methods of orders four and five will be constructed.
2. to derive the order conditions of Runge-Kutta type method for directly solving special fourth-order ODEs, known as RKFD methods. Based on the order conditions, RKFD methods of orders four, five and six will be derived.
3. to construct embedded RKFD methods of orders 5(4) and 6(5) for directly solving special fourth-order ODEs using variable step size codes.
4. to compare the efficiency of the new proposed methods with the existing methods.
5. to apply the new IRKD and RKFD methods to solve physical problem and engineering problem respectively.

1.7 Outline of the Thesis

This thesis consists of eight chapters which are organized as follows:

Chapter 1 gives a brief introduction on the development of the numerical methods for solving differential equations, which involves the definitions and properties of ODEs. Numerical methods particularly Runge-Kutta methods, Runge-Kutta-Nyström methods, Improved Runge-Kutta methods and Improved Runge-Kutta-Nyström methods will also be introduced.

Chapter 2 deals with the review of the earlier works on the numerical methods for solving ODEs, which covers the literature review on numerical methods for first-order and second-order ODEs. Followed by the literature review on numerical methods for solving third-order and fourth-order ODEs.

Chapter 3 devotes to the derivation of Improved Runge-Kutta type method for solving third order ODEs, denoted as IRKD methods by finding the order conditions using Taylor series expansions. The order conditions up to the sixth-order are presented.

Chapter 4 is focused on the derivation of a three-stage fourth-order and four-stage fifth-order IRKD methods. Comparison of the numerical results using IRKD methods and the existing methods will also be given. The application of the new IRKD methods for solving the physical problem in thin film flow is shown.

Chapter 5 focuses on the derivation of the order conditions of Runge-Kutta type methods for directly solving special fourth-order ODEs, denoted as RKFD methods using two techniques; the first technique is using the Taylor series expansion and the second technique is using the relevant-colored trees and the corresponding B-series theory. The order conditions up to order seven are also presented.

Chapter 6 is devoted to the derivation of the explicit three-stage fourth-order RKFD method, followed by the derivation of the explicit three-stage fifth-order and four-stage sixth-order RKFD methods. Based on the constant step-size code the new RKFD methods are used for solving special fourth-order ODEs, and numerical results are compared with the results obtained by the existing RKN methods and RK methods after converting the fourth-order ODEs to a system of second-order ODEs and to a system of first order ODEs respectively. The implementation of the new RKFD methods to solve the engineering problem in an ill-posed problem of a beam on the elastic foundation is presented.

Chapter 7 presents the derivation of the two pairs of embedded RKFD methods for the direct solution of special fourth- order ODEs of the form $y^{(iv)} = f(x,y)$. The first pair is the RKFD5(4) which is fourth order RKFD method embedded in fifth order method. The second pair is the RKFD6(5) pair which is fifth order RKFD method embedded in sixth order method. Based on the newly proposed methods a variable step-size code is developed for solving special fourth-order ODEs.

Finally, the summary of the thesis, conclusion and recommendation for future research are given in Chapter 8.

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