

## UNIVERSITI PUTRA MALAYSIA

DIAGONALLY IMPLICIT TWO AND THREE DERIVATIVE RUNGE-KUTTA METHODS FOR SOLVING FIRST ORDER OSCILLATORY ORDINARY AND DELAY DIFFERENTIAL EQUATIONS

NUR AMIRAH BINTI AHMAD



UNIVERSITI PUTRA MALAYSIA
BERILMU BERBAKTI

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## By

## NUR AMIRAH BINTI AHMAD

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## DEDICATIONS

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## By

## NUR AMIRAH BINTI AHMAD

## December 2020

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In this study, Diagonally Implicit Two Derivative Runge-Kutta (DITDRK) methods and Diagonally Implicit Three Derivative Runge-Kutta (DIThDRK) methods are constructed for the numerical integration of first-order Initial Value Problems (IVPs). For DITDRK methods, the methods derived are also used in the solution of stiff Ordinary Differential Equations (ODEs) and Delay Differential Equations (DDEs). Three new methods with a minimum number of function evaluations are derived for DITDRK methods. Meanwhile for DIThDRK methods also, three new methods are constructed with a minimum number of function evaluations.

Solving ODEs which have periodic or oscillatory solutions in nature are more convenient with the implementation of trigonometrically-fitted and phase-fitted and amplification-fitted techniques. Hence, taking this idea into account, we implemented these techniques into DITDRK and DIThDRK methods. Two new methods each for DITDRK and DIThDRK methods for both oscillatory techniques are derived. They are fourth and fifth-order for DITDRK methods and sixth and seventh-order for DIThDRK methods. The Local Truncation Error (LTE) for each method is computed.

Stiff system of ODEs are solved using implicit formulae and required the use of Newton-like iteration, which needs a lot of computational effort. Here, we focused on the derivation of DITDRK methods for both constant and variable step-size. For constant step-size, three new methods of order three, four and six are constructed. For variable step-size, two new embedded methods of 3(2) and 4(3) DITDRK methods are derived. The stability of these methods are discussed along with their stability regions.

A brief introduction on Delay Differential Equations (DDEs) is given. The stability properties of DITDRK methods when applied to DDEs, using Lagrange interpolation to evaluate the
delay term are investigated. The P-stability and Q-stability of fourth and fifth-order DITDRK methods are discussed along with the boundary of the region. In solving first-order DDEs, Newton Divided Difference Interpolation (NDDI) is used to approximate the delay term. As for solving periodic DDEs, we use Trigonometric interpolation which is specially design to solve oscillatory problems due to its periodic properties. Hence, two methods of fourth and fifth-order Trigonometrically-Fitted DITDRK (TFDITDRK) methods are used to solve these types of problems.

Numerical experiments show that the newly derived methods are more efficient and accurate in comparison with existing Diagonally Implicit Runge-Kutta (DIRK) methods of the same order and properties in the literature in terms of maximum global error, number of function evaluation per step and execution time.

# KAEDAH RUNGE-KUTTA DUA DAN TIGA TERBITAN PEPENJURU TERSIRAT UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA DAN LENGAH BERAYUN PERINGKAT PERTAMA 

Oleh

## NUR AMIRAH BINTI AHMAD

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Dalam kajian ini, kaedah Runge-Kutta Dua Terbitan Pepenjuru Tersirat (RKDTPT) dan kaedah Runge-Kutta Tiga Terbitan Pepenjuru Tersirat (RKTTPT) dibina untuk penyelesaian pengamiran berangka Masalah Nilai Awal (MNA) peringkat pertama. Untuk kaedah RKDTPT, kaedah yang diterbitkan juga diguna dalam penyelesaian Persamaan Pembezaan Biasa (PPB) kaku dan Persamaan Pembezaan Lengah (PPL). Tiga kaedah baharu dengan jumlah penilaian fungsi yang minima diterbitkan untuk kaedah RKDTPT. Sementara itu, untuk kaedah RKTTPT juga, tiga kaedah baharu dibina dengan jumlah penilaian fungsi yang minima.

Menyelesaikan PPB yang mempunyai penyelesaian semulajadi berkala atau berayun adalah lebih sesuai dengan pelaksanaan teknik suai-trigonometri dan suai-fasa dan suai-pembesaran. Oleh itu, dengan mengambil kira idea ini, kami melaksanakan teknik-teknik ini ke dalam kaedah RKDTPT dan RKTTPT. Dua kaedah baharu untuk setiap kaedah RKDTPT dan RKTTPT untuk kedua-dua teknik berkala diterbitkan. Mereka adalah peringkat empat dan lima untuk kaedah RKDTPT dan peringkat enam dan tujuh untuk kaedah RKTTPT. Ralat Pangkasan Tempatan (RPT) untuk setiap kaedah dikira.

Sistem PPB kaku diselesaikan menggunakan formula tersirat dan memerlukan penggunaan lelaran Newton, yang memerlukan pengiraan yang sangat banyak. Di sini, kami memfokuskan kepada penerbitan kaedah RKDTPT untuk kedua-dua saiz langkah tetap dan berubah. Untuk saiz langkah tetap, tiga kaedah baharu peringkat tiga, empat dan enam dibina. Untuk saiz langkah berubah, dua kaedah terbenam 3(2) dan 4(3) kaedah RKDTPT diterbitkan. Kestabilan kaedah-kaedah ini dibincangkan bersama-sama dengan rantau kestabilan.

Pengenalan ringkas terhadap Persamaan Pembezaan Lengah (PPL) diberikan. Sifat kestabilan kaedah RKDTPT apabila digunakan kepada PPL menggunakan interpolasi Lagrange
untuk mengira sebutan lengah dikaji. Kestabilan-P dan kestabilan-Q peringkat empat dan lima kaedah RKDTPT dibincangkan bersama-sama dengan sempadan rantaunya. Dalam menyelesaikan PPB peringakat pertama, Interpolasi Pembezaan Pembahagian Newton (IPPN) digunakan untuk menganggarkan sebutan lengah. Bagi menyelesaikan PPL berkala, kami menggunakan interpolasi Trigonometri yang direka khas untuk menyelesaikan masalah berayun oleh kerana sifat berkalanya. Oleh itu, dua kaedah RKDTPT suai-trigonometri peringkat empat dan lima digunakan untuk menyelesaikan masalah jenis ini.

Keputusan berangka menunjukkan bahawa kaedah-kaedah yang baharu diterbitkan adalah lebih jitu dan cekap dalam perbandingan dengan kaedah-kaedah Runge-Kutta Pepenjuru Tersirat (RKPT) sedia ada peringkat sama dan sifat dalam sorotan litratur dalam ralat global maksima, jumlah penilaian fungsi setiap langkah dan perlaksanaan masa.

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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. The members of the Supervisory Committee were as follows:

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## LIST OF ABBREVIATIONS

| ODEs | Ordinary Differential Equations |
| :---: | :---: |
| DDEs | Delay Differential Equations |
| IVPs | Initial Value Problems |
| PDEs | Partial Differential Equations |
| FSAL | First Same As Last |
| LTE | Local Truncation Error |
| RK | Runge-Kutta method |
| RKN | Runge-Kutta Nyström method |
| DIRK | Diagonally Implicit Runge-Kutta method |
| SIRK | Singly Implicit Runge-Kutta method |
| TDRK | Two Derivative Runge-Kutta method |
| DITDRK | Diagonally Implicit Two Derivative Runge-Kutta method |
| ThDRK | Three Derivative Runge-Kutta method |
| DIThDRK | Diagonally Implicit Three Derivative Runge-Kutta method |
| $h$ | Step-size |
| FE | Total of function evaluations |
| Time | Execution time |
| TOL | The chosen tolerance |
| TS | Total of successful steps |
| FS | Total of failed steps |
| Jaco | Total of Jacobian evaluations |
| MAXERR | Maximum global error |

## CHAPTER 1

## INTRODUCTION

### 1.1 The Initial Value Problem

The Initial Value Problems (IVPs) for a system of $s$ first-order Ordinary Differential Equations (ODEs) is defined as:

$$
\begin{equation*}
y^{\prime}=f(x, y), \quad y(u)=\omega \tag{1.1}
\end{equation*}
$$

where

$$
\begin{aligned}
\mathbf{y}(x) & =\left[y_{1}(x), y_{2}(x), \ldots, y_{c}(x)\right]^{T} \\
\mathbf{f}(x, y) & =\left[f_{1}(x, y), f_{2}(x, y), \ldots, f_{c}(x, y)\right]^{T}, \quad x \in[u, w]
\end{aligned}
$$

and $\omega=\left[\omega_{1}, \omega_{2}, \ldots, \omega_{s}\right]^{T}$ is the vector of initial conditions.

