UNIVERSITI PUTRA MALAYSIA

EXPLICIT TWO-DERIVATIVE RUNGE-KUTTA TYPE METHODS FOR SOLVING THIRD-ORDER ORDINARY AND RETARDED DELAY DIFFERENTIAL EQUATIONS

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By

LEE KHAI CHIEN

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

This humble work is dedicated to my beloved family lecturers, friends and future researchers.

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

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LEE KHAI CHIEN

June 2022

Chairman : **Assoc. Prof. Norazak Senu, PhD**
Institute : **Mathematical Research**

In this study, two types of explicit two-derivative Runge-Kutta type (GTDRKT and TDRKT) methods are constructed for the numerical integration of general and special type of third-order ordinary differential equations (ODEs). Improved two-derivative Runge-Kutta type (TDIRKT) methods are derived for solving third-order ODEs in the form of $f(u,u',u'')$. B-series and rooted tree theory are used to derive order conditions and coefficients for GTDRKT and TDRKT methods. Stability, consistency and convergence analysis of the proposed methods are investigated. The Local Truncation Error (LTE) for GTDRKT, TDRKT and TDIRKT methods are computed and analysed for u,u' and u''. For TDIRKT methods, the previous term, k_{-i} is implemented in the formulation and the relevant order conditions are introduced for constructing the proposed methods. Exponentially-fitting and trigonometrically-fitting techniques are implemented into both GTDRKT and TDIRKT methods by constructing coefficients with principle frequency based. These proposed methods are developed based on the idea of integrating initial value problems (IVPs) exactly with numerical solution in the form linear composition of the set functions $e^{\omega x}$ and $e^{-\omega x}$ for exponentially-fitted and $e^{i\omega x}$ and $e^{-i\omega x}$ for trigonometrically-fitted for solving third-order ordinary differential equations with exponential and oscillatory solutions.

Brief introduction on Retarded Delay Differential Equations (RDDEs) is provided. Stability, consistency and D-convergence for both TDRKT and TDIRKT methods when applied to RDDEs with constant delay, using Newton interpolation methods to evaluate the delay term are discussed and analysed. In solving third-order RDDEs, Newton interpolation is used to approximate the delay term and solve the subsequent equations through TDRKT and TDIRKT methods. In numerical test, numerical results are illustrated using efficiency curves where maximum global error versus the CPU time taken. Number of function evaluations for all proposed methods and selected existing methods are computed with different endpoints and step size. Results exhibited the proposed methods work effectively for solving general and special type of third-order ODEs as well as third-order RDDEs.

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

KAEDAH JENIS RUNGE-KUTTA DUA TERBITAN TAK TERSIRAT UNTUK MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA DAN LENGAH TERLAMBAT PERINGKAT KETIGA

Oleh

LEE KHAI CHIEN

Jun 2022

Pengerusi : **Profesor Madya Norazak Senu, PhD**
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Dalam kajian ini, dua jenis kaedah jenis Runge-Kutta dua terbitan tak tersirat (RKDTTTU dan RKDTTT) diterbitkan untuk menyelesaikan persamaan pembezaan biasa (PBB) umum dan istimewa peringkat ketiga. Kaedah jenis Runge-Kutta Dua Terbitan Tak Tersirat penambahbaikan (RKDTTTP) diterbitkan untuk menyelesaikan persamaan pembezaan biasa peringkat ketiga dalam bentuk $f(u,u',u'')$. Siri-B dan teori pokok berakar digunakan untuk memperoleh syarat peringkat dan pekali bagi kaedah RKDTTTU dan RKDTTT. Analisis kestabilan, kekonsistenan dan penumpuan bagi kaedah tersebut dikaji. Ralat pangkasan setempat bagi kaedah RKDTTTU, RKDTTT dan RKDTTTP ditafsir dan dianalisis untuk u,u' dan u''. Bagi kaedah RKDTTTP, Sebutan sebelum, k_{-i} ditambah ke dalam formulasi dan syarat peringkat diperkenalkan untuk membina kaedah tersebut. Teknik suai-eksponen dan suai-trigonometri diaplikasi ke dalam kaedah RKDTTTU dan RKDTTT dengan menerbitkan pekali yang berasaskan prinsip frekuensi. Kaedah tersebut diterbitkan berdasarkan idea mengintegrasikan masalah nilai awal dengan penyelesaian berangka dalam bentuk komposisi linear bagi set fungsi $e^{\omega x}$ dan $e^{-\omega x}$ untuk suai-eksponen dan $e^{i\omega x}$ dan $e^{-i\omega x}$ untuk suai-trigonometri bagi menyelesaikan persamaan pembezaan biasa peringkat ketiga yang mempunyai penyelesaian berbentuk eksponen dan ayunan.

