Alexandria Engineering Journal (2020) 59, 2449–2467

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Alexandria Engineering Journal

www.elsevier.com/locate/aej
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ORIGINAL ARTICLE

Numerical study of third-order ordinary differential equations using a new class of two derivative Runge-Kutta type methods

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Received 3 December 2019; revised 6 March 2020; accepted 7 March 2020
Available online 17 April 2020

KEYWORDS

Runge-Kutta type methods;
B-series;
Rooted tree;
Third-order ordinary differential equations;
Algebraic order

Abstract This study introduces new special two-derivative Runge-Kutta type (STDRKT) methods involving the fourth derivative of the solution for solving third-order ordinary differential equations. In this regards, rooted tree theory and the corresponding B-series theory is proposed to derive order conditions for STDRKT methods. Besides, explicit two-stages fifth order and three-stages sixth order STDRKT methods are derived and stability,consistency and convergence of STDRKT methods are analysed in details. Accuracy and effectiveness of the proposed techniques are validated by a number of various test problems and compared to existing methods in the literature.

1. Introduction

In this paper, we focus on initial value problems of third order ordinary differential equations (ODEs):

$$\begin{cases} u'''(x) = f(x, u(x), u'(x), u''(x)), \\ u(x_0) = \alpha, \quad u'(x_0) = \beta, \quad u''(x_0) = \gamma, \quad x \in [x_0, x_{end}], \end{cases} \tag{1.1}$$

where $u \in \Re^N, f := \Re \times \Re^N \times \Re^N \times \Re^N \to \Re^N$is a continuous vector functions.

Third-order ordinary differential equations are often utilised to forecast applied scientific obstacles in the fields of physics, economics, biology and other disciplines. The usual approach used to solve third-order ODEs is convert the problem into first-order ODEs system with initial conditions $u(x_0) = u_0,\ u'(x_0) = u'_0,\ u''(x_0) = u''_0$ and solved it using particular first-order methods such as linear multistep methods and Runge-Kutta methods. However, local truncation error and rounding error are generated and caused inaccuracy in

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Peer review under responsibility of Faculty of Engineering, Alexandria University.

https://doi.org/10.1016/j.aej.2020.03.008
1110-0168

approximating the numerical problems. Several direct methods are widely proposed by researchers in solving third-order ODEs such as iterative method, Traub's method, residual power series method, block method and more (see Chun and Kim [1], Sharma and Sharma [2], Omar et al.[3], Mehrkanoon[4]).

One of the application problems related to third-order ODEs is nonlinear Genesio equation, which is widely used to represent jerk dynamical system and major characteristics of regular and chaotic motion for jerk system are presented (see Umut and Yasar [5]). Direct solution was proposed for solving third-order nonlinear Genesio equation through block hybrid collocation method (see Yap et al. [6]). Runge-Kutta type direct integrators with collocation technique for solving third-order ODEs for a class of implicit RKT methods was proposed (see You and Chen [7]).

In this research paper, a Runge-Kutta scheme which comprises of fourth derivatives for the direct solution of general third order ODEs is proposed. This method is modified from existing two derivative Runge-Kutta type methods whereby the multiple increment function $\sum_{i=1}^{n} b_i k_i$ in third derivative is removed and replaced by single function $f(x, u, u', u'')$ from the third order numerical problem. The benefits of this method is to deduct the amount of function evaluation and enhance the accuracy since the increment function contains of numerical errors based on the number of stages. Several effective two derivative Runge-Kutta-Nyström methods with inclusion of second derivative has been proposed to solve second order ODEs (see Fang et al. [8], Chen et al. [9], Ehigie et al. [10] and Mohamed et al. [11]).

The aim of this paper is to derive high order STDRKT methods with minimal amount of stage k, consists of two-stages fifth-order and three-stages sixth-order methods. In Section 2, general formulation of STDRKT methods is proposed. In Section 3, B-series and rooted tree theories of proposed method will be shown and elements of B-series such as integer function, fundamental differential and density will be derived. STDRKT methods are developed based on the order conditions obtained from B-series and the stability and convergence analysis of STDRKT methods is discussed in Section 4 to exhibit the capability of STDRKT. In Section 5, different types of numerical test are proposed and used to compare with existing methods to examine the efficiency of STDRKT methods. Numerical results are shown in Section 6 and the paper ends with discussion and conclusion in Section 7.

2. The formulation of STDRKT methods

In deriving STDRKT methods, a fourth derivative is comprised in the formulation as follow:

$$
\begin{aligned}
u^{(iv)}(x) &= g(x, u(x), u'(x), u''(x)) \\
&= f_x(x, u, u'(x), u''(x)) \\
&\quad + f_u(x, u(x), u'(x), u''(x))u'(x) \\
&\quad + f_{u'}(x, u(x), u'(x), u''(x))u''(x) \\
&\quad + f_{u''}(x, u(x), u'(x), u''(x))f(x, u(x), u'(x), u''(x)).
\end{aligned} \tag{2.2}
$$

Evaluation $g(x, u, u', u'')$ is derived from the derivative of third derivative. A s-stage special two derivative Runge-Kutta type method for third-order IVPs is prescribed as follow:

$$
\begin{aligned}
u_{n+1} &= u_n + hu'_n + \frac{h^2}{2}u''_n + \frac{h^3}{6}f(x_n, u_n, u'_n, u''_n) \\
&\quad + h^4\sum_{i=1}^{s} b_i g(x_n + c_i h, U_i, U'_i, U''_i),
\end{aligned}
$$

$$
\begin{aligned}
u'_{n+1} &= u'_n + hu''_n + \frac{h^2}{2}f(x_n, u_n, u'_n, u''_n) \\
&\quad + h^3\sum_{i=1}^{s} b'_i g(x_n + c_i h, U_i, U'_i, U''_i),
\end{aligned}
$$

$$
u''_{n+1} = u''_n + hf(x_n, u_n, u'_n, u''_n) + h^2\sum_{i=1}^{s} b''_i g(x_n + c_i h, U_i, U'_i, U''_i),
$$

where

$$
\begin{aligned}
U_i &= u_n + c_i hu'_n + \tfrac{(c_i h)^2}{2}u''_n + \tfrac{(c_i h)^3}{6}f(x_n, u_n, u'_n, u''_n) \\
&\quad + h^4\sum_{j=1}^{s} A_{i,j} g\left(x_n + c_i h, U_j, U'_j, U''_j\right), \\
U'_i &= u'_n + c_i hu''_n + \tfrac{(c_i h)^2}{2}f(x_n, u_n, u'_n, u''_n) \\
&\quad + h^3\sum_{j=1}^{s} \widehat{A}_{i,j} g\left(x_n + c_i h, U_j, U'_j, U''_j\right), \\
U''_i &= u''_n + c_i hf(x_n, u_n, u'_n, u''_n) \\
&\quad + h^2\sum_{j=1}^{s} \overline{A}_{i,j} g\left(x_n + c_i h, U_j, U'_j, U''_j\right),
\end{aligned} \tag{2.3}
$$

where $c_i, b_i, b'_i, b''_i, \overline{A}_{i,j} \widehat{A}_{i,j}, A_{i,j}, i,j = 1, \ldots, s$ are positive integers. This method is able to be converted into Butcher's tableau as shown in Table 1.

STDRKT methods are explicit methods if $A_{i,j}$, $\widehat{A}_{i,j}$ and $\overline{A}_{i,j}$ equal to 0 for $i \leqslant j$, and are implicit methods otherwise. It just comprises of one evaluation of f and multiple evaluations of g for every step, in which total number of function evaluations is much less than the existing two derivative RK methods which consist of numerious evaluations of f and g for every step depending on the amount of stages.