Theorem 1.1 (Existence and Uniqueness)
Let $f(x, y)$ are defined and continous for every points $(x, y)$ in the region $R$-defined by $u \leq x \leq$ $w,-\infty<y<\infty$, where $u$ and $w$ are finite, and there exist a constant $L$ such that for all $x, y, y^{*}$, $(x, y)$ and $\left(x, y^{*}\right)$ are both in $R$.

$$
\begin{equation*}
\left|f(x, y)-f\left(x, y^{*}\right)\right| \leq L\left|y-y^{*}\right| . \tag{1.2}
\end{equation*}
$$

Then, let say if $\omega$ is any given random number, there exist a solution $y(x)$ which is unique where $y(x)$ is continuous and differentiable for all $(x, y) \in R$.

The condition (1.2) is known as Lipschitz condition, and the constant $L$ as Lipschitz constant. For proof and justification, refer to Henrici (1962). Hence, in this research, the conditions of the theorem are assumed to be satisfied which contribute to the existence of a unique solution of (1.1).

### 1.2 The Delay Differential Equation

Delay Differential Equations (DDEs) can be divided into four different classes namely retarded DDE (Baker, 2000), neutral DDE (Jackiewicz and Lo, 2006), distributed DDE (Augeraud-Véron and Leandri, 2014) and stochastic DDE (Fan, 2011). Among these four type of DDEs, the retarded type has become the most well-known class of DDEs.

Generally, a DDE refers to both a retarded DDE (RDDE) and a neutral DDE (NDDE) . RDDE is an ODE involving solution of the delay term $y(t-\tau(t, y(t))))$ and is given by

$$
\left.\begin{array}{ll}
y^{\prime}(t)=f(t, y(t), y(t-\tau(t, y(t)))), & t \in[u, w]  \tag{1.3}\\
y(t)=\varphi(t), & t \leq u
\end{array}\right\}
$$

A NDDE is an ODE involving both solutions of the delay term $y(t-\tau(t, y(t))))$ and the derivative of the delay term itself $y^{\prime}(t-\sigma(t, y(t)))$, given by

$$
\left.\begin{array}{ll}
y^{\prime}(t)=f\left(t, y(t), y(t-\tau(t, y(t))), y^{\prime}(t-\sigma(t, y(t)))\right), & t \in[u, w],  \tag{1.4}\\
y(t)=\varphi(t), & t \leq u, \\
y^{\prime}(t)=\varphi^{\prime}(t), & t \leq u .
\end{array}\right\}
$$

The delays or lags $\tau$ and $\sigma$ are measurable as a physical quatities that is scalar in function. Function $f$ is assumed to be continuous and it is always non-negative and satisfies the Lipschitz condition in $y(t)$ for all $t \in[u, w] . \varphi(t)$ is the initial function which is known to be defined in [ $\rho, t_{0}$ ], where

$$
\begin{equation*}
\rho=\min _{1 \leq i \leq n}\left\{\min \left(t-\tau_{t \geq t_{0}}\right)\right\} . \tag{1.5}
\end{equation*}
$$

There are three conditions that the delay can be represent which are a constant (the constant delay case), a function of $t, \tau_{i}=\tau_{i}(t)$ (the variable or time-dependent delay case) and a function of both $t$ and $y, \tau_{i}=\tau_{i}(t, y(t))$ (the state-dependent delay case) (Bellen and Zennaro, 2013; Hayashi, 1996).

Since DDE is always refererred to as both RDDE and NDDE, many authors refer the DDE as the RDDE only. In this thesis, we are only concerned with RDDE, hence it will therefore be referred to as DDE only.

### 1.3 Stiff System of Ordinary Differential Equation

Stiffness is a phenomenon identified in the numerical integration of ODEs that arise in various real life applications including the study of spring and damping system, problems in chemical kinetics and the analysis of control system. In correspond to a stable solution, it is often characterized in terms of the largest and smallest real parts of the zero of the stability function. Firstly, the eigenvalues of the Jacobian matrix of (1.1) is defined

Definition 1.1 (Lambert, 1973)
The eigenvalues $\lambda_{m}, m=1, \ldots, s$, of the (1.1) at $(x, y)$ is defined as the eigenvalues of the Jacobian matrix, $J=\left(\frac{\partial f}{\partial y}\right)$ evaluated at $(x, y)$.

With respect to the linear system of first order equations, various definitions of stiffness have been given in the literature.

$$
\begin{equation*}
\underline{y}^{\prime}=A \underline{y}+\underline{\phi}(x), \quad \underline{y}(u)=\underline{\eta}, \quad u \leq x \leq w, \tag{1.6}
\end{equation*}
$$

where

$$
\underline{y}^{T}=\left(y_{1}, \ldots, y_{s}\right) \text { and } \underline{\eta}^{T}=\left(\eta_{1}, \ldots, \eta_{s}\right) .
$$

Lambert (1973) has given the most widely accepted definitions on stiffness as follows:

Definition 1.2 (Lambert, 1973)
The linear system (1.6) is said to be stiff if

1. $\operatorname{Re} \lambda_{i}<0, i=1, \ldots, s$ and
2. $\max _{i}\left|\operatorname{Re}\left(\lambda_{i}\right)\right| \gg \min _{i}\left|\operatorname{Re}\left(\lambda_{i}\right)\right|$, where $\lambda_{i}$ are the eigenvalues of $A$ and the ratio $\frac{\max _{i}\left|\operatorname{Re}\left(\lambda_{i}\right)\right|}{\min _{i}\left|\operatorname{Re}\left(\lambda_{i}\right)\right|}$ is called the stiffness ratio or the stiffness index.

The general solution to (1.6) is in the form of

$$
y(x)=\sum_{i=1}^{s} c_{i} e^{\lambda_{i} x} u_{i}+\psi(x)
$$

where $y(x)=\sum_{i=1}^{s} c_{i} e^{\lambda_{i} x} u_{i}$ is the transient solution and $\psi(x)$ is the steady state solution.
Nonlinear system $\underline{y}^{\prime}=f(x, \underline{y})$ exhibits stiffness if the eigenvalues of the Jacobian $\frac{\partial f}{\partial \underline{y}}$ behaves in a similar manner. The eigenvalues are no longer constant, but depend on the solution and therefore vary with $x$. Accordingly, the system $y^{\prime}=f(x, y)$ is considered stiff in an interval $I$ of $x$ if for $x \in I$, the eigenvalues $\lambda_{i}(x)$ of $\frac{\partial f}{\partial y}$ satisfy Definition 1.2 above.

At the beginning of the integration, the solution can be rapidly varying due to the rapidly decreasing transient solution. This phase is referred to as the transient phase and accuracy rather than stability restricts the stepsize of any integration method. Thus the structure of the solutions suggest the application of non-stiff methods in the transient phase and stiff methods in the steady-state region hoping for computational cost saving.