Pengenalan ringkas terhadap Persamaan Pembezaan Lengah Terencat (PPLT) dibekalkan. Kestabilan, konsistensi dan penumpuan-D bagi kaedah RKDTTT and RKDTTTP dibincangkan dan dikaji, di mana kaedah tersebut diaplikasi terhadap PPLT dengan lengah malar dan kaedah interpolasi Newton digunakan untuk menilai sebutan lengah. Dalam penyelesaian PPLT peringkat ketiga, interpolasi Newton digunakan untuk menganggar sebutan lengah dan diselesaikan selanjutnya dengan menggunakan kaedah RKDTTT dan RKDTTTP. Dalam ujian berangka, keputusan berangka digambarkan menggunakan lengkung kecekapan di mana logaritma ralat

sejagat maksimum berbanding masa CPU diambil. Bilangan penilaian fungsi bagi semua kaedah yang diterbitkan dan kaedah sedia ada yang terpilih dikira dengan titik akhir dan saiz langkah yang berbeza. Keputusan menunjukkan kaedah yang diterbitkan dalam kajian ini cekap dalam menyelesaikan persamaan pembezaan biasa umum dan istimewa peringkat ketiga dan juga PPLT peringkat ketiga.

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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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Declaration by Members of Supervisory Committee

This is to confirm that:

- the research conducted and the writing of this thesis was under our supervision;
- supervision responsibilities as stated in the Universiti Putra Malaysia (Graduate Studies) Rules 2003 (Revision 2012-2013) are adhered to.

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LIST OF ABBREVIATIONS

ATDRKT6	Explicit four-stage sixth-order trigonometrically-fitted two-derivative Runge-Kutta method
IVP	Initial value problem
ODEs	Ordinary differential equations
DDEs	Delay differential equations
EFRKT5	Explicit exponential-fitted Runge-Kutta type method with four stage fifth-order
EFRKT5	Explicit exponential-fitted Runge-Kutta type method with four stage fifth-order
ERK6	Enhanced Runge-Kutta with seven stage sixth-order method
EFTDIRKT6	Explicit exponential-fitted two-derivative improved Runge-Kutta type method with three stage sixth-order developed in Chapter 7
EFTDRKT5	Explicit exponential-fitted two-derivative Runge-Kutta typemethod with two stage fifth-order developed in Chapter 5
EFTDRKT6	Explicit exponential-fitted two-derivative Runge-Kutta typemethod with three stage sixth-order developed in Chapter 5
GTDRKT6	Three-stage two-derivative Runge-Kutta type method of six algebraic order developed in Chapter 3
GTDRKT5	Two-stage two-derivative Runge-Kutta type method of five algebraic order developed in Chapter 3
Hussain4	Fourth order improved Runge-Kutta direct method
Hussain5	Fifth order improved Runge-Kutta direct method
IRKD5	Four stage fifth-order improved Runge-Kutta direct method
KTDRKT5	Explicit four-stage fifth-order trigonometrically-fitted two-derivative Runge-Kutta method with FSAL property
Mechee4	Explicit two stage fourth-order direct method

Mechee5	Explicit three stage fifth-order direct method
PTDRKT6	Explicit three-stage sixth-order phase-fitted three-derivative Runge-Kutta method
RK4	Runge-Kutta four stage fourth-order method
RK5	Runge-Kutta six-stage fifth-order method
RK6	Runge-Kutta seven-stage sixth-order method
RK6S	Runge-Kutta seven-stage sixth-order method
RK6N	Runge-Kutta seven-stage sixth-order method
RK6Z	Six stage sixth-order Runge-Kutta method
RKD5	Explicit three stage fifth-order direct method
RKF45	Runge-Kutta-Fehlberg method
TFRKT5	Explicit trigonometrically-fitted Runge-Kutta type method with four stage fifth-order
TDRKT5	Explicit two-derivative Runge-Kutta type method with three stage fifth-order developed in Chapter 4
TFTDIRKT6	Explicit trigonometrically-fitted two-derivative improved Runge-Kutta type method with three stage sixth-order developed in Chapter 7
TFTDRKT5	Explicit trigonometrically-fitted two-derivative Runge-Kutta type method with two stage fifth-order developed in Chapter 5
TFTDRKT6	Explicit trigonometrically-fitted two-derivative Runge-Kutta type method with three stage sixth-order developed in Chapter 5
h	Step-size
FE	Total number of function evaluations
TIME	CPU time
MAXXER	Maximum global error
MTD	Methods