3. Rooted trees, B-series and order conditions for STDRKT methods

Definition 3.1. STDRKT methods in (2.3) has order p for all smooth initial value problems in the form (1.1), local truncation errors for solution and its derivative obey

$$
||u(x_0 + h) - u_1|| = ||u'(x_0 + h) - u'_1|| = ||u''(x_0 + h) - u''_1|| = O(h^{p+1}).
$$

Table 1 STDRKT methods in Butcher tableau.

C	A	$\widehat{A}$	$\overline{A}$
	b^T	b'^T	b''^T

3.1. Rooted trees and theory for B-series

For simplicity purpose, the dependence of u on x will be ignored in deriving rooted tree for STDRKT methods. Thus, non-autonnomous problem (1.1) converted into following autonomous system

$$\begin{cases} v''' = \begin{pmatrix} 0 \\ 0 \\ \bar{f}(v, v', v'') \end{pmatrix}, \\ v(x_0) = \begin{pmatrix} x_0 \\ u_0 \\ v_0 \end{pmatrix}, \quad v'(x_0) = \begin{pmatrix} 1 \\ u'_0 \\ v'_0 \end{pmatrix}, \quad v''(x_0) = \begin{pmatrix} 0 \\ 1 \\ v''_0 \end{pmatrix}, \end{cases} \tag{3.5}$$

where $v = (x, u^T)^T$ and $\bar{f}(v, v', v'') = f(x, u, u', u'')$. Then, STDRKT method (2.3) is applied to the autonomous system (3.5) to yield

$$\begin{aligned}
X_i &= x_0 + c_i h, \quad X'_i = 1, \quad X''_i = 0, \\
U_i &= u_0 + c_i h u'_0 + \tfrac{(c_i h)^2}{2} u''_0 + \tfrac{(c_i h)^3}{6} f_0 + h^4 \sum_{j=1}^{s} A_{i,j} g\left(X_j, U_j, U'_j, U''_j,\right) \\
U'_i &= u'_0 + c_i h u''_0 + \tfrac{(c_i h)^2}{2} f_0 + h^3 \sum_{j=1}^{s} \widehat{A}_{i,j} g\left(X_j, U_j, U'_j, U''_j\right), \\
U''_i &= u''_0 + c_i h f_0 + h^2 \sum_{j=1}^{s} \overline{A}_{i,j} g\left(X_j, U_j, U'_j, U''_j\right), \\
i &= 1, \ldots, s, \\
x_1 &= x_0 + h, \\
u_1 &= u_0 + h u'_0 + \tfrac{h^2}{2} u''_0 + \tfrac{h^3}{6} f_0 + h^4 \sum_{i=1}^{s} b_i g\left(X_i, U_i, U'_i, U''_i,\right) \\
x'_1 &= 1, \\
u'_1 &= u'_0 + h u''_0 + \tfrac{h^2}{2} f_0 + h^3 \sum_{i=1}^{s} b'_i g\left(X_i, U_i, U'_i, U''_i\right), \\
x''_1 &= 0, \\
u''_1 &= u''_0 + h f_0 + h^2 \sum_{i=1}^{s} b''_i g\left(X_i, U_i, U'_i, U''_i\right).
\end{aligned} \tag{3.6}$$

By comparing (3.6) and (2.3), application of STDRKT methods (2.3) to non-autonomous problem (1.1) provides the same numerical solution as autonomous form (3.5) (see Chen et al. [9]). Hence, autonomous problem will be considered as follow

$$\begin{aligned} & u''' = f(u, u', u'') \\ & u(x_0) = u_0, \quad u'(x_0) = u'_0, \quad u''(x_0) = u''_0. \end{aligned} \tag{3.7}$$

For obtaining a general formula for higher derivatives of analytical solution of problem (3.7), we consider the expression of first to seventh derivatives of the analytical solution $u(x)$ at $x = x_0$.

$$\begin{aligned}
u^{(1)} &= u', u^{(2)} = u'', \; u^{(3)} = f, \; u^{(4)} = g, \\
u^{(5)} &= g'_u u' + g'_{u'} u'' + g'_{u''} f, \\
u^{(6)} &= g^{(2)}_{uu} u'^2 + 2g^{(2)}_{uu'} u' u'' + 2g^{(2)}_{uu''} u' f + g^{(2)}_{u'u'} u''^2 \\
&\quad + 2g^{(2)}_{u'u''} u'' f + g^{(2)}_{u''u''} f^2 + g'_u u'' + g'_{u'} f + g'_{u''} g, \\
u^{(7)} &= g^{(3)}_{uuu} u'^3 + 3g^{(3)}_{uuu'} u'^2 u'' + 3g^{(3)}_{uuu''} u'^2 f + 3g^{(3)}_{uu'u'} u' u''^2 \\
&\quad + 6g^{(3)}_{uu'u''} u' u'' f g^{(3)}_{uu''u''} u' f^2 + g^{(3)}_{u'u'u'} u''^3 + 3g^{(3)}_{u'u'u''} u''^2 f + 3g^{(3)}_{u'u''u''} u'' f^2 + g^{(3)}_{u''u''u''} f^3 \\
&\quad + 3g^{(2)}_{uu} u' u'' + 3g^{(2)}_{uu'} u' f + 3g^{(2)}_{uu''} u' g + 3g^{(2)}_{uu''} u'' f + 3g^{(2)}_{u'u'} u'' f + 3g^{(2)}_{u'u''} u'' g \\
&\quad + 3g^{(2)}_{u''u''} f g + g_{u''} g^{(2)}_{uu} u'^2 + 2g_{u''} g^{(2)}_{uu'} u' u'' + 2g_{u''} g^{(2)}_{uu''} u' f + g_{u''} g^{(2)}_{u'u'} u''^2 \\
&\quad + 2g_{u''} g^{(2)}_{u'u''} u'' f + g_{u''} g^{(2)}_{u''u''} f^2 + g_{u''} g'_u u'' + g_{u''} g'_{u'} f + g_{u''} g'_{u''} g, \\
&\quad + g_u f + g_{u'} g + 3g_{uu'} u''^2 + 3g_{u'u''} f^2,
\end{aligned} \tag{3.8}$$

where the arguments (x_0) and $(u(x_0), u'(x_0), u''(x_0))$ are suppressed. The complexity of the expression increases as the order increases. Thus, geometric representation is utilised to simplify the expression. There are four types of vertices with branches connecting them, including "black circle", "white rectangle", "white circle" and "black triangle".

1. A black circle vertex, white rectangle, white circle and black triangle are used to represent u', u'', f and g respectively.
2. A black triangle vertex comprised of k branches connecting up to black circle vertex, followed by heading up to white rectangle vertex with l branches, white circle vertex branches with m branches and black triangle vertex with n branches, is used to represent each $g^{(k+l+m+n)}_{u \ldots uu' \ldots u'u'' \ldots u'' f \ldots f}$, the k-th partial derivative in terms of u, l-th partial derivative in terms of y', m-th partial derivative with respect to u'' and n-th partial derivative in terms of f.

Following describes the essences of the set of rooted trees for STDRKT methods.

Definition 3.2. The set RT of rooted trees is recursively interpreted as

1. The graph "black circle vertex" containing of root with one black circle vertex, expressed as τ_1, belongs to rooted tree; the graph comprises a black circle vertex subsequently by a white rectangle vertex, expressed as τ_2; the graph comprises a black circle vertex subsequently by a white rectangle vertex and subsequently followed by white circle vertex, denoted as τ_3 and lastly, the graph comprises a black circle vertex followed by a white rectangle vertex and succeeded by white circle vertex and black triangle vertex, denoted as τ_4;
2. If $t_1, \ldots, t_r, t_{r+1}, \ldots, t_m, t_{m+1}, \ldots, t_n, t_{n+1}, \ldots, t_s \in RT, t_{n+1}, \ldots, t_s$ different from τ_1, then the graph can be obtained as the roots of $t_1, \ldots, t_r$ connecting downward to white rectangle vertex, combining the roots of $t_{r+1}, \ldots, t_m$ into this white rectangle vertex, followed by joining the roots $t_{m+1}, \ldots, t_n$ downward to white circle vertex and sequently to the roots $t_n, t_{n+1}, \ldots, t_s$ into a new black circle vertex, which are components of RT. It is expressed as

$$t = [t_1, \ldots, t_r, < t_{r+1}, \ldots, t_m >, < t_{m+1}, \ldots, t_n >, < t_{n+1}, \ldots, t_s >]_4, \tag{3.9}$$

in which new black circle vertex is root of the rooted tree t.