### 1.4 Problem Statement

Our attention will be focused on deriving DITDRK and DIThDRK methods for solving firstorder ODEs (1.1) and DDEs (1.3) for the numerical solution of periodic and non-periodic problems. There are quite a number of research papers discussing on explicit TDRK and ThDRK methods but there are none on DITDRK and DIThDRK methods. Furthermore, there are none ongoing research on DITDRK and DIThDRK methods for solving stiff and non-stiff ODEs as well as oscillating and non-oscillating DDEs. Hence, taking this golden opportunity, we try to go one step further, digging into diagonally implicit methods since it is theoretically known that implicit methods are more accurate and precise compared to explicit methods. Moreover, we believed with the existence of $g$ and $\hat{g}$ parameter in their general formula will help in achieving higher order method with a lower stage number.

### 1.5 The Objectives of the Thesis

The derivation of highly improved and efficient numerical methods based on the DITDRK method and DIThDRK method for the numerical integration of first order ODEs and DDEs
in the form of (1.1) and (1.3) respectively for constant step-size and some variable step-size mode. The main objectives of this thesis are proposed as follows:

1. To derive DITDRK and DIThDRK methods using order conditions for solving firstorder ODEs.
2. To construct trigonometrically-fitted and phase-fitted and amplification-fitted DITDRK and DIThDRK methods for the solution of first-order ODEs for the numerical solutions of periodic problems.
3. To develop DITDRK methods for solving first-order stiff ODEs for constant and variable step-size.
4. To derive and analyse P-Stability and Q-Stability for DITDRK methods for the numerical solution of first-order DDEs of constant type.
5. To solve first-order DDEs of constant type for the numerical solutions of periodic problems using trigonometrically-fitted DITDRK methods and Trigonometric interpolation to approximate the delay term.

### 1.6 Scope of the Study

This thesis concentrates on the derivation of DITDRK and DIThDRK methods for solving first-order ODEs and DDEs of the form (1.1) and (1.3) respectively. We are also going to solve first-order stiff ODEs. This study focus on the development of efficient methods in solving ODEs problems which are oscillatory in nature by trigonometrically-fitted and phasefitted and amplification-fitted techniques and non-periodic solutions using order conditions. In addition, Trigonometric interpolation will be used to approximate the delay term for solving periodic DDEs problems. Note that the second-order IVPs of ODEs and DDEs will be solved by reducing them to system of first-order ODEs and DDEs. The proposed methods will be derived using constant and variable step-size approach to produce the approximated solutions.

### 1.7 Outline of the Study

The background of numerical integration of first order ODEs and DDEs are discussed briefly in Chapter 1. A brief explanation on IVPs as well as the existence and uniqueness theorem are given in this chapter. Diagonally Implicit Two Derivative Runge-Kutta method and Diagonally Implicit Three Derivative Runge-Kutta method along with their algebraic order conditions are discussed. The local truncation error for both DITDRK and DIThDRK methods are also presented. In addition, the stability analysis for these two methods are discussed thoroughly. In Chapter 2, the literature review is given where this section contains a brief history about Two Derivative Runge-Kutta method, Three Derivative Runge-Kutta method, oscillatory techniques, DDEs and stiff ODEs.

Three DITDRK methods which are fourth-order two-stage, fifth-order three-stage and sixth-order four-stage respectively and three DIThDRK methods which are sixth-order two-stage, seventh-order three-stage and eighth-order four-stage are constructed using order conditions are proposed in Chapter 3. The stability of the developed methods are analyzed
and their stability regions are plotted. Numerical experiments are carried out to show their effectiveness and accuracy compared with other existing DIRK methods of the same order.

In Chapter 4, two DITDRK methods of fourth-order and fifth-order each are constructed using trigonometrically-fitted and phase-fitted and amplification-fitted techniques. The algebraic order as well as the local truncation error for these methods are further discussed in this chapter. Numerical results are presented and compared with other existing DIRK methods with the same oscillatory properties in the literature. In Chapter 5, two DIThDRK methods of sixth-order and seventh-order each are constructed using trigonometrically-fitted and phase-fitted and amplification-fitted techniques. The algebraic order and the local truncation error for these new methods are briefly discussed in this chapter. Numerical results are presented and compared with other existing DIRK methods with the same periodic properties in the literature.

Meanwhile in Chapter 6, three DITDRK methods of third-order two-stage, fourth-order three-stage and sixth-order four-stage respectively are developed using constant step-size approach to solve first-order stiff ODEs. As for variable step-size approach, two new embedded methods of 3(2) and 4(3) DITDRK methods are derived. The stability of these proposed methods is discussed along with their stability regions. Numerical experiments are carried out to show their effectiveness and accuracy in comparison with other existing DIRK methods of the same order.

Next, in Chapter 7, the P-stability and Q-stability of fourth and fifth-order DITDRK methods are discussed along with the boundary of the region. As for solving periodic DDEs, we use Trigonometric interpolation which is specially design to solve oscillatory problems due to its periodic properties. Hence, two methods of fourth and fifth-order Trigonometrically-Fitted DITDRK (TFDITDRK) methods are used to solve these types of problems. Numerical experiments are carried out to show their effectiveness and accuracy in comparison with other existing DIRK methods of the same order. Finally, the summary of this thesis and future work are discussed in Chapter 8.

### 1.8 Two Derivative Runge-Kutta (TDRK) Method

A Two Derivative Runge-Kutta method is a Runge-Kutta method designed for solving first-order ODEs in the form of (1.1). A TDRK method can be divided into two kind which is explicit TDRK methods and implicit TDRK methods. If $a_{i j}=0$ for $i \leq j$, a TDRK method is an explicit method and if $a_{i j}=\delta$ where $i=j, \delta \in \mathfrak{R}$, it is denoted as diagonally implicit or also known as singly implicit. In our research context, we concentrate mainly on diagonally implicit TDRK method.

Consider the scalar ODEs (1.1) with $f: \mathfrak{R}^{N} \rightarrow \mathfrak{R}^{N}$. In this case, the second derivative is also assumed to be known where

$$
\begin{equation*}
y^{\prime \prime}=g(y):=f^{\prime}(y) f(y), \quad g: \mathfrak{R}^{N} \rightarrow \mathfrak{R}^{N} . \tag{1.7}
\end{equation*}
$$

An implicit TDRK method for the numerical integration of IVPs (1.1) is given by

$$
\begin{align*}
Y_{i} & =g\left(x_{n}+c_{i} h, y_{n}+h \sum_{j=1}^{s} a_{i j} f\left(Y_{j}\right)+h^{2} \sum_{j=1}^{s} \hat{a}_{i j} Y_{j}\right),  \tag{1.8}\\
y_{n+1} & =y_{n}+h \sum_{i=1}^{s} b_{i} f\left(Y_{i}\right)+h^{2} \sum_{i=1}^{s} \hat{b}_{i} Y_{i}, \tag{1.9}
\end{align*}
$$

where $i=1, \ldots, s$.

The implicit TDRK method with the coefficients in (1.8) and (1.9) are presented using the Butcher tableau as follows:

| c | A | $\hat{A}$ |
| :---: | :---: | :---: |
|  | $b^{T}$ | $\hat{b}^{T}$ |

Diagonally implicit methods with a minimal number of function evaluations can be developed by considering the methods in the form

$$
\begin{align*}
Y_{i} & =g\left(x_{n}+c_{i} h, y_{n}+h c_{i} f\left(x_{n}, y_{n}\right)+h^{2} \sum_{j=1}^{s} \hat{a}_{i j} Y_{j}\right),  \tag{1.10}\\
y_{n+1} & =y_{n}+h f\left(x_{n}, y_{n}\right)+h^{2} \sum_{i=1}^{s} \hat{b}_{i} Y_{i}, \tag{1.11}
\end{align*}
$$

where $i=1, \ldots, s$.