CHAPTER 1

INTRODUCTION

1.1 Differential Equations

Differential equations are mathematical equations or formulas for unknown functions comprise of one or a few variables that associate with the values of the function itself to its derivatives of various orders. Also, differential equations can be expressed as the equations which comprise of dependent variables with respect to other independent variable. Various disciplines such as physics, medicines, biology, economics and astronomy can be formulated through differential equations. In medical field, differential equations are utilised to model spread of disease, outlining dynamics of infectious diseases and constructing control strategies to limit evolution and spread of diseases. In economics, differential equations are used to figure out optimum investments strategies, gross domestic product, consumption, income and investment. In biology, differential equations can be utilised to model biological processes on various levels ranging from DNA molecules or biosynthesis phospholipids on the cellular level. There are numerous types of differential equations, consist of ordinary, delay, partial and fractional differential equations.

1.1.1 Ordinary differential equations

Ordinary differential equations (ODEs) with initial value problem(IVPs) can be defined as:

$$u^{(n+1)} = f(t, u(t), u'(t), u''(t), ..., u^{(n)}(t)) \tag{1.1}$$

where

$$u(0) = u_0, u'(0) = u'_0, ..., u^{(n)}(0) = u_0^{(n)}, \quad t \geq 0.$$

and n is the order of differential equation.

Theorem 1.1 Let $m_1, m_2, ..., m_n$, f all continuous functions on the open interval, I such that $x_0 \in I$. Then the linear differential equation with order-n, $u^{(n)} + m_1 u^{(n-1)} + ... + m_{n-1}u' + m_n u = f(t)$ with the initial conditions $u(x_0) = u_0, u'(x_0) = u'_0, ..., u^{(n-1)}(x_0) = u_0^{(n-1)}$, has a unique solution $u = \phi(x)$ throughout the interval (Gustafson and Wilcox, 1998).

In this research, the conditions of the theorem are satisfied by the third-order linear ordinary differential equations in (1.1) with n=3.

1.1.1.1 Criteria of Oscillatory and Nonoscillatory for Third-order Linear Differential Equations

Criteria of oscillatory and nonoscillatory for third-order ordinary differential equations referred to Ghawadri et al. (2018) are mentioned as follow

$$u'''(x) + \alpha(t)u'(x) + \beta(x)u(x) = 0. \tag{1.2}$$

The solution of equation (1.2) is oscillatory if both $\alpha(x)$ and $\beta(x)$ are constant, negative and fulfil the following requirement:

$$-\beta(x) - \frac{2}{3\sqrt{3}}(-\alpha(x))^{3/2} > 0, \tag{1.3}$$

then two linear independent oscillatory solutions are exist and zeroes of any oscillatory solutions are split in which the oscillatory solution of equation (1.3) is linear combination of them. The solution of equation (1.3) is oscillatory iff it has infinity of zeroes clustering in $(0, +\infty)$ and nonoscillatory if and only if it has finite number of zeroes in $(0, +\infty)$ (Lazer, 1966). We focus on the condition $\beta(x) = 0$ as follow:

1. $u'''(x) = \alpha(x)u'(x), \alpha(x) > 0$, the solution of characteristic roots equations contains exponential function if that equations are real and one of them is zero.

2. $u'''(x) = -\alpha(x)u'(x), \alpha(x) > 0$, the solution of characteristic roots equations contains oscillatory function if that equations are real and another two are conjugate roots.