Definition 3.3. The order for the integer function $\rho : RT \to \mathbb{N}$, is recursively denoted as:

1. $\rho(\tau_1) = 1,\ \rho(\tau_2) = 2,\ \rho(\tau_3) = 3,\ \rho(\tau_4) = 4,$
2. for $t = [t_1, \ldots, t_r, < t_{r+1}, \ldots, t_m >, < t_{m+1}, \ldots, t_n >]_3 \in RT$

$$\rho(t) = 4 + \sum_{i=1}^{r} \rho(t_i) + \sum_{i=r+1}^{m} (\rho(t_i) - 1) + \sum_{i=m+1}^{n} (\rho(t_i) - 2).$$

For every $t \in RT$, the order ρ represents the amount of vertices t. The set comprised of all rooted trees with order k is expressed as RT_k.

Definition 3.4. For every tree $t \in RT$, the fundamental differential is a vector function $F(t) : \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$, that is recursively expressed as follow:

1. $F(\tau_1)(u, u', u'') = y', F(\tau_2)(u, u', u'') = u'', F(\tau_3)(u, u', u'') = f(u, u', u''), F(\tau_4)(u, u', u'') = f'(u, u', u'') = g(u, u', u'')$
2. for $t = [t_1, \ldots, t_r, < t_{r+1}, \ldots, t_m >, < t_{m+1}, \ldots, t_n >, < t_{n+1}, \ldots, t_s >]_4 \in RT$

$$F(t)(u, u', u'') = \frac{\partial^n g}{\partial u^r \partial u'^{m-r} \partial u''^{m-m}}(u, u', u'')[F(t_1)(u, u', u''), \ldots, F(t_n)(u, u', u'')]. \tag{3.10}$$

Definition 3.5. An integer function, $\sigma : RT \to \mathbb{N}$ is recursively described as follow:

1. $\sigma(\tau_1) = \sigma(\tau_2) = \sigma(\tau_3) = \sigma(\tau_4) = 1,$
2. for $t = \left[t_1^{\mu_1}, \ldots, t_r^{\mu_r}, < t_{r+1}^{\mu_{r+1}}, \ldots, t_m^{\mu_m} >, < t_{m+1}^{\mu_{m+1}}, \ldots, t_n^{\mu_n} >\right] \in RT,$ with the condition of $t_1, \ldots, t_r$, $t_{r+1}, \ldots, t_m$ and $t_{m+1}, \ldots, t_n$ distinct,

$$\sigma(t) = \prod_{i=1}^{n} \mu_i!(\sigma(t_i)^{\mu_i}),$$

in which μ_i is product of t_i for $i = 1, \ldots, n$. Referring the rooted trees of B-series for Runge-Kutta methods developed by Hairer et al. [12], the set RK of STDRKT methods in B-series is defined.

Definition 3.6. For function $\beta : RT \cup \{\varnothing\} \to \mathbb{R}$, the form

$$B(\beta, u, u', u'') = \beta(\varnothing)y + \sum_{t \in RT} \frac{h^{\rho(t)}}{\sigma(t)} \beta(t)F(t)(u, u', u''),$$

is labeled as B-series.

The lemma below is utilised for deriving the order conditions for STDRKT methods.

Lemma 3.1. *Let three mappings,* $\bar{\beta} : RT \cup \{\varnothing\} \to \mathbb{R}, \hat{\beta} : RT \to \mathbb{R}$ *and* $\beta : RT \to \mathbb{R}$ *satisfy* $\bar{\beta}(\varnothing) = 1, \hat{\beta}(\tau_1) = 1$ *and* $\beta(\tau_2) = 1$*, then* $h^4 g\left(B(\bar{\beta}, u, u', u''), B\left(\frac{\rho}{h}\hat{\beta}, u, u', u''\right), B\left(\frac{\rho(\rho-1)}{h^2}\beta, u, u', u''\right)\right)$ *is also B-series.*

$$h^4 g\left(B(\bar{\beta}, u, u', u''), B\left(\frac{\rho}{h}\hat{\beta}, u, u', u''\right), B\left(\frac{\rho(\rho - 1)}{h^2}\beta, u, u', u''\right)\right) = B\left(\beta^{(4)}, u, u', u''\right),$$

with

$$\beta^{(4)}(\varnothing) = \beta^{(4)}(\tau_1) = \beta^{(4)}(\tau_2) = \beta^{(4)}(\tau_3) = 0,\ \beta^{(4)}(\tau_4) = 1,$$

and for $\rho(t) \geqslant 5$.

$$\beta^{(4)} = \sum_{\bar{t}} \left(\prod_{i=1}^{r} \bar{\beta}(\bar{t}_i) \times \prod_{i=r+1}^{m} \rho(\bar{t}_i)\hat{\beta}(\bar{t}_i) \times \prod_{i=m+1}^{n} \rho(\bar{t}_i)(\rho(\bar{t}_i) - 1)\beta(\bar{t}_i)\right),$$

in which the summation replaces all the trees t with

$$\bar{t} = [\bar{t}_1, \ldots, \bar{t}_r, < \bar{t}_{r+1}, \ldots, \bar{t}_m >, < \bar{t}_{m+1}, \ldots, \bar{t}_n >]_3 = [t \setminus \tau_4]_3.$$

Theorem 3.1. *Given the analytical solution* $u(x_0 + h)$ *of Eq. (1.1) is B-series* $B\left(e, u_0, u_0', u_0''\right)$ *with real function e prescribed on* $RT \cup \{\varnothing\}$*, then*

$$e(\varnothing) = 1,\ e(\tau_1) = 1,\ e(\tau_2) = \frac{1}{2},\ e(\tau_3) = \frac{1}{6},$$

and for $t = [t_1, \ldots, t_r, < t_{r+1}, \ldots, t_m >, < t_{m+1}, \ldots, t_n >]_3$,

$$e(t) = \frac{1}{\rho(t)(\rho(t) - 1)(\rho(t) - 2)} \prod_{i=1}^{r} e(t_i) \prod_{i=r+1}^{m} \rho(t_i)e(t_i) \prod_{i=m+1}^{n} \rho(t_i) \times (\rho(t_i) - 1)e(t_i).$$

Proof of Theorem 3.1 By assumption,

$$\begin{aligned} u(x_0 + h) = B\left(e, u_0, u_0', u_0''\right) &= e(\varnothing)u_0 + he(\tau_1)u'(0) + h^2 e(\tau_2)u_0'' \\ &+ h^3 e(\tau_3) f\left(u_0, u_0', u_0''\right) \\ &+ \sum_{t \in RT \setminus \{\tau_1, \tau_2, \tau_3\}} \frac{h^{\rho(t)}}{\sigma(t)} e(t)F(t)\left(u_0, u_0', u_0''\right). \end{aligned} \tag{3.11}$$