The above method is denoted as a special DITDRK method. The unique part of this method is that it involves only one evaluation of $f$ and many evaluations of $g$ per step compared to many evaluations of $f$ per step in traditional RK methods. Its Butcher tableau is given as follows:

| c | $\hat{A}$ |
| :---: | :---: |
|  | $\hat{b}^{T}$ |

The DITDRK parameters $a_{i j}, \hat{a}_{i j}, b_{i}, \hat{b}_{i}$ and $c_{i}$ are assumed to be real and $s$ is the number of stage of the method. The $s$-dimensional vectors $\mathbf{b}, \hat{\mathbf{b}}, \mathbf{c}$ and $s \times s$ matrix, $\mathbf{A}$ and $\hat{\mathbf{A}}$ are introduced where $\mathbf{b}=\left[b_{1}, b_{2}, \ldots, b_{s}\right]^{T}, \hat{\mathbf{b}}=\left[\hat{b}_{1}, \hat{b}_{2}, \ldots, \hat{b}_{s}\right]^{T}, \mathbf{c}=\left[c_{1}, c_{2}, \ldots, c_{s}\right]^{T}, \mathbf{A}=\left[a_{i j}\right]$ and $\hat{\mathbf{A}}=\left[\hat{a}_{i j}\right]$ respectively.

### 1.9 Algebraic Conditions and Local Truncation Error for TDRK Method

The DITDRK methods (1.10) and (1.11) can be written as the following:

$$
\begin{equation*}
y_{n+1}=y_{n}+h y_{n}^{\prime}+h^{2} \sum_{i=1}^{s} \hat{b}_{i} k_{i} \tag{1.12}
\end{equation*}
$$

where

$$
\begin{equation*}
k_{i}=g\left(x_{n}+c_{i} h, y_{n}+h c_{i} y_{n}^{\prime}+h^{2} \sum_{j=1}^{i} \hat{a}_{i j} k_{j}\right) . \tag{1.13}
\end{equation*}
$$

The order conditions for DITDRK methods can be easily obtained by expanding the local truncation error in a direct way. The DITDRK method (1.10) and (1.11) can be expressed as:

$$
\begin{equation*}
y_{n+1}=y_{n}+h \psi\left(x_{n}, y_{n}, h\right), \tag{1.14}
\end{equation*}
$$

where the increment function $\psi\left(x_{n}, y_{n}, h\right)$ is denoted as

$$
\begin{equation*}
\psi\left(x_{n}, y_{n}, h\right)=y_{n}^{\prime}+h \sum_{i=1}^{s} \hat{b}_{i} k_{i}, \tag{1.15}
\end{equation*}
$$

and $k_{i}$ is given in (1.13).

The Taylor series increment function is denoted as $\Delta$. After substracting the computed solution, $y_{n+1}$ with the exact solution, $y\left(x_{n+1}\right)$, the local truncation errors of $y_{n}$ can be obtained where

$$
\begin{equation*}
L T E_{n+1}=h(\psi-\Delta) \tag{1.16}
\end{equation*}
$$

The Taylor series increment function of $y_{n}$ is expressed as

$$
\begin{equation*}
\Delta=y_{n}^{\prime}+\frac{1}{2} h y_{n}^{\prime \prime}+\frac{1}{6} h^{2} y_{n}^{\prime \prime \prime}+\frac{1}{24} h^{3} y_{n}^{(i v)}+\frac{1}{120} h^{4} y_{n}^{(v)}+\ldots+\frac{1}{p!} h^{p-1} y_{n}^{(p)} . \tag{1.17}
\end{equation*}
$$

The above equations are expressed in terms of elementary differentials. A few elementary differentials are given as follows:

$$
\begin{align*}
& y^{\prime}= F_{1}^{(1)}=f, \\
& y^{\prime \prime}= F_{1}^{(2)}=f_{x}+f_{y} y^{\prime}, \\
& y^{\prime \prime \prime}= F_{1}^{(3)}=  \tag{1.18}\\
& f_{x x}+2 f_{x y} y^{\prime}+f_{y y} y^{\prime \prime}+f_{y y}\left(y^{\prime}\right)^{2}, \\
& y^{(i v)}= F_{1}^{(4)}= \\
& f_{x x x}+3 f_{x x y} y^{\prime}+3 f_{x y y}\left(y^{\prime}\right)^{2}+3 f_{x y} y^{\prime \prime}+3 f_{y y} y^{\prime} y^{\prime \prime}+ \\
& f_{y y y}\left(y^{\prime}\right)^{3}+f_{y y} y^{\prime \prime \prime} .
\end{align*}
$$

Expressing $\Delta$ in terms of the elementary differential leads to:

$$
\begin{equation*}
\Delta=F_{1}^{(1)}+\frac{1}{2} h F_{1}^{(2)}+\frac{1}{6} h^{2} F_{1}^{(3)}+\frac{1}{24} h^{3} F_{1}^{(4)}+\mathscr{O}\left(h^{4}\right) . \tag{1.19}
\end{equation*}
$$

Substituting (1.18) into (1.15), the increment function $\psi$ for DITDRK method becomes

$$
\begin{equation*}
\sum_{i=1}^{s} \hat{b}_{i} k_{i}=\sum_{i=1}^{s} \hat{b}_{i} F_{1}^{(2)}+h \sum_{i=1}^{s} \hat{b}_{i} c_{i} F_{1}^{(3)}+\frac{1}{2} h^{2} \sum_{i=1}^{s} \hat{b}_{i} c_{i}^{2} F_{1}^{(4)}+\mathscr{O}\left(h^{3}\right) \tag{1.20}
\end{equation*}
$$

Using (1.15) and (1.17), the LTE can be written as:

$$
\left.\left.\begin{array}{rl}
L T E_{n+1}= & h^{2}
\end{array}\right]\left(\sum_{i=1}^{s} \hat{b}_{i} F_{1}^{(2)}+h \sum_{i=1}^{s} \hat{b}_{i} c_{i} F_{1}^{(3)}+\frac{1}{2} h^{2} \sum_{i=1}^{s} \hat{b}_{i} c_{i}^{2} F_{1}^{(4)}+\ldots\right)\right] .
$$

Simplifying (1.21)
$L T E_{n+1}=h^{2}\left[\left(\sum_{i=1}^{s} \hat{b}_{i}-\frac{1}{2}\right) F_{1}^{(2)}+\left(\sum_{i=1}^{s} \hat{b}_{i} c_{i}-\frac{1}{6}\right) h F_{1}^{(3)}+\left(\frac{1}{2} h^{2} \sum_{i=1}^{s} \hat{b}_{i} c_{i}^{2}-\frac{1}{24}\right) h^{2} F_{1}^{(4)}+\ldots\right]$.

The order conditions for a $s$-stage DITDRK method by using (1.22) up to order seven as proposed by Chan and Tsai (2010) are given as follows:

$$
\begin{array}{ll}
\text { Order 2: } & \sum \hat{b}_{i}=\frac{1}{2}, \\
\text { Order 3: } & \sum \hat{b}_{i} c_{i}=\frac{1}{6}, \\
\text { Order 4: } & \sum \hat{b}_{i} c_{i}^{2}=\frac{1}{12} \\
\text { Order 5: } & \sum \hat{b}_{i} c_{i}^{3}=\frac{1}{20} \\
& \sum \hat{b}_{i} \hat{a}_{i j} c_{j}=\frac{1}{120} \\
& \sum \hat{b}_{i} c_{i}^{4}=\frac{1}{30}, \\
\text { Order 6: } & \sum \hat{b}_{i} c_{i} \hat{a}_{i j} c_{j}=\frac{1}{180} \\
& \sum \hat{b}_{i} \hat{a}_{i j} c_{j}^{2}=\frac{1}{360} \tag{1.30}
\end{array}
$$