1.1.2 Delay differential equations

Delay differential equations (DDEs) is differential equations where the state variable appears with delayed term and the time derivatives at the current time depend on the solution and its derivative at previous times. There are various type of DDEs, comprised of retarded DDE, variable DDE, state-dependent DDE, neutral DDE and stochastic DDE (Bellen and Zennaro, 2003). Among these DDEs, retarded DDEs, has been widely used in various fields, including disease modelling, homoclinic and heteroclinic bifurcations, population dynamics. The solution of this type of DDE depends on not only a single initial condition at time, $t = t_0$, but also on the former history of the system. Time delay, τ in the constant time-delay system can be categorized into a discrete delay, derivative-dependent delay, state-dependent delay and time-dependent delay, which serves as the previous critical information that is important to approximate the solutions at forthcoming times. In engineering field, time delays are utilised in controlling feedback loops which is crucial to stabilise and control output system. Several methods arised to solve delay differential equations. Variational iteration and homotopy perturbation methods are used to solve delay differential equations in electrodynamics (Kocak and Yildirim, 2009). Pseudo-inverse method with Galerkin approximations can be used to predict feedback gain for closed-loop control system which includes time-periodic delay. (Kandala and Vyasarayani, 2018).

In general, retarded delay differential equation consists of delay value, $u^{(n)}(x-\tau_i)$, $\tau_i = \tau_i(x, u(x), ..., u^{(n-1)}(x))$, $i = 0, ..., n-1$ without the delay in state derivative value and is given by

$$u^{(n)} = f(x, u(x), u'(x), u''(x), ..., u^{(n-1)}(x), u(x-\tau_0), u'(x-\tau_1), u''(x-\tau_2), ..., u^{(n-1)}(x-\tau_{n-1})), \quad x \in [v, w]. \tag{1.4}$$

where

$$u^{(k)}(t) = \phi^{(k)}(t), \quad k = 0, 1, ..., n-1, \quad x \leq v,$$

and n is the order of differential equation, τ is the delay term of the system, $x - \tau$ is the delay argument.

Meanwhile, neutral delay differential equation involve both solutions of the delay values, $u^{(k)}(x-\tau_k)$, $k = 0, ..., n-1$ and the derivative of state variable itself, $u^{(n)}(x-\tau_n)$, which can be presented as follow:

$$u^{(n)} = f(x, u(x), u'(x), u''(x), ..., u^{(n-1)}(x), u(x-\tau_0), u'(x-\tau_1), ..., u''(x-\tau_2), ..., u^{(n-1)}(x-\tau_{n-1}), u^{(n)}(x-\tau_n)), \quad x \in [v, w], \tag{1.5}$$

where

$$u^{(k)}(t) = \phi^{(k)}(t), \quad k = 0, 1, ..., n, \quad x \leq v.$$
$$\tau_i = \tau_i(x, u(x), ..., u^{(n-1)}(x)), \quad i = 0, ..., n.$$

n is the order of differential equation, τ_i is the delay term of the system.

The delay term, τ_k is measurable as physical quantity that is scalar in function. Function f in both equations (1.4) and (1.5) are assumed to be continuous and non-negative as well as satisfies the *Lipschitz condition* in $u(t)$ for all $x \in [v, w]$. Initial function, $\phi(t)$ which is known to be defined in $[\rho, x_0]$, where

$$\rho = \min_{1 \leq i \leq n} \{ \min_{1 \leq i \leq n} (x - \tau_k) \}. \tag{1.6}$$

Based on the idea derived by Bellen and Zennaro (2003), the delay term can be categorised into three conditions, comprising constant delay case (τ_k is a constant), variable or time-dependent delay case ($\tau_k = \tau_k(t)$) and state-dependent delay case ($\tau_k = \tau_k(t, u(t), ..., u^{(n-1)}(t))$). In this thesis, we focus on solving general and special type of third-order ordinary differential equations and third-order retarded delay differential equations with constant delay. The types of third-order retarded DDEs we focus throughout the thesis are as follow:

Type I RDDE:

$$\begin{aligned} u''' &= f(x, u(x), u(x-\tau)), \quad x \in [x_0, x_n], \\ u(x_0) &= u_0, \quad u'(x_0) = u'_0, \quad u''(x_0) = u''_0. \end{aligned} \tag{1.7}$$

Type II RDDE:

$$\begin{aligned} u''' &= f(x, u(x), u'(x-\tau), u''(x-\tau)), \quad x \in [x_0, x_n], \\ u(x_0) &= u_0, \quad u'(x_0) = u'_0, \quad u''(x_0) = u''_0. \end{aligned} \tag{1.8}$$