First two derivatives of $y(x_0 + h)$ are shown below

$$\begin{aligned} (u(x_0+h))' &= \frac{d}{dh}(u(x_0+h)) \\ & e(\tau_1)u'(0) + 2he(\tau_2)u_0'' + 3h^2 e(\tau_3) f\left(u_0, u_0', u_0''\right) \\ &+ \sum_{t \in RT \setminus \{\tau_1, \tau_2, \tau_3\}} \frac{\rho(t)h^{\rho(t)-1}}{\sigma(t)} e(t)F(t)\left(u_0, u_0', u_0''\right) \\ &= \left(\frac{\rho}{h}e, u_0, u_0', u_0''\right) \\ (u(x_0+h))'' &= \frac{d^2}{dh^2}(u(x_0+h)) = 2e(\tau_2)u_0'' + 6he(\tau_3) f\left(u_0, u_0', u_0''\right) \\ &+ \sum_{t \in RT \setminus \{\tau_1, \tau_2, \tau_3\}} \frac{\rho(t)(\rho(t)-1)h^{\rho(t)-2}}{\sigma(t)} e(t)F(t)\left(u_0, u_0', u_0''\right) \\ &= B\left(\frac{\rho(\rho-1)}{h^2}e, u_0, u_0', u_0''\right) \end{aligned} \tag{3.12}$$

From Lemma 3.1,

$$g\left(B(e,u_0,u_0',u_0''),B\left(\frac{\rho}{h}e,u,u',u''\right),B\left(\frac{\rho(\rho-1)}{h^2}e,u,u',u''\right)\right)$$
$$=e''(\tau_3)f(u_0,u_0',u_0'')+\sum_{t\in RT\setminus\{\tau_1,\tau_2,\tau_3\}}\frac{h^{\rho)-2}}{\sigma(t)}e''(t)F(t)(u_0,u_0',u_0'')$$

where $e''(\tau_2)=1$ and for $t=[t_1,\ldots,t_r,<t_{r+1},\ldots,t_m>,<t_{m+1},\ldots,t_n>]_3\in RT\setminus\{\tau_1,\tau_2,\tau_3\}$

$$e''(t)=\prod_{i=1}^{r}e(t_i)\prod_{i=r+1}^{m}\rho(t_i)e(t_i)\prod_{i=m+1}^{n}\rho(t_i)(\rho(t_i)-1)e(t_i) \tag{3.13}$$

Combining (3.11) and (3.12) into autonomous problem of (1.1) and coefficients of the fundamental differential are compared on the both sides, yield

$$e(\tau_2)=\frac{1}{2},\quad e(\tau_3)=\frac{1}{6}$$

and for $t=[t_1,\ldots,t_r,<t_{r+1},\ldots,t_m>,<t_{m+1},\ldots,t_n>]_3\in RT\setminus\{\tau_1,\tau_2,\tau_3\}$

$$e(t)=\frac{1}{\rho(t)(\rho(t)-1)(\rho(t)-2)}\prod_{i=1}^{r}e(t_i)\prod_{i=r+1}^{m}\rho(t_i)e(t_i)\prod_{i=m+1}^{n}\rho(t_i)$$
$$\times(\rho(t_i)-1)e(t_i).\quad\square$$

Lastly, by referring to Taylor series expansion of $u(x_0+h)$ around $h=0$, $e(\varnothing)=e(\tau_1)=1$, $e(\tau_2)=2$, $e(\tau_3)=6$.

For each $t\in RT$, both density and positive integer can be defined as $\gamma(t)=\frac{1}{e(t)}$ and $\alpha(t)=\frac{\rho(t)!}{\sigma(t)\gamma(t)}$. Two propositions can be derived based on Theorem 3.1.

Proposition 3.1. *For every tree $t\in RT$, density $\gamma(t)$ is defined as positive integer function on set RT with*

1. $\gamma(\tau_1)=1,\ \gamma(\tau_2)=2,\ \gamma(\tau_3)=6,$
2. for $t=[t_1,\ldots,t_r,<t_{r+1},\ldots,t_m>,<t_{m+1},\ldots,t_n>]_3\in RT$, $\gamma(t)=\rho(t)(\rho(t)-1)(\rho(t)-2)\prod_{i=1}^{r}\gamma(t_i)\prod_{i=r+1}^{m}\frac{\gamma(t_i)}{\rho(t_i)}\prod_{i=m+1}^{n}\frac{\gamma(t_i)}{\rho(t_i)(\rho(t_i)-1)}$.

Proposition 3.2. *For every tree $t\in RT$, positive integer $\alpha(t)$ fulfils*

1. $\alpha(\tau_1)=1,\ \alpha(\tau_2)=1, \alpha(\tau_3)=1,$
2. for $t=\left[t_1^{\mu_1},\ldots,t_r^{\mu_r},<t_{r+1}^{\mu_{r+1}},\ldots,t_m^{\mu_m}>,<t_{m+1}^{\mu_{m+1}},\ldots,t_n^{\mu_n}>\right]_3\in RT$, whereby $t_1,\ldots,t_r$ distinct, $t_{r+1},\ldots,t_m$ distinct and $t_{m+1},\ldots,t_n$ distinct,

$$\alpha(t)=(\rho(t)-3)!\prod_{i=1}^{r}\frac{1}{\mu_i!}\left(\frac{\alpha(t_i)}{\rho(t_i)!}\right)^{\mu_i}\prod_{i=r+1}^{m}\frac{1}{\mu_i!}\left(\frac{\alpha(t_i)}{(\rho(t_i)-1)!}\right)^{\mu_i}\cdot\prod_{i=m+1}^{n}\frac{1}{\mu_i!}\left(\frac{\alpha(t_i)}{(\rho(t_i)-2)!}\right)^{\mu_i}, \tag{3.14}$$

where μ_i is the product of $t_i, i=1,\ldots,n$.

Here, *B*-series can be defined as

$$B(\beta,u,u',u'')=\beta(\varnothing)u+\sum_{t\in RT}\frac{h^{\rho(t)}}{\rho(t)!}\beta(t)\gamma(t)\alpha(t)F(t)(u,u',u''), \tag{3.15}$$

and $g\left(B(\bar\beta,u,u',u''),B\left(\hat\beta,u,u',u''\right),B(\beta,u,u',u'')\right)$ can be denoted as

$$g\left(B(\bar\beta,u,u',u''),B\left(\hat\beta,u,u',u''\right),B(\beta,u,u',u'')\right)$$
$$=\sum_{t\in RT\setminus\{\tau_1,\tau_2,\tau_3\}}\frac{h^{\rho(t)-4}}{\rho(t)!}\beta^{(4)}(t)\gamma(t)\alpha(t)F(t)(u,u',u''). \tag{3.16}$$

3.2. Analytical solution and exact derivative on B-series

Theorem 3.2. *The analytical solution $u(x_0+h)$ and the derivative $u'(x_0+h)$ and $u''(x_0+h)$ of the problem (3.7) have the forms as follow*

$$\begin{aligned}u(x_0+h)&=u_0+\sum_{t\in RT}\tfrac{h^{\rho(t)}}{\rho(t)!}\alpha(t)F(t)(u_0,u_0',u_0'')=B\left(\tfrac{\alpha\sigma}{\rho!},u_0,u_0',u_0''\right)\\&=B\left(\tfrac{1}{\gamma},u_0,u_0',u_0''\right),\end{aligned} \tag{3.17}$$

$$\begin{aligned}u'(x_0+h)&=u_0'+\sum_{t\in RT}\tfrac{h^{\rho(t)-1}}{(\rho(t)-1)!}\alpha(t)F(t)(u_0,u_0',u_0'')\\&=B\left(\tfrac{\alpha\sigma}{h(\rho-1)!},u_0,u_0',u_0''\right)\\&=B\left(\tfrac{\rho}{h\gamma},u_0,u_0',u_0''\right),\end{aligned} \tag{3.18}$$

$$\begin{aligned}u''(x_0+h)&=u_0''+\sum_{t\in RT}\tfrac{h^{\rho(t)-2}}{(\rho(t)-2)!}\alpha(t)F(t)(u_0,u_0',u_0'')\\&=B\left(\tfrac{\alpha\sigma}{h^2(\rho-2)!},u_0,u_0',u_0''\right)\\&=B\left(\tfrac{\rho(\rho-1)}{h^2\gamma},u_0,u_0',u_0''\right).\end{aligned} \tag{3.19}$$

Proof of Theorem 3.2. The conclusion is based on Theorem 3.1 and the expression (3.15). $\square$