Order 7: $\quad \sum \hat{b}_{i} c_{i}^{5}=\frac{1}{42}$,

$$
\begin{equation*}
\sum \hat{b}_{i} c_{i}^{2} \hat{a}_{i j} c_{j}=\frac{1}{252} \tag{1.31}
\end{equation*}
$$

$$
\begin{equation*}
\sum \hat{b}_{i} c_{i} \hat{a}_{i j} c_{j}^{2}=\frac{1}{504} \tag{1.32}
\end{equation*}
$$

$$
\begin{equation*}
\sum \hat{b}_{i} \hat{a}_{i j} c_{j}^{3}=\frac{1}{840} \tag{1.33}
\end{equation*}
$$

$$
\begin{equation*}
\sum \hat{b}_{i} \hat{a}_{i j}^{2} c_{j}=\frac{1}{5040} \tag{1.34}
\end{equation*}
$$

For DITDRK methods, the following simplifying assumption as proposed by Chan and Tsai (2010) to simplify the order conditions is imposed:

$$
\begin{equation*}
\sum_{j=1}^{i} \hat{a}_{i j}=\frac{1}{2} c_{i}^{2}, \quad i=1, \ldots, s \tag{1.36}
\end{equation*}
$$

Minimizing the error norms is one of the finest strategy to acquire a particular order accuracy as stated in Dormand (1996). The norm of the local truncation error is:

$$
\begin{equation*}
\left\|\tau^{(\zeta+1)}\right\|_{2}=\sqrt{\sum_{j=1}^{\zeta+1}\left(\tau_{j}^{(\zeta+1)}\right)^{2}} \tag{1.37}
\end{equation*}
$$

The increment function of a DITDRK method can be expressed as follows

$$
\begin{equation*}
\Phi=\sum_{i=1}^{\infty} h^{i-2}\left\{\sum_{j=1}^{n_{i}} \rho_{j}^{(i)} F_{j}^{(i)}\right\} \tag{1.38}
\end{equation*}
$$

where the $\rho_{j}^{(i)}$ are the functions of the DITDRK parameters $\hat{a}_{i j}, \hat{b}_{i}, c_{i}$ and the simplifying assumption (1.36) is satisfied. By using the equations (1.16) and (1.18) with (1.38), for any DITDRK methods, the local truncation error can be written as

$$
\begin{align*}
L T E_{n+1} & =\sum_{i=2}^{\infty} h^{i}\left\{\sum_{j=1}^{n_{i}}\left(\rho_{j}^{(i)}-\frac{\gamma_{j}^{(i)}}{i!}\right) F_{j}^{(i)}\right\} \\
& =\sum_{i=2}^{\infty} h^{i}\left\{\sum_{j=1}^{n_{i}} \tau_{j}^{(i)} F_{j}^{(i)}\right\} \tag{1.39}
\end{align*}
$$

where

$$
\tau_{j}^{(i)}=\rho_{j}^{(i)}-\frac{\gamma_{j}^{(i)}}{i!}, \quad i=2,3, \ldots ; \quad j=1,2, \ldots, n_{i}
$$

are the error coefficients. Hence, the error coefficients up to order seven for DITDRK methods are given below:

Order 2: $\quad \tau_{1}^{(2)}=\sum \hat{b}_{i}-\frac{1}{2}$,
Order 3: $\quad \tau_{1}^{(3)}=\sum \hat{b}_{i} c_{i}-\frac{1}{6}$,
Order 4: $\quad \tau_{1}^{(4)}=\sum \hat{b}_{i} c_{i}^{2}-\frac{1}{12}$,
Order 5: $\quad \tau_{1}^{(5)}=\sum \hat{b}_{i} c_{i}^{3}-\frac{1}{20}$,

$$
\begin{equation*}
\tau_{2}^{(5)}=\sum \hat{b}_{i} \hat{a}_{i j} c_{j}-\frac{1}{120} \tag{1.43}
\end{equation*}
$$

Order 6: $\quad \tau_{1}^{(6)}=\sum \hat{b}_{i} c_{i}^{4}-\frac{1}{30}$,

$$
\begin{equation*}
\tau_{2}^{(6)}=\sum \hat{b}_{i} c_{i} \hat{a}_{i j} c_{j}-\frac{1}{180} \tag{1.45}
\end{equation*}
$$

$$
\begin{align*}
\tau_{3}^{(6)} & =\sum \hat{b}_{i} \hat{a}_{i j} c_{j}^{2}-\frac{1}{360}  \tag{1.47}\\
\text { Order 7: } \quad \tau_{1}^{(7)} & =\sum \hat{b}_{i} c_{i}^{5}-\frac{1}{42},  \tag{1.48}\\
\tau_{2}^{(7)} & =\sum \hat{b}_{i} c_{i}^{2} \hat{a}_{i j} c_{j}-\frac{1}{252},  \tag{1.49}\\
\tau_{3}^{(7)} & =\sum \hat{b}_{i} c_{i} \hat{a}_{i j} c_{j}^{2}-\frac{1}{504},  \tag{1.50}\\
\tau_{4}^{(7)} & =\sum \hat{b}_{i} \hat{a}_{i j} c_{j}^{3}-\frac{1}{840}  \tag{1.51}\\
\tau_{5}^{(7)} & =\sum \hat{b}_{i} \hat{a}_{i j}^{2} c_{j}-\frac{1}{5040} \tag{1.52}
\end{align*}
$$

### 1.10 Stability of TDRK Method

When a DITDRK method is applied to the model equation

$$
\begin{equation*}
y^{\prime}=f(x, y)=\lambda y, \quad y^{\prime \prime}=f^{\prime}(x, y) f(x, y)=\lambda^{2} y, \quad \lambda \in \mathbb{C}, \tag{1.53}
\end{equation*}
$$

the resulting difference equation is

$$
\begin{equation*}
y_{n+1}=H(v) y_{n}, \quad v=\lambda h, \tag{1.54}
\end{equation*}
$$

where $H(v)$ is the stability polynomial of the DITDRK method. It can be clearly seen that $y_{n} \rightarrow 0$ as $n \rightarrow \infty$ if and only if

$$
\begin{equation*}
|H(v)|<1, \tag{1.55}
\end{equation*}
$$

and the method will be absolutely stable for $v$ values for which (1.55) holds.

Applying the test equation (1.53) to DITDRK method (1.10)-(1.11) yields

$$
\begin{align*}
Y_{i} & =y_{n}+c_{i} v y_{n}+v^{2} \sum_{j=1}^{i} \hat{a}_{i j} Y_{j},  \tag{1.56}\\
y_{n+1} & =y_{n}+v y_{n}+v^{2} \sum_{i=1}^{s} \hat{b}_{i} Y_{i}, \tag{1.57}
\end{align*}
$$

where $i=1, \ldots, s$.

Define $Y, e \in \mathfrak{R}^{s}$ by $e=(1,1, \ldots, 1)^{T}$ and $Y=\left(Y_{1}, Y_{2}, \ldots, Y_{S}\right)^{T}$, then (1.56) and (1.57) can be written in the form

$$
\begin{align*}
Y & =y_{n} e+c_{i} v y_{n}+v^{2} \hat{A} Y,  \tag{1.58}\\
y_{n+1} & =y_{n}+v y_{n}+v^{2} \hat{b}^{T} Y . \tag{1.59}
\end{align*}
$$

Solving for (1.58) and substituting into (1.59) gives

$$
\begin{equation*}
y_{n+1}=\left[(1+v)+v^{2} \hat{b}^{T}(e+c v)\left(I-v^{2} \hat{A}\right)^{-1}\right] y_{n}, \tag{1.60}
\end{equation*}
$$

$I$ is the $s \times s$ unit matrix $\hat{b}=\left(\hat{b}_{1}, \hat{b}_{2}, \ldots, \hat{b}_{s}\right)^{T}$ and $c=\left(c_{1}, c_{2}, \ldots, c_{s}\right)^{T}$. The stability function is then given by

$$
\begin{equation*}
H(v)=1+v^{2} \hat{b}^{T}\left(I-v^{2} \hat{A}\right)^{-1} e+v\left(1+v^{2} \hat{b}^{T} c\left(I-v^{2} \hat{A}\right)^{-1}\right) \tag{1.61}
\end{equation*}
$$