1.2 Two-derivative Runge-Kutta method

The general formula of s-stage explicit two-derivative Runge-Kutta method for numerical integration of first-order initial value problems (IVPs) as proposed by Chan and Tsai (2010) in the form of

$$\begin{aligned} u_{n+1} &= u_n + h\sum_{i=1}^{s} b_i f\left(t_n + c_i h, U_i\right) + h^2 \sum_{i=1}^{s} B_i g\left(t_n + c_i h, U_i\right), \\ U_i &= u_n + h\sum_{j=1}^{s} a_{i,j} f\left(t_n + c_i h, U_j\right) + h^2 \sum_{j=1}^{s} A_{i,j} g\left(t_n + c_i h, U_j\right), \end{aligned} \tag{1.9}$$

where $i = 1, ..., s$ for $i \geq j$ and g-evaluation is the derivative of f-evaluation.

General formula of s-stage explicit two-derivative Runge-Kutta Nyström method for numerical integration of second-order initial value problems (IVPs) as proposed by Chen et al. (2015b) is as follow

$$\begin{aligned} u_{n+1} &= u_n + hu'_n + h^2 \sum_{i=1}^{s} b_i f\left(t_n + c_i h, U_i, U'_i\right) + h^3 \sum_{i=1}^{s} B_i g\left(t_n + c_i h, U_i\right), \\ U_i &= u_n + hc_i u'_n + h^2 \sum_{j=1}^{s} a_{i,j} f\left(t_n + c_i h, U_j, U_i\right) + h^3 \sum_{j=1}^{s} A_{i,j} g\left(t_n + c_i h, U_j\right), \end{aligned} \tag{1.10}$$

$i = 1, ..., s$ for $i \geq j$.

Lately, there are some modifications are done for the classical two-derivative Runge-Kutta methods into special form in order to reduce the computational cost by replacing multiple f-evaluations reduced into one (Chan and Tsai, 2010). The s-stage explicit two-derivative Runge-Kutta method for solving first-order ODEs is defined as

$$u_{n+1} = u_n + hf(t_n, u_n) + h^2 \sum_{i=1}^{s} b_i g(t_n + c_i h, U_i),$$
$$U_i = u_n + c_i hf(t_n, u_n) + h^2 \sum_{j=1}^{s} a_{i,j} g(t_n + c_i h, U_j), \quad (1.11)$$

where $i = 1, ..., s$ for $i \geq j$. The coefficients of b_i, c_i and $a_{i,j}$ can be represented in Butcher tableau in Table 1.1.

Table 1.1: Two-derivative Runge-Kutta methods for integrating first-order ODEs in Butcher tableau

$$\begin{array}{c|cccccc} 0 & 0 & & & & \\ c_1 & a_{2,1} & 0 & & & \\ c_2 & a_{3,1} & a_{3,2} & 0 & & \\ \vdots & \vdots & \vdots & \ddots & \ddots & \\ c_s & a_{s,1} & a_{s,2} & \ddots & a_{s,s-1} & 0 \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array}$$

The general formula of s-stage explicit two-derivative Runge-Kutta method for numerical integration of second-order initial value problems (IVPs)

$$u_{n+1} = u_n + hu'_n + \frac{h^2}{2} f(t_n, u_n, u'_n) + h^3 \sum_{i=1}^{s} b_i g(t_n + c_i h, U_i, U'_i),$$
$$U_i = u_n + c_i hu'_n + \frac{h^2}{2} f(t_n, u_n, u'_n) + h^3 \sum_{j=1}^{s} a_{i,j} g\left(t_n + c_i h, U_j, U'_j\right),$$
$$U'_i = u'_n + c_i hf(t_n, u_n, u'_n) + h^2 \sum_{j=1}^{s} a'_{i,j} g\left(t_n + c_i h, U_j, U'_j\right),$$

where $i = 1, ..., s$ for $i \geq j$ and g-evaluation is the derivative of f-evaluation. The coefficients of b_i, c_i, $a_{i,j}$ and $a'_{i,j}$ can be represented in Butcher tableau in Table 1.2.