3.3. Numerical solution and numerical derivative on B-series

For setting up B-series concerning of numerical solution of u_1 and its numerical derivatives, u_1' and u_1'' of the problem (3.7) produced by STDRKT methods, U_i, U_i' and U_i'' are expanded as B-series as $U_i=B(\bar\Psi_i,u_0,u_0',u_0'')$, $U_i'=B\left(\frac{\rho}{h}\hat\Psi_i,u_0,u_0',u_0''\right)$ and $U_i''=B\left(\frac{\rho(\rho-1)}{h^2}\Psi_i,u_0,u_0',u_0''\right)$ respectively. Hence, the first three equations in (2.3) become

$$\begin{aligned}&B(\bar\Psi_i,u_0,u_0',u_0'')=u_0+c_ihu_0'+\tfrac{(c_ih)^2}{2}u_0''+\tfrac{(c_ih)^3}{6}f_0\\&\quad+h^4\sum_{j=1}^{s}A_{i,j}g\left(B(\bar\Psi_j,u_0,u_0',u_0''),B\left(\tfrac{\rho}{h}\hat\Psi_j,u_0,u_0',u_0''\right),B\left(\tfrac{\rho(\rho-1)}{h^2}\Psi_j,u_0,u_0',u_0''\right)\right),\\&B\left(\tfrac{\rho}{h}\hat\Psi_i,u_0,u_0',u_0''\right)=u_0'+c_ihu_0''+\tfrac{(c_ih)^2}{2}f_0\\&\quad+h^3\sum_{j=1}^{s}\hat A_{i,j}g\left(B(\bar\Psi_j,u_0,u_0',u_0''),B\left(\tfrac{\rho}{h}\hat\Psi_j,u_0,u_0',u_0''\right),B\left(\tfrac{\rho(\rho-1)}{h^2}\Psi_j,u_0,u_0',u_0''\right)\right),\\&B\left(\tfrac{\rho(\rho-1)}{h^2}\Psi_i,u_0,u_0',u_0''\right)=u_0''+c_ihf_0\\&\quad+h^2\sum_{j=1}^{s}\bar A_{i,j}g\left(B(\bar\Psi_j,u_0,u_0',u_0''),B\left(\tfrac{\rho}{h}\hat\Psi_j,u_0,u_0',u_0''\right),B\left(\tfrac{\rho(\rho-1)}{h^2}\Psi_j,u_0,u_0',u_0''\right)\right).\end{aligned} \tag{3.20}$$

Referring to (3.15) and (3.16), the previous three equations can be expressed as

$$
\begin{aligned}
&\bar{\Psi}_i(\emptyset)u+\sum_{t\in RT}\tfrac{h^{\rho(t)}}{\rho(t)!}\bar{\Psi}_i(t)\gamma(t)\alpha(t)F(t)u_0,u_0',u_0'')\\
&=u_0+c_ihu_0'+\tfrac{(c_ih)^2}{2}u_0''+\tfrac{(c_ih)^3}{6}f_0\\
&\quad+\sum_{j=1}^{s}\sum_{RT\setminus\{\tau_1,\tau_2,\tau_3\}}\tfrac{h^{\rho(t)}}{\rho(t)!}A_{i,j}\Psi_j^{(4)}(t)\gamma(t)\alpha(t)F(t)\big(u_0,u_0',u_0''\big),\\
&\sum_{t\in RT}\tfrac{h^{\rho(t)-1}}{(\rho(t)-1)!}\hat{\Psi}_i(t)\gamma(t)\alpha(t)F(t)\big(u_0,u_0',u_0''\big)\\
&=u_0'+c_ihu_0''+\tfrac{(c_ih)^2}{2}f_0\\
&\quad+\sum_{j=1}^{s}\sum_{RT\setminus\{\tau_1,\tau_2,\tau_3\}}\tfrac{h^{\rho(t)-1}}{\rho(t)!}\widehat{A}_{i,j}\Psi_j^{(4)}(t)\gamma(t)\alpha(t)F(t)\big(u_0,u_0',u_0''\big),\\
&\sum_{t\in RT}\tfrac{h^{\rho(t)-2}}{(\rho(t)-2)!}\Psi_i(t)\gamma(t)\alpha(t)F(t)u_0,u_0',u_0'')\\
&=u_0''+c_ihf_0+\sum_{j=1}^{s}\sum_{RT\setminus\{\tau_1,\tau_2,\tau_3\}}\tfrac{h^{\rho(t)-2}}{\rho(t)!}\overline{A}_{i,j}\Psi_j^{(4)}(t)\gamma(t)\alpha(t)F(t)\big(u_0,u_0',u_0''\big),
\end{aligned}
\tag{3.21}
$$

It follows

$$
\begin{aligned}
&\bar{\Psi}_i(\emptyset)=1,\ \bar{\Psi}_i(\tau_1)=c_i,\ \bar{\Psi}_i(\tau_2)=\tfrac{(c_i)^2}{2},\ \bar{\Psi}_i(\tau_3)=\tfrac{(c_i)^3}{6},\\
&\bar{\Psi}_i(\tau_4)=\sum_{j=1}^{s}A_{i,j}\Psi_j^{(4)}=\sum_{j=1}^{s}A_{i,j},\ \hat{\Psi}_i(\tau_1)=1,\ \hat{\Psi}_i(\tau_2)=c_i,\\
&\hat{\Psi}_i(\tau_3)=\tfrac{(c_i)^2}{2},\\
&\hat{\Psi}_i(\tau_4)=\sum_{j=1}^{s}\widehat{A}_{i,j}\Psi_j^{(4)}=\sum_{j=1}^{s}\widehat{A}_{i,j},\ \Psi_i(\tau_2)=1,\ \Psi_i(\tau_3)=c_i,\\
&\Psi_i(\tau_4)=\sum_{j=1}^{s}\overline{A}_{i,j}\Psi_j^{(4)}=\sum_{j=1}^{s}\overline{A}_{i,j},
\end{aligned}
\tag{3.22}
$$

and

$$
\bar{\Psi}_i(t)=\sum_{j=1}^{s}A_{i,j}\Psi_j^{(4)}(t),\ \hat{\Psi}_i(t)=\sum_{j=1}^{s}\widehat{A}_{i,j}\Psi_j^{(4)}(t),\ \Psi_i(t)=\sum_{j=1}^{s}\overline{A}_{i,j}\Psi_j^{(4)}(t).
\tag{3.23}
$$

Moreover, for trees $t=[t_1,\dots,t_r,<t_{r+1},\dots,t_m>,<t_{m+1},\dots,t_n>]_3\in RT$ and $\rho(t)\geqslant 5$, Lemma 3.1 obtains

$$
\Psi_j^{(4)}(t)=\sum_{\bar{t}}\left(\prod_{i=1}^{r}\bar{\Psi}_j(\bar{t}_i)\prod_{i=r+1}^{m}\hat{\Psi}_j(\bar{t}_i)\prod_{i=m+1}^{n}\Psi_j(\bar{t}_i)\right),
\tag{3.24}
$$

in which the sum replaces all trees $\bar{t}$ satiating $t=[t_1,\dots,t_r,<t_{r+1},\dots,t_m>,<t_{m+1},\dots,t_n>]_3=[t\setminus\tau_4]_3$. Inserting (3.23) into (3.24), yields

$$
\Psi_j^{(4)}(t)=um_{\bar{t}}\left(\prod_{i=1}^{r}\sum_{k=1}^{s}A_{j,k}\Psi_k^{(4)}(\bar{t}_i)\times\prod_{i=r+1}^{m}\sum_{k=1}^{s}\widehat{A}_{j,k}\Psi_k^{(4)}(\bar{t}_i)\times\prod_{i=m+1}^{n}\sum_{k=1}^{s}\overline{A}_{j,k}\Psi_k^{(4)}(\bar{t}_i)\right).
\tag{3.25}
$$

Denote $\Psi_j^{(4)}(t)=\Phi_j(t)$ for all trees $t=[t_1,\dots,t_r,<t_{r+1},\dots,t_m>,<t_{m+1},\dots,t_n>]_3\in RT$ and $\rho(t)\geqslant 5$. Then (27) can be transcribed as

$$
\Phi_j(t)=\sum_{\bar{t}}\left(\prod_{i=1}^{r}\sum_{k=1}^{s}A_{j,k}\Phi_k(\bar{t}_i)\times\prod_{i=r+1}^{m}\sum_{k=1}^{s}\widehat{A}_{j,k}\Phi_k(\bar{t}_i)\times\prod_{i=m+1}^{n}\sum_{k=1}^{s}\overline{A}_{j,k}\Phi_k(\bar{t}_i)\right).
\tag{3.26}
$$

where $t=[t_1,\dots,t_r,<t_{r+1},\dots,t_m>,<t_{m+1},\dots,t_n>]_3=[t\setminus\{\tau_4\}]$. Propositions below shows the values of $\Phi_i(t)$ for all trees in RT.