According to Cramer's rule, the stability function of DITDRK method can be written as

$$
\begin{equation*}
H(v)=\frac{P(v)}{Q(v)}=\frac{(1+v) \operatorname{det}\left[\left(I-v^{2} \hat{A}\right)+\left(v^{2} /(1+v)\right) e \hat{b}^{T}+\left(v^{3} /(1+v)\right) c \hat{b}^{T}\right]}{\operatorname{det}\left(I-v^{2} \hat{A}\right)} . \tag{1.62}
\end{equation*}
$$

It can be seen that $y_{n} \rightarrow 0$ as $n \rightarrow \infty$ if and only if

$$
\begin{equation*}
|H(v)|<1, \tag{1.63}
\end{equation*}
$$

and the method is absolutely stable for those $v$ values for which (1.63) holds. The stability region is defined as $\{v \in \mathbb{C}:|H(v)| \leq 1\}$ or the set of points in the complex plane given that the computed solution remains bounded after many computation steps as in Wolfram (1991).

Definition 1.3 (Butcher, 1987)
A Runge-Kutta method is said to be absolutely stable for a given $v$, if for all that $v$, all the roots of the stability polynomial have modulus less than or equal to one, with those of modulus one being simple.

Definition 1.4 (Butcher, 1987)
A Runge-Kutta method is said to be A-stable if its stability region contains $C^{-}$, the nonpositive half-plane $\{v \mid \operatorname{Re}(v)<0\}$.

Absolute stability property will ensure that the decreasing solution will be approximated by non-increasing function. Meanwhile, the A-stable method can be regarded as trying to produce an approximate to the exponential function whose modulus is bounded by unity.

When solving the IVP (1.53), a more satisfactory approximation to the exponential will be the one that is not only A-stable, but also satisfies the property that as $|v| \rightarrow \infty$, with $\operatorname{Re}(z)<0$, its modulus approaches zero, which leads to the definition below.

Definition 1.5 (Wanner and Hairer, 1996)
A method is called L-stable if it is A-stable and if in addition $\lim _{v \rightarrow \infty} H(v)=0$. If an Implicit Runge-Kutta (IRK) method is A-stable, then it is L-stable if and only if $H(v)=\frac{P(v)}{Q(v)}$, such that the degree of $P(v)<$ degree of $Q(v)$.

### 1.11 Three Derivative Runge-Kutta (ThDRK) Method

A Three Derivative Runge-Kutta method is a Runge-Kutta method designed for solving first-order ODEs in the form of (1.1) other than TDRK method. A ThDRK method can be divided into two form which is explicit ThDRK methods and implicit ThDRK methods. If $a_{i j}=0$ for $i \leq j$, a ThDRK method is an explicit method and if $a_{i j}=\delta$ where $i=j, \delta \in \mathfrak{R}$, it is denoted as diagonally implicit or also known as singly implicit. In our research context, we concentrate mainly on diagonally implicit ThDRK method.

Consider the scalar ODEs (1.1) with $f: \mathfrak{R}^{N} \rightarrow \mathfrak{R}^{N}$. In this case, the second and third derivative are also assumed to be known where

$$
\begin{array}{ll}
y^{\prime \prime}=g(y):=f^{\prime}(y) f(y), & g: \mathfrak{R}^{N} \rightarrow \mathfrak{R}^{N}, \\
y^{\prime \prime \prime}=\hat{g}(y):=f^{\prime \prime}(y)(f(y), f(y))+f^{\prime}(y) f^{\prime}(y) f(y), & \hat{g}: \mathfrak{R}^{N} \rightarrow \mathfrak{R}^{N} . \tag{1.64}
\end{array}
$$

An implicit ThDRK method for the numerical integration of IVPs (1.1) is given by

$$
\begin{align*}
Y_{i} & =\hat{g}\left(x_{n}+c_{i} h, y_{n}+h \sum_{j=1}^{s} a_{i j} f\left(Y_{j}\right)+\frac{h^{2}}{2} \sum_{j=1}^{s} \hat{a}_{i j} g\left(Y_{j}\right)+h^{3} \sum_{j=1}^{s} \bar{a}_{i j} Y_{j}\right),  \tag{1.65}\\
y_{n+1} & =y_{n}+h \sum_{i=1}^{s} b_{i} f\left(Y_{i}\right)+\frac{h^{2}}{2} \sum_{i=1}^{s} \hat{b}_{i} g\left(Y_{i}\right)+h^{3} \sum_{i=1}^{s} \bar{b}_{i} Y_{i}, \tag{1.66}
\end{align*}
$$

where $i=1, \ldots, s$.

The implicit ThDRK method with the coefficients in (1.65) and (1.66) are presented using the Butcher tableau as follows:

| c | A | $\hat{A}$ | $\bar{A}$ |
| :---: | :---: | :---: | :---: |
|  | $b^{T}$ | $\hat{b}^{T}$ | $\bar{b}^{T}$ |

Diagonally implicit methods with a minimal number of function evaluations can be developed by considering the methods in the form

$$
\begin{align*}
Y_{i} & =\hat{g}\left(x_{n}+c_{i} h, y_{n}+h c_{i} f\left(x_{n}, y_{n}\right)+\frac{h^{2}}{2} c_{i}^{2} g\left(x_{n}, y_{n}\right)+h^{3} \sum_{j=1}^{s} \bar{a}_{i j} Y_{j}\right),  \tag{1.67}\\
y_{n+1} & =y_{n}+h f\left(x_{n}, y_{n}\right)+\frac{h^{2}}{2} g\left(x_{n}, y_{n}\right)+h^{3} \sum_{i=1}^{s} \hat{b}_{i} Y_{i}, \tag{1.68}
\end{align*}
$$

where $i=1, \ldots, s$.

The above method is denoted as a special DIThDRK method. The unique part of this method is that it involves only one evaluation of $f$ and $g$ and many evaluations of $\hat{g}$ per step compared to a number of evaluations of $f$ per step in traditional RK methods. Its Butcher tableau is given as follows:

The DIThDRK parameters $a_{i j}, \hat{a}_{i j}, \bar{a}_{i j}, b_{j}, \hat{b}_{j}$ and $\bar{b}_{j}$ are assumed to be real and $s$ is the number of stage of the method. The $s$-dimensional vectors $\mathbf{b}, \hat{\mathbf{b}}, \overline{\mathbf{b}}, \mathbf{c}$ and $s \times s$ matrix $\mathbf{A}, \hat{\mathbf{A}}$ and $\overline{\mathbf{A}}$, are introduced where $\mathbf{b}=\left[b_{1}, b_{2}, \ldots, b_{s}\right]^{T}, \hat{\mathbf{b}}=\left[\hat{b}_{1}, \hat{b}_{2}, \ldots, \hat{b}_{s}\right]^{T}, \overline{\mathbf{b}}=\left[\bar{b}_{1}, \bar{b}_{2}, \ldots, \bar{b}_{s}\right]^{T}, \mathbf{c}=$ $\left[c_{1}, c_{2}, \ldots, c_{s}\right]^{T}, \mathbf{A}=\left[a_{i j}\right], \hat{\mathbf{A}}=\left[\hat{a}_{i j}\right]$ and $\overline{\mathbf{A}}=\left[\bar{a}_{i j}\right]$ respectively.