Table 1.2: Two-derivative Runge-Kutta methods for integrating second-order ODEs in Butcher tableau

$$
\begin{array}{c|ccccc||ccccc}
0 & 0 & & & & & 0 & & & & \\
c_1 & a_{2,1} & 0 & & & & a'_{2,1} & 0 & & & \\
c_2 & a_{3,1} & a_{3,2} & 0 & & & a'_{3,1} & a'_{3,2} & 0 & & \\
\vdots & \vdots & \vdots & \ddots & \ddots & & \vdots & \vdots & \ddots & \ddots & \\
c_s & a_{s,1} & a_{s,2} & \ddots & a_{s,s-1} & 0 & a'_{s,1} & a'_{s,2} & \ddots & a'_{s,s-1} & 0 \\
\hline
 & b_1 & b_2 & \dots & b_{s-1} & b_s & b'_1 & b'_2 & \dots & b'_{s-1} & b'_s
\end{array}
$$

1.3 B-series and Rooted tree theory

B-series, also indicated as Butcher series, is a well-known algebraic method for interpreting numerical solutions of ordinary differential equations, which comprised of approximate solutions. The numerical properties of the numerical methods can be determined and assessed through the formulation and interpretation of B-series. In recent, B-series is highly utilised as the apporach to construct high-order and effective methods, particularly Runge-Kutta methods and multivalue methods.

For general first-order ODEs, let $u : \mathbb{R} \to \mathbb{R}^d$ be an analytic function satisfying an ordinary differential equation $u'(t) = f(u(t))$, we can denote the B-series of u in the form as follow:

$$B(a,u) = a(\emptyset)u + \sum_{t \in RT} \frac{h^{\rho(t)}}{\sigma(t)} a(t)F(t)(u). \tag{1.12}$$

where $F(t)(u)$ is called elementary differential attached with the tree t provided that the differential equations $u' = f((u(t))$ and evaluated at point u, RT is the set of rooted trees, $a(t) \in \mathbb{R}$ is the coefficient for the series with tree t, $\sigma(t) \in \mathbb{R}$ is the integer function of tree t, $h \in \mathbb{R}$ is the stepsize of t and $\rho(t)$ is the order of the tree t.

In the B-series for the results computed by Runge-Kutta method, $a(t)$ represents the elementary weight based on the coefficients of the Runge-Kutta method. Given Runge-Kutta method defined by the Butcher tableau (see Table 1.3)

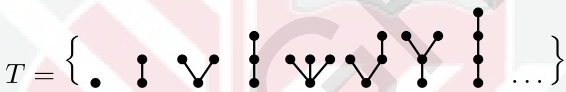
Table 1.3: Runge-Kutta method in Butcher tableau

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

where the interrelated elementary weight for the stage number i, elementary weight $\Psi(t)$ for the method that are corresponding to a tree t can be formulated as follow:

$$\begin{aligned}
\Psi_i(\tau) &= c_i, \\
\Psi(\tau) &= \sum_{i=1}^{s} b_i \\
\Psi_i([t_1,t_2,...,t_n]) &= \sum_{j=1}^{s} a_{i,j}\Psi_j(t_1)\Psi_j(t_2)\cdots\Psi_j(t_n) \\
\Psi([t_1,t_2,...,t_n]) &= \sum_{j=1}^{s} b_i\Psi_j(t_1)\Psi_j(t_2)\cdots\Psi_j(t_n) \qquad (1.13)
\end{aligned}$$

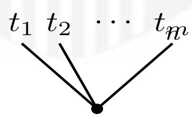
Rooted tree is a connected acyclic graph which contains of specific vertex designated to be the root. The tree $t = [t_1,t_2,\cdots t_n]$ is formed by defining a vertex, which consist of the root t, attaching the original roots of $t_1,t_2,...,t_n$ to the root of t. The set of the rooted trees can be presented as follow:



Set T can be generated by starting with

$$\tau = \bullet$$

and the operation for $[t_1,t_2,...,t_n]$ can be defined by the diagram below:



The tree $t = [t_1,t_2,...,t_n]$ is formed by introducing a vertex, which contains root of t and connecting the set of trees, $t_1,t_2,...,t_n$. If there exists repetitions in tree t, it can be writen as

$$t = \left[t_1^{k_1}, t_n^{k_n}, ..., t_n^{k_n}\right]. \qquad (1.14)$$

The order of rooted tree, which represents the number of vertices of tree t can be denoted as $\rho(t)$ satisfies the recursion function

$$\rho(t) = \begin{cases} 1, & t = \tau \\ 1 + \rho(t_1) + \rho(t_2) + ... + \rho(t_n), & t = [t_1, t_2, ..., t_n]. \end{cases} \tag{1.15}$$