Proposition 3.3. *The function Φ_i on $RT\setminus\{\tau_1,\tau_2\}$ can be calculated coercively as follow:*

1. $\Phi_i(\tau_3)=0,\ \Phi_i(\tau_4)=1,$
2. for $t=\left[t_1^{\mu_1},\dots,t_r^{\mu_r},<t_{r+1}^{\mu_{r+1}},\dots,t_m^{\mu_m}>,<t_{m+1}^{\mu_{m+1}},\dots,t_n^{\mu_n}>\right]_3\in RT$, with $t_2,\dots,t_r$ distinct and disperate from $\tau_1,t_{r+1},\dots,t_m$ distinct and $t_{m+1},\dots,t_n$ distinct,

$$
\Phi_i(t)=c_i^{\mu_1}\prod_{k=2}^{r}\left(\sum_{j=1}^{s}A_{i,j}\Phi_j(\bar{t}_i)\right)^{\mu_k}\times\prod_{k=r+1}^{m}\left(\sum_{j=1}^{s}\widehat{A}_{i,j}\Phi_j(\bar{t}_i)\right)^{\mu_k}\times\prod_{k=m+1}^{n}\left(\sum_{j=1}^{s}\overline{A}_{i,j}\Phi_j(\bar{t}_i)\right)^{\mu_k},
\tag{3.27}
$$

   where μ_1 is the product of τ_1 and μ_k is the product of t_k for $k=2,\dots,n$,
3. for $t\in RT$ and $\rho(t)\geqslant 5,\bar{t}=\left[\tau_1^{\mu_1},\bar{t}_2^{\mu_2},\dots,\bar{t}_r^{\mu_r},<\bar{t}_{r+1}^{\mu_{r+1}},\dots,\bar{t}_m^{\mu_m}>,<\bar{t}_{m+1}^{\mu_{m+1}},\dots,\bar{t}_n^{\mu_n}>\right]_3=[t\setminus\tau_4]_3$ *with $\bar{t}_2,\dots,\bar{t}_r$ distinct and disparate from τ_1 and $\bar{t}_{r+1},\dots,\bar{t}_n$ distinct,*

$$
\bar{\Phi}_i(t)=\sum_{\bar{t}}\Phi_i(\bar{t}),
$$

   where μ_1 is the product of τ_1 and μ_k is the product of t_k for $k=2,\dots,n$.

Hereby, we indicate the vectors $\Phi(t)=(\Phi_1(t),\dots,\Phi_s(t))^T$ for $t\in RT\setminus\{\tau_1,\tau_2,\tau_3\}$. The rooted trees with order up to nine with the values of related functions are listed in Table 2. Elementary weight for y_1, expressed as $\phi(t)$ and can be formed as follow

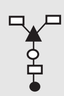
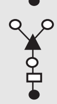
$$
\phi(t)=\sum_{i=1}^{s}b_i\Phi_i(t)=b^T\Phi(t),
$$

and elementary weight for u' and u'' are expressed as $\phi'(t)$ and $\phi''(t)$ respectively.

$$
\phi'(t)=\sum_{i=1}^{s}b_i'\Phi_i(t)=b'^T\Phi(t),\quad \phi''(t)=\sum_{i=1}^{s}b_i''\Phi_i(t)=b''^T\Phi(t).
\tag{3.28}
$$

Therefore, the numerical solution u_1 and its numerical derivative, u_1' and u_1'' of the numerical problem generated by STDRKT methods have following B-series

Table 2 Root trees for STDRKT methods up to order nine.

Order $\rho(t)$	Tree t	Graph	$\alpha(t)$	Density $\gamma(t)$	$\phi(t)$	Elementary differential
1		τ_1	1	1		u'
2		τ_2	1	2		u''
3		τ_3	1	6		f
4		τ_4	1	24	e	g
5		$\tau_{5,1}$	1	120	c	$g_u u'$
		$\tau_{5,2}$	1	120	c	$g_{u'} u''$
		$\tau_{5,3}$	1	120	c	$g_{u''} f$
6		$\tau_{6,1}$	1	360	c^2	$g_{uu}(u', u')$
		$\tau_{6,2}$	2	360	c^2	$g_{uu'}(u', u'')$
		$\tau_{6,3}$	2	360	c^2	$g_{uu''}(u', f)$
		$\tau_{6,4}$	1	360	c^2	$g_{u'u'}(u'', u'')$
		$\tau_{6,5}$	2	360	c^2	$g_{u'u''}(u'', f)$
		$\tau_{6,6}$	1	360	c^2	$g_{u''u''}(f, f)$
		$\tau_{6,7}$	1	360	c^2	$g_u u''$
		$\tau_{6,8}$	1	360	c^2	$g_{u'} f$

(*continued on next page*)

Table 2 (*continued*)

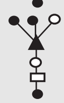
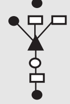
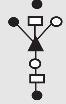
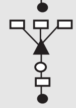
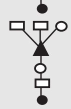
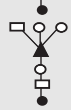
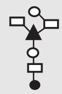
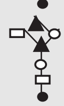
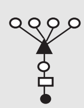
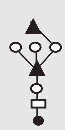
Order $\rho(t)$	Tree t	Graph	$\alpha(t)$	Density $\gamma(t)$	$\phi(t)$	Elementary differential
6		$\tau_{6,9}$	1	720	$\bar{A}e$	$g_{u''}g$
7		$\tau_{7,1}$	1	840	c^3	$g_{uuu}(u',u',u')$
		$\tau_{7,2}$	3	840	c^3	$g_{uuu'}(u',u',u'')$
		$\tau_{7,3}$	3	840	c^3	$g_{uuu''}(u',u',f)$
		$\tau_{7,4}$	3	840	c^3	$g_{uu'u'}(u',u'',u'')$
		$\tau_{7,5}$	6	840	c^3	$g_{uu'u''}(u',u'',f)$
		$\tau_{7,6}$	3	840	c^3	$g_{uu''u''}(u',f,f)$
		$\tau_{7,7}$	1	840	c^3	$g_{u'u'u'}(u'',u'',u'')$
		$\tau_{7,8}$	3	840	c^3	$g_{u'u'u''}(u'',u'',f)$
		$\tau_{7,9}$	3	840	c^3	$g_{u'u''u''}(u'',f,f)$
		$\tau_{7,10}$	1	840	c^3	$g_{u''u''u''}(f,f,f)$
		$\tau_{7,11}$	3	840	c^3	$g_{uu}(u',u'')$
		$\tau_{7,12}$	3	840	c^3	$g_{uu'}(u',f)$

Table 2 (*continued*)