### 1.12 Algebraic Conditions and Local Truncation Error for ThDRK Method

The ThDRK methods (1.67) and (1.68) can be written as the following:

$$
\begin{equation*}
y_{n+1}=y_{n}+h y_{n}^{\prime}+\frac{h^{2}}{2} y_{n}^{\prime \prime}+h^{3} \sum_{i=1}^{s} \bar{b}_{i} k_{i}, \tag{1.69}
\end{equation*}
$$

where

$$
\begin{equation*}
k_{i}=\hat{g}\left(x_{n}+c_{i} h, y_{n}+h c_{i} y_{n}^{\prime}+\frac{h^{2}}{2} c_{i}^{2} y_{n}^{\prime \prime}+h^{3} \sum_{j=1}^{i} \bar{a}_{i j} k_{j}\right) \tag{1.70}
\end{equation*}
$$

The order conditions for DIThDRK methods can be easily obtained by expanding the local truncation error in a direct way. The DIThDRK method (1.69) and (1.70) can be expressed as:

$$
\begin{equation*}
y_{n+1}=y_{n}+h \psi\left(x_{n}, y_{n}, h\right) \tag{1.71}
\end{equation*}
$$

where the increment function $\psi\left(x_{n}, y_{n}, h\right)$ is denoted as

$$
\begin{equation*}
\psi\left(x_{n}, y_{n}\right)=y_{n}^{\prime}+\frac{h}{2} y_{n}^{\prime \prime}+h^{2} \sum_{i=1}^{s} \bar{b}_{i} k_{i} \tag{1.72}
\end{equation*}
$$

and $k_{i}$ is given in (1.70).

The Taylor series increment function is denoted as $\Delta$. After substracting the computed solution, $y_{n+1}$ with the exact solution, $y\left(x_{n+1}\right)$, the local truncation errors of $y_{n}$ can be obtained where

$$
\begin{equation*}
L T E_{n+1}=h(\psi-\Delta) \tag{1.73}
\end{equation*}
$$

The Taylor series increment function of $y_{n}$ is expressed as

$$
\begin{equation*}
\Delta=y_{n}^{\prime}+\frac{1}{2} h y_{n}^{\prime \prime}+\frac{1}{6} h^{2} y_{n}^{\prime \prime \prime}+\frac{1}{24} h^{3} y_{n}^{(i v)}+\frac{1}{120} h^{4} y_{n}^{(v)}+\frac{1}{720} h^{5} y_{n}^{(v i)}+\ldots+\frac{1}{p!} h^{p-1} y_{n}^{(p)} \tag{1.74}
\end{equation*}
$$

The above equations are expressed in terms of elementary differentials. A few elementary differentials are given in (1.18) and as follows:

$$
\begin{aligned}
y^{(v)}=F_{1}^{(5)}= & f_{y y y y}\left(y^{\prime}\right)^{4}+6 y^{\prime \prime}\left(y^{\prime}\right)^{2} f_{y y y}+4 y^{\prime \prime \prime} f_{x y y y}+3\left(y^{\prime \prime}\right)^{2} f_{y y}+12 y^{\prime \prime} y^{\prime} f_{x y y}+ \\
& 4 y^{\prime \prime \prime} y^{\prime} f_{y y}+6\left(y^{\prime}\right)^{2} f_{x x y y}+6 f_{x x y} y^{\prime \prime}+4 f_{x y} y^{\prime \prime \prime}+f_{y} y^{(i v)}+4 f_{x x x y} y^{\prime}+ \\
& f_{x x x x}
\end{aligned}
$$

Express $\Delta$ in terms of the elementary differential lead to:

$$
\begin{equation*}
\Delta=F_{1}^{(1)}+\frac{1}{2} h F_{1}^{(2)}+\frac{1}{6} h^{2} F_{1}^{(3)}+\frac{1}{24} h^{3} F_{1}^{(4)}+\frac{1}{120} h^{4} F_{1}^{(5)}+\mathscr{O}\left(h^{5}\right) \tag{1.76}
\end{equation*}
$$

Substituting (1.75) into (1.72), the increment function $\psi$ for DIThDRK method becomes

$$
\begin{equation*}
\sum_{i=1}^{s} \bar{b}_{i} k_{i}=\sum_{i=1}^{s} \bar{b}_{i} F_{1}^{(3)}+h \sum_{i=1}^{s} \bar{b}_{i} c_{i} F_{1}^{(4)}+\frac{1}{2} h^{3} \sum_{i=1}^{s} \bar{b}_{i} c_{i}^{2} F_{1}^{(5)}+\mathscr{O}\left(h^{4}\right) \tag{1.77}
\end{equation*}
$$

Using (1.72) and (1.74), the LTE can be written as:

$$
\left.\left.\begin{array}{rl}
L T E_{n+1}= & h^{3}
\end{array}\right]\left(\sum_{i=1}^{s} \bar{b}_{i} F_{1}^{(3)}+h \sum_{i=1}^{s} \bar{b}_{i} c_{i} F_{1}^{(4)}+\frac{1}{2} h^{2} \sum_{i=1}^{s} \bar{b}_{i} c_{i}^{2} F_{1}^{(5)}+\ldots\right)\right] .
$$

Simplifying (1.78)

$$
\begin{align*}
L T E_{n+1}= & h^{3}\left[\left(\sum_{i=1}^{s} \bar{b}_{i}-\frac{1}{6}\right) F_{1}^{(3)}+\left(\sum_{i=1}^{s} \bar{b}_{i} c_{i}-\frac{1}{24}\right) h F_{1}^{(4)}\right. \\
& \left.+\left(\frac{1}{2} h^{2} \sum_{i=1}^{s} \bar{b}_{i} c_{i}^{2}-\frac{1}{120}\right) h^{2} F_{1}^{(5)}+\ldots\right] \tag{1.79}
\end{align*}
$$

The order conditions for a $s$-stage DIThDRK method by using (1.79) up to order eight as proposed by Turacı and Öziş (2015) are given as follows:

Order 3: $\quad \sum \bar{b}_{i}=\frac{1}{6}$,
Order 4: $\quad \sum \bar{b}_{i} c_{i}=\frac{1}{24}$,
Order 5: $\quad \sum \bar{b}_{i} c_{i}^{2}=\frac{1}{60}$,
Order 6: $\quad \sum \bar{b}_{i} c_{i}^{3}=\frac{1}{120}$,
Order 7: $\quad \sum \bar{b}_{i} \bar{a}_{i j} c_{j}=\frac{1}{5040}$,

$$
\begin{equation*}
\sum \bar{b}_{i} c_{i}^{4}=\frac{1}{210} \tag{1.84}
\end{equation*}
$$

$$
\begin{array}{ll}
\text { Order 8: } & \sum \bar{b}_{i} c_{i}^{5}=\frac{1}{336}, \\
& \sum \bar{b}_{i} \bar{a}_{i j} c_{j}^{2}=\frac{1}{20160}, \\
& \sum \bar{b}_{i} c_{i} \bar{a}_{i j} c_{j}=\frac{1}{8064} . \tag{1.88}
\end{array}
$$

For DIThDRK methods, the following simplifying assumption as proposed by Turacı and Öziş (2015) to simplfy the order conditions is imposed:

$$
\begin{equation*}
\sum_{j=1}^{i} \bar{a}_{i j}=\frac{1}{6} c_{i}^{3}, \quad i=1, \ldots, s \tag{1.89}
\end{equation*}
$$

The norm of local truncation error is given in (1.37).