The symmetry, $\sigma(t)$ is defined from the recursion

$$\sigma(t) = \begin{cases} 1, & t = \tau \\ 1 + \prod_{i=1}^{n} k_i! \sigma(t_i)^{k_i}, & t = [t_1, t_2, ..., t_n]. \end{cases} \tag{1.16}$$

Also, the real function $a(t)$ can be prescribed as

$$a(\emptyset) = 1, \quad a(t) = \frac{1}{\gamma(t)}, \quad t \in T \tag{1.17}$$

where the density, $\gamma(t)$ is defined as

$$\gamma(t) = \begin{cases} 1, & t = \tau \\ \rho(t)\gamma_1(t)\gamma_2(t)\cdots\gamma_n(t), & t = [t_1, t_2, ..., t_n]. \end{cases} \tag{1.18}$$

Autonomous initial value problem of first order ODEs is given by

$$u'(t) = f(u(t)), \quad u(t_0) = u_0, \tag{1.19}$$

elementary differentials $F(t)(u_0)$ arise in the Taylor series for this problem. The elementary differential is defined making use of f, f', f'' with $u(t)$ replaced by u_0

$$F(t)(u_0) = \begin{cases} f, & t = \tau \\ f^{(n)}(F(t_1)(u_0),), & t = [t_1, t_2, ..., t_n]. \end{cases} \tag{1.20}$$

The tree function of Runge-Kutta method is demostrated in figure below (see Table 1.4).

Table 1.4: Tree function of Runge-Kutta method up to four vertices

t	$\rho(t)$	$\sigma(t)$	$\gamma(t)$	$F(t)(u_0)$
τ	1	1	1	$\mathbf{f}$
$[\tau]$	2	1	2	$\mathbf{f}'\mathbf{f}$
$[\tau^2]$	3	2	3	$\mathbf{f}''(\mathbf{f},\mathbf{f})$
$[[\tau]]$	3	1	6	$\mathbf{f}'\mathbf{f}'\mathbf{f}$
$[\tau^3]$	4	6	4	$\mathbf{f}'''(\mathbf{f},\mathbf{f},\mathbf{f})$
$[\tau[\tau]]$	4	1	8	$\mathbf{f}''(\mathbf{f},\mathbf{f}'\mathbf{f})$
$[[\tau^2]]$	4	2	12	$\mathbf{f}'\mathbf{f}''(\mathbf{f},\mathbf{f})$
$[[[\tau]]]$	4	1	24	$\mathbf{f}'\mathbf{f}'\mathbf{f}'\mathbf{f}$

1.4 Problem Statement

We consider the solution of general and special third-order ordinary differential equations (ODEs) and delay differential equations (DDEs) with both oscillatory and nonoscillatory solutions using two-derivative Runge-Kutta type methods. A lot of Runge-Kutta type methods are derived recently with high algebraic order to acquire less dispersion and dissipation error for solving particular ODEs and DDEs. Hence, various fitting techniques are implemented to the classical Runge-Kutta type methods to produce some methods with zero dispersion and dissipation. Hence, two-derivative approach is implemented into the formulation of Runge-Kutta type methods to improve the accuracy of the solutions with less computational cost.

We concern about constructing two-derivative Runge-Kutta type methods with yielding less error and less computational cost. The conventional approach is by developing two-derivative Runge-Kutta type method using Taylor series expansion and algebraic simplification method and mainly deals with second-order ordinary differential equations. However, not much two-derivative Runge-Kutta type methods are developed by researchers to solve third-order ODEs and some application problems such as thin-film flow and genesio problems. Hence we are motivated to propose two-derivative Runge-Kutta type methods with classical and improved version which acquire higher accuracy and less computational time.

It is possible to extend the works into the derivation of two-derivative Runge-Kutta type methods with fitting techniques for solving third-order ODEs with exponential and trigonometrical solutions. Exponentially-fitting and trigonometrically-fitting techniques are implemented into both classical and improved two-derivative Runge-Kutta type methods which should provide significant improvement in accuracy numerically.