Order $\rho(t)$	Tree t	Graph	$\alpha(t)$	Density $\gamma(t)$	$\phi(t)$	Elementary differential
7		$\tau_{7,13}$	3	840	c^3	$g_{uu''}(u'', f)$
		$\tau_{7,14}$	3	840	c^3	$g_{u'u'}(u'', f)$
		$\tau_{7,15}$	3	1680	$c \cdot \bar{A}e$	$g_{uu''}(u', f)$
		$\tau_{7,16}$	3	1680	$c \cdot \bar{A}e$	$g_{uu''}(u', g)$
		$\tau_{7,17}$	3	1680	$c \cdot \bar{A}e$	$g_{uu''}(u', g)$
		$\tau_{7,18}$	3	1680	$c \cdot \bar{A}e$	$g_{u''u''}(f, g)$
		$\tau_{7,19}$	3	1680	$c \cdot \bar{A}e$	$g_{u'u''}(u'', g)$
		$\tau_{7,20}$	1	5040	$\bar{A}c$	$g_{u''}g_{u}u'$
		$\tau_{7,21}$	1	5040	$\bar{A}c$	$g_{u''}g_{u''}f$
		$\tau_{7,22}$	1	5040	$\hat{A}e$	$g_{u'}g$
8		$\tau_{8,1}$	1	1680	c^4	$g_{u''u''u''u''}(f, f, f, f)$
		$\tau_{8,2}$	6	3360	$c^2 \cdot \bar{A}e$	$g_{u''u''u''}(f, f, g)$

(*continued on next page*)

Table 2 (*continued*)

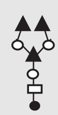
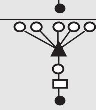
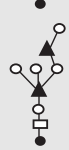
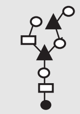
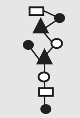
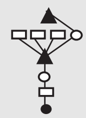
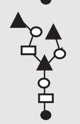
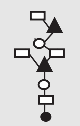
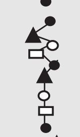
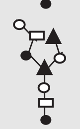
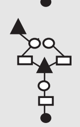
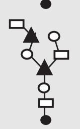
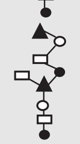
Order $\rho(t)$	Tree t	Graph	$\alpha(t)$	Density $\gamma(t)$	$\phi(t)$	Elementary differential
8		$\tau_{8,3}$	1	40320	$\frac{1}{2}\bar{A}c^2 + c\cdot\bar{A}c$	$g_{u''u''}g_{u''}(f,f)$
		$\tau_{8,4}$	12	3360	$c^2\cdot Ae$	$g_{uu''u''}(u',f,g)$
		$\tau_{8,5}$	10	4032	$\frac{1}{2}c^2\bar{A}e + c\cdot\hat{A}e$	$g_{u'u''}(f,g)$
		$\tau_{8,6}$	1	40320	$\frac{1}{2}\bar{A}c^2 + \hat{A}c$	$g_{u'}g_{u''}f$
		$\tau_{8,7}$	1	40320	Ae	$g_u g$
		$\tau_{8,8}$	3	13440	$\frac{1}{2}(\bar{A}e)^2 + \bar{A}\cdot\bar{A}e$	$g_{u''u''}(g,g)$
		$\tau_{8,9}$	1	40320	$\bar{A}\cdot\bar{A}e$	$g_{u''}g_{u''}g$
9		$\tau_{9,1}$	1	3024	c^5	$g_{u''u''u''u''u''}(f,f,f,f,f)$
		$\tau_{9,2}$	15	24192	$\frac{1}{2}c\cdot(\bar{A}e)^2$ $+c\cdot\bar{A}\cdot\bar{A}e$	$g_{uu''u''}(u',g,g)$
		$\tau_{9,3}$	2	181440	$\frac{1}{3}\bar{A}c^3 + c^2\bar{A}c$	$g_{u''u''u''}g_{u''}(f,f,f)$

Table 2 (*continued*)

Order $\rho(t)$	Tree t	Graph	$\alpha(t)$	Density $\gamma(t)$	$\phi(t)$	Elementary differential
9		$\tau_{9,4}$	3	120960	$\frac{1}{2}\left(\bar{A}c^3+c^2\bar{A}c\right)+c\cdot\hat{A}c$	$g_{u'u''}g_{u''}(f,f)$
		$\tau_{9,5}$	8	45360	$c\cdot\bar{A}c^2$	$g_{uu''}g_u(u',u'')$
		$\tau_{9,6}$	10	6048	$c^3\bar{A}e$	$g_{u'u'u'u''}(u'',u'',u'',g)$
		$\tau_{9,7}$	10	36288	$\bar{A}\cdot\hat{A}e+\hat{A}\cdot\bar{A}e$	$g_{u'u''}(g,g)$
		$\tau_{9,8}$	1	362880	$\frac{1}{2}\hat{A}c^2+c\cdot\hat{A}c$	$g_{u'u'}g_{u'}(u'',u'')$
		$\tau_{9,9}$	1	362880	Ac	$g_u g_u u'$
		$\tau_{9,10}$	50	72576	$\frac{1}{2}c^3\bar{A}e+c^2\hat{A}e$	$g_{uu'u''}(u',f,g)$
		$\tau_{9,11}$	15	24192	$\frac{1}{6}c^3\bar{A}e+c\cdot Ae$	$g_{uu''}(f,g)$
		$\tau_{9,12}$	10	36288	$c^2\cdot\hat{A}e$	$g_{u'u'}(f,g)$
		$\tau_{9,13}$	6	60480	$\frac{1}{2}c\cdot\bar{A}c^2+\hat{A}c^2$	$g_{u'u''}g_{u'}(u'',f)$
		$\tau_{9,14}$	15	24192	$\frac{1}{2}c^2\hat{A}e+c\cdot Ae$	$g_{uu'}(u'',g)$

$$\begin{aligned} u_1(x_0+h) = {} & u_0 + hu_0' + \tfrac{h^2}{2}u_0'' + \tfrac{h^3}{6}f_0 \\ & + \sum_{t\in RT\setminus\{\tau_1,\tau_2,\tau_3\}} \tfrac{h^{\rho(t)}}{\rho(t)!}\phi(t)\gamma(t)\alpha(t)F(t)\left(u_0,u_0',u_0''\right), \\ u_1'(x_0+h) = {} & y_0' + hy_0'' + \tfrac{h^2}{2}f_0 \\ & + \sum_{t\in RT\setminus\{\tau_1,\tau_2,\tau_3\}} \tfrac{h^{\rho(t)-1}}{\rho(t)!}\phi(t)\gamma(t)\alpha(t)F(t)\left(u_0,u_0',u_0''\right), \\ u_1''(x_0+h) = {} & y_0'' + hf_0 + \sum_{t\in RT\setminus\{\tau_1,\tau_2,\tau_3\}} \tfrac{h^{\rho(t)-2}}{\rho(t)!}\phi(t)\gamma(t)\alpha(t)F(t)\left(u_0,u_0',u_0''\right). \end{aligned} \tag{3.29}$$

All the rooted trees for STDRKT methods up to order seven and selected rooted trees comprised of all order conditions for STDRKT methods with order eight and nine are shown in Table 2. The selection of rooted trees with order eight and nine is based on the terms of $\phi(t)$ that crucial in deriving all order conditions with order eight and nine. Duplication of the term for $\phi(t)$ will be eliminated and that rooted trees are not listed in Table 2 due to the concern of yielding large quantity of pages.

4. Development of STDRKT methods

Coefficients of STDRKT methods are determined as given in (3.5).

Order conditions for explicit STDRKT methods are listed as follow.

The order conditions for u:

Fourth order:

$$b^T e = \frac{1}{24}. \tag{4.29}$$

Fifth order:

$$b^T c = \frac{1}{120}. \tag{4.30}$$

Sixth order:

$$b^T c^2 = \frac{1}{360}, \qquad b^T \overline{A}e = \frac{1}{720}. \tag{4.31}$$

Seventh order:

$$b^T c^3 = \frac{1}{840}, \qquad b^T \widehat{A}e = \frac{1}{5040}, \qquad b^T \overline{A}c = \frac{1}{5040}, \qquad b^T c\overline{A}e = \frac{1}{1680}. \tag{4.32}$$

The order conditions for u':

Third order:

$$b'^T e = \frac{1}{6}. \tag{4.33}$$

Fourth order:

$$b'^T c = \frac{1}{24}. \tag{4.34}$$

Fifth order:

$$b'^T c^2 = \frac{1}{60}, \qquad b'^T \overline{A}e = \frac{1}{120}. \tag{4.35}$$

Sixth order:

$$b'^T c^3 = \frac{1}{120}, \qquad b'^T \widehat{A}e = \frac{1}{720}, \qquad b'^T \overline{A}c = \frac{1}{720}, \qquad b'^T c\overline{A}e = \frac{1}{240}. \tag{4.36}$$

Seventh order:

$$\begin{aligned} & b'^T c^4 = \tfrac{1}{210}, \qquad b'^T\left(\tfrac{1}{2}\overline{A}c^2 + \widehat{A}c\right) = \tfrac{1}{5040}, \qquad b'^T Ae = \tfrac{1}{5040}, \\ & b'^T c^2\overline{A}e = \tfrac{1}{420}, \qquad b'^T\overline{A}\cdot\left(\overline{A}e\right) = \tfrac{1}{5040}, \qquad b'^T c\widehat{A}e = \tfrac{1}{1260}, \\ & b'^T\left(c\cdot\overline{A}c + \overline{A}c^2\right) = \tfrac{1}{2520}, \qquad b'^T\left(\overline{A}e\right)^2 = \tfrac{1}{1260}. \end{aligned} \tag{4.37}$$

The order conditions for u'':

Second order:

$$b''^T e = \frac{1}{2}. \tag{4.38}$$

Third order:

$$b''^T c = \frac{1}{6}. \tag{4.39}$$

Fourth order:

$$b''^T c^2 = \frac{1}{12}, \qquad b''^T \overline{A}e = \frac{1}{24}. \tag{4.40}$$

Fifth order:

$$b''^T c^3 = \frac{1}{20}, \qquad b''^T \widehat{A}e = \frac{1}{120}, \qquad b''^T \overline{A}c = \frac{1}{120}, \qquad b''^T c\overline{A}e = \frac{1}{40}. \tag{4.41}$$

Sixth order:

$$\begin{aligned} & b''^T c^4 = \tfrac{1}{30}, \qquad b_i''^T\left(\tfrac{1}{2}\overline{A}c^2 + \widehat{A}c\right) = \tfrac{1}{720}, \qquad b''^T Ae = \tfrac{1}{720}, \\ & b''^T c^2\overline{A}e = \tfrac{1}{60}, \qquad b''^T\overline{A}\cdot\left(\overline{A}e\right) = \tfrac{1}{720}, \qquad b''^T c\widehat{A}e = \tfrac{1}{180}, \\ & b''^T\left(c\cdot\overline{A}c + \overline{A}c^2\right) = \tfrac{1}{360}, \qquad b''^T\left(\overline{A}e\right)^2 = .\tfrac{1}{180} \end{aligned} \tag{4.42}$$

Seventh order:

$$\begin{aligned} & b''^T c^5 = \tfrac{1}{42}, \quad b''^T c\left(\tfrac{1}{2}\left(\overline{A}e\right)^2 + \overline{A}\cdot\overline{A}e\right) = \tfrac{1}{336}, \quad b''^T c\cdot\overline{A}c^2 = \tfrac{1}{630}, \\ & b''^T\left(\tfrac{1}{3}\overline{A}c^3 + c^2\cdot\overline{A}c\right) = \tfrac{1}{2520}, \quad b''^T\left(\tfrac{1}{2}\overline{A}c^3 + \tfrac{1}{2}c^2\cdot\overline{A}c + c\cdot\widehat{A}c\right) = \tfrac{1}{1680}, \\ & b''^T c^3\cdot\overline{A}e = \tfrac{1}{84}, \quad b''^T\left(\tfrac{1}{2}c\cdot\overline{A}c^2 + Ac^2\right) = \tfrac{1}{840}, \quad b''^T c^2\cdot\widehat{A}e = \tfrac{1}{252} \\ & b''^T\left(\tfrac{1}{2}\widehat{A}c^2 + c\cdot\widehat{A}c\right) = \tfrac{1}{2520}, \quad b''^T\left(\widehat{A}\cdot\overline{A}e + \overline{A}\cdot\widehat{A}e\right) = \tfrac{1}{504}, \\ & b''^T\left(\tfrac{1}{6}\overline{A}c^3 + Ac\right) = \tfrac{1}{5040}, \quad b''^T c\cdot Ae = \tfrac{1}{1008}, \\ & b''^T\left(\overline{A}c\cdot\overline{A}e + c\overline{A}\cdot\overline{A}e\right) = \tfrac{1}{720}. \end{aligned} \tag{4.43}$$

The simplifying assumption is utilised in generating parameters of STDRKT methods as follow:

$$\sum_{i}^{n} A_{i,j} = \frac{c_i^4}{24}. \tag{4.44}$$

4.1. Two stage STDRKT method of order five

Order conditions up to order five in the equations u, u' and u'', comprised of Eqs. (4.29), (4.30), (4.33), (4.34) and (4.35), (4.38), (4.39), (4.40), (4.41) and (4.42) are used to derive the fifth-order STDRKT method. Simplified assumption (4.44) is used to obtain parameters of the methods. This system has no free parameter but yield a unique solution. Truncation error norms for u_n, u_n' and u_n'' are given by

$||\tau^{(6)}|| = 1.389 \times 10^{-3}, ||\tau'^{(6)}|| = 2.196 \times 10^{-3}, ||\tau''^{(6)}|| = 1.440 \times 10^{-2}$ with the global truncation error term, $||\tau_g^{(6)}||_2 = 1.463 \times 10^{-2}$. Parameters of the new method are given in Butcher tableau and denoted by STDRKT2(5) shown in Table 3:

4.2. Three stage STDRKT method of order six

Order conditions up to order six in the equations u, u' and u'' comprised of Eqs. (4.29), (4.30) and (4.31), (4.33), (4.34), (4.35) and (4.36), (4.38), (4.39), (4.40), (4.41) and (4.42) are used to derive the sixth-order STDRKT method. The resulting system contains two free parameters, $A_{3,1}$ and $A_{3,2}$.

$$A_{2,1} = -5\left(\frac{1}{2} - \frac{1}{10}\sqrt{5}\right)A_{3,1} - 5\left(\frac{1}{2} - \frac{1}{10}\sqrt{5}\right)A_{3,2} + A_{3,1} + A_{3,2} + \frac{1}{120} - \frac{1}{600}\sqrt{5} \tag{4.45}$$

Minimizing error equations of seventh order conditions are utilised to select the parameters that generate minimum value of truncation error norms for u_n, u'_n and u''_n. Minimising error equations generate $||\tau^{(7)}|| = 1.141 \times 10^{-4}$, $||\tau'^{(7)}|| = 1.731 \times 10^{-3}$ and $||\tau''^{(7)}|| = 3.460 \times 10^{-3}$ with the global truncation error of $||\tau_g^{(7)}||_2 = 3.871 \times 10^{-3}$, yielding, $A_{3,1} = \frac{2144}{223443}$, $A_{3,2} = \frac{225}{101651}$. Then, these values are substituted into (4.44) and obtain $A_{2,1} = \frac{6167}{64229898}$ The coefficients of the new method presented in Butcher tableau and denoted by STDRKT3(6) as seen in Table 4:

Next, we discuss the properties of STDRKT methods, including zero stability, consistency and convergence.

Definition 4.1. The numerical method with order p is zero stable if numerical solutions remain bounded in the limit $h \to 0$, with the modulus of roots for the first characteristic polynomial are less than or equal to zero. [13]

STDRKT methods can be transformed