The increment function of a ThDRK method can be expressed as follows

$$
\begin{equation*}
\Phi=\sum_{i=3}^{\infty} h^{i-3}\left\{\sum_{j=1}^{n_{i}} \rho_{j}^{(i)} F_{j}^{(i)}\right\} \tag{1.90}
\end{equation*}
$$

where the $\rho_{j}^{(i)}$ are the functions of the DIThDRK parameters $\bar{a}_{i j}, \bar{b}_{i}, c_{i}$ and the simplifying assumption (1.89) is satisfied. By using the equations (1.16) and the elementary differentials given in (1.18) and (1.76) with (1.90), for any DIThDRK methods, the local truncation error can be written as

$$
\begin{align*}
L T E_{n+1} & =\sum_{i=3}^{\infty} h^{i}\left\{\sum_{j=1}^{n_{i}}\left(\rho_{j}^{(i)}-\frac{\gamma_{j}^{(i)}}{i!}\right) F_{j}^{(i)}\right\} \\
& =\sum_{i=3}^{\infty} h^{i}\left\{\sum_{j=1}^{n_{i}} \tau_{j}^{(i)} F_{j}^{(i)}\right\} \tag{1.91}
\end{align*}
$$

where

$$
\tau_{j}^{(i)}=\rho_{j}^{(i)}-\frac{\gamma_{j}^{(i)}}{i!}, \quad i=3,4, \ldots ; \quad j=1,2, \ldots, n_{i}
$$

are the error coefficients. Hence, the error coefficients up to order eight for DIThDRK processes are given below:

Order 3: $\quad \tau_{1}^{(3)}=\sum \bar{b}_{i}-\frac{1}{6}$,
Order 4: $\quad \tau_{1}^{(4)}=\sum \bar{b}_{i} c_{i}-\frac{1}{24}$,
Order 5: $\quad \tau_{1}^{(5)}=\sum \bar{b}_{i} c_{i}^{2}-\frac{1}{60}$,
Order 6: $\quad \tau_{1}^{(6)}=\sum \bar{b}_{i} c_{i}^{3}-\frac{1}{120}$,

$$
\begin{align*}
\text { Order 7: } \quad \tau_{1}^{(7)} & =\sum \bar{b}_{i} \bar{a}_{i j} c_{j}-\frac{1}{5040},  \tag{1.96}\\
\tau_{2}^{(7)} & =\sum \bar{b}_{i} c_{i}^{4}-\frac{1}{210}  \tag{1.97}\\
\text { Order 8: } \quad \tau_{1}^{(8)} & =\sum \bar{b}_{i} c_{i}^{5}-\frac{1}{336},  \tag{1.98}\\
\tau_{2}^{(8)} & =\sum \bar{b}_{i} \bar{a}_{i j} c_{j}^{2}-\frac{1}{20160},  \tag{1.99}\\
\tau_{3}^{(8)} & =\sum \bar{b}_{i} c_{i} \bar{a}_{i j} c_{j}-\frac{1}{8064} \tag{1.100}
\end{align*}
$$

### 1.13 Stability of ThDRK Method

When a DIThDRK method is applied to the model equation

$$
\begin{equation*}
y^{\prime}=\lambda y, \quad y^{\prime \prime}=\lambda^{2} y, \quad y^{\prime \prime \prime}=\lambda^{3} y, \quad \lambda \in \mathbb{C}, \tag{1.101}
\end{equation*}
$$

the resulting difference equation is given by (1.54).

Applying the test equation (1.101) to DIThDRK method (1.67)-(1.68) yields

$$
\begin{align*}
Y_{i} & =y_{n}+c_{i} v y_{n}+\frac{v^{2}}{2} c_{i}^{2} y_{n}+v^{3} \sum_{j=1}^{i} \bar{a}_{i j} Y_{j},  \tag{1.102}\\
y_{n+1} & =y_{n}+v y_{n}+\frac{v^{2}}{2} y_{n}+v^{3} \sum_{i=1}^{s} \bar{b}_{i} Y_{i}, \tag{1.103}
\end{align*}
$$

where $i=1, \ldots, s$.

Define $Y, e \in \mathfrak{R}^{s}$ by $e=(1,1, \ldots, 1)^{T}$ and $Y=\left(Y_{1}, Y_{2}, \ldots, Y_{S}\right)^{T}$, then (1.102) and (1.103) can be written in the form

$$
\begin{align*}
Y & =y_{n} e+c_{i} v y_{n}+\frac{v^{2}}{2} c_{i}^{2} y_{n}+v^{3} \bar{A} Y,  \tag{1.104}\\
y_{n+1} & =y_{n}+v y_{n}+\frac{v^{2}}{2} y_{n}+v^{2} \bar{b}^{T} Y . \tag{1.105}
\end{align*}
$$

Solving for (1.104) and substituting into (1.105) gives

$$
\begin{equation*}
y_{n+1}=\left[\left(1+v+\frac{v^{2}}{2}\right)+v^{3} \bar{b}^{T}\left(e+c v+\frac{v^{2}}{2} c^{2}\right)\left(I-v^{3} \bar{A}\right)^{-1}\right] y_{n} \tag{1.106}
\end{equation*}
$$

The stability function is then given by

$$
\begin{align*}
H(v)= & 1+v^{3} \bar{b}^{T}\left(I-v^{3} \bar{A}\right)^{-1} e+v\left(1+v^{3} \bar{b}^{T} c\left(I-v^{3} \bar{A}\right)^{-1}\right)+ \\
& \frac{v^{2}}{2}\left(1+v^{3} \bar{b}^{T} c^{2}\left(I-v^{3} \bar{A}\right)^{-1}\right) . \tag{1.107}
\end{align*}
$$

According to Cramer's rule, the stability function of DIThDRK method can be written as $H(v)=\frac{P(v)}{Q(v)}$, where

$$
\begin{align*}
P(v)= & \left(1+v+\frac{v^{2}}{2}\right) \operatorname{det}\left[\left(I-v^{3} \bar{A}\right)+\left(v^{3} /\left(1+v+\frac{v^{2}}{2}\right)\right) e \bar{b}^{T}+\left(v^{4} /\left(1+v+\frac{v^{2}}{2}\right)\right) c \bar{b}^{T}\right. \\
& \left.+\frac{1}{2}\left(v^{5} /\left(1+v+\frac{v^{2}}{2}\right)\right) c^{2} \bar{b}^{T}\right]  \tag{1.108}\\
Q(v)= & \operatorname{det}\left(I-v^{3} \bar{A}\right) \tag{1.109}
\end{align*}
$$

which will be used in the derivation of the DIThDRK methods in the following chapter.

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## BIODATA OF STUDENT

Born on the $16^{\text {th }}$ of February 1992 in Tanjong Karang Selangor, Nur Amirah binti Ahmad started her primary education at Sekolah Kebangsaan Batu 9 Jalan Bomba, Tanjong Karang in 1999 from standard one to standard six.

She then continued her secondary education at Sekolah Menengah Kebangsaan Dato’ Harun, Tanjong Karang in 2005 until Form Three and went to Sekolah Menengah Sains Kuala Selangor, Kuala Selangor in 2008 due to her excellent performance in Penilaian Menengah Rendah (PMR) in 2007 and completed in 2009.

She passed her Sijil Pelajaran Malaysia (SPM) with flying colors and was offered to pursue her studies in the area of pure science at the Centre for Foundation Studies in Science, Universiti Malaya, Kuala Lumpur in 2010. A year later, she went to Universiti Putra Malaysia to pursue her first degree in 2011 under Biasiswa Khas Tenaga Akademik (BKTA) offered by Ministry of Higher Education. She obtained her Bachelor Degree in Science (Mathematics) in 2015.

She later continued her studies at Universiti Putra Malaysia under Institute for Mathematical Research (INSPEM), sponsored by Ministry of Higher Education (MyBrainSc) and obtained her Master of Science Degree (Computational Mathematics) in 2017.

In the same year, she pursued her education in PhD. in Computational Mathematics at Universiti Putra Malaysia supervised by Assoc. Prof. Dr. Norazak Senu. Her main works are based on Applied Mathematics (Numerical Analysis).

## LIST OF PUBLICATIONS

The following are the list of publications that arise from this study.

## Journal articles:

Ahmad, N. A., Senu, N., Ibrahim, Z. B. and Othman, M. (2019). Diagonally Implicit Two Derivative Runge-Kutta methods for solving First Order Initial Value Problems, Journal of Abstract and Computational Mathematics 4(1): 18-36.

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