1.5 Objectives of the Study

The construction of efficient direct methods based on Explicit Two-Derivative Runge-Kutta type methods and Explicit Two-Derivative Improved Runge-Kutta type methods for numerical integration of general and special type third-order ODEs, type I and type II RDDEs for constant step size mode. Both methods are extended to solve exponential and oscillatory third-order ODEs by the implementation of fitting techniques. The main objectives of this thesis are proposed as below:

1. To develop two-derivative Runge-Kutta type method for solving general third-order ODEs through B-series and rooted tree theory.
2. To develop two-derivative Runge-Kutta type method for solving special third-order ODEs in the form of $u''' = f(x, u(x))$ through B-series and rooted tree theory and extended to solve type I RDDEs with Newton interpolation.
3. To construct exponentially-fitted and trigonometrically-fitted two-derivative Runge-Kutta type method for integrating third-order ODEs with exponential and oscillatory solutions.
4. To develop two-derivative Improved Runge-Kutta type with inclusive of previous increment term for solving special third-order ODEs and type II RDDEs with Newton interpolation.
5. To construct exponentially-fitted and trigonometrically-fitted two-derivative Improved Runge-Kutta type methods for numerical integrating third-order ODEs with exponential and oscillatory solutions.

1.6 Scope of Study

This study focuses on the derivation of GTDRKT methods for solving general third-order ODEs. Then, TDRKT methods are constructed based on B-series and rooted tree theory and solve third-order special type of ODEs and retarded DDEs. In addition, exponentially-fitted and trigonometrically-fitted TDRKT methods is developed using order condition and frequency principle and these methods are used to solve third-order ODEs with exponential and oscillatory solutions. Then, we concentrate on developing improved TDRKT methods, whereby the previous terms, b_{-i}, k_{-i} are included in the formulation and utilised to solve third-order ODEs in the form of $u''' = f(x, u'(x), u''(x))$. Improved TDRKT methods are then extended to solve third-order ODEs with exponential and oscillatory solutions by implementing exponentially and trigonometrically fitting techniques.

1.7 Outline of the Thesis

In this section, we provide a brief description of the thesis. Chapter 1 begins with the introduction of the general formulation of two-derivative Runge-Kutta type method. B-series and rooted tree theory, which are crucial to develop order conditions for Runge-Kutta methods are introduced subsequently. Chapter 2 provides the reviews of previous works on B-series and numerical solutions for solving third-order ODEs and DDEs.

In Chapter 3, the derivation of explicit two-derivative Runge-Kutta type methods are presented for solving third-order general ordinary differential equations (ODEs). The derivation of order conditions for two-derivative Runge-Kutta type method using B-series and rooted tree theory are proposed. Stability, consistency and convergence of purposed methods are studied and the methods are used to solve general third-order ODEs. In Chapter 4, B-series and rooted tree theory is applied again for the derivation of explicit two-derivative Runge-Kutta type, TDRKT methods are presented for solving third-order ODEs in the form of $u''' = f(t, u(t))$ and type I RDDEs. Stability and D-convergence for TDRKT methods applied to type I RDDEs are discussed. The applications of the purposed methods in comparison with other existing methods are shown for solving numerical problems.

In Chapter 5, exponentially-fitted and trigonometrically-fitted two-derivative Runge-Kutta type methods are derived for solving third-order ODEs with exponential and oscillatory solutions. Fifth-order and sixth-order proposed methods are developed based on idea of integrating IVPs exactly with numerical solution in the form linear composition of the set functions $e^{\omega t}$ and $e^{-\omega t}$ for exponentially-fitted and $e^{i\omega t}$ and $e^{-i\omega t}$ for trigonometrically-fitted. Numerical solutions illustrate efficiency of the purposed methods compared to existing methods for integrating third-order ODEs with exponential and oscillatory solutions. Chapter 6 discussed the technique of implementation of previous term, k_{-i} and b_{-i} into the formulation to derive improved two-derivative Runge-Kutta type methods for solving third-order ODEs. Fifth-order and sixth-order with improved Runge-Kutta type methods is presented and used to solve third-order ODEs and type II RDDEs in this chapter.

Chapter 7 begins with the construction of improved two-derivative Runge-Kutta type method with exponentially-fitting and trigonometrially-fitting technique. Coefficients of the proposed methods with principle frequency based are derived. Error analysis of the purposed methods is investigated. The applications of these proposed methods for solving exponential and oscillatory ODEs are shown. Finally, conclusion of the thesis is provided in Chapter 8 and future work is also recommended.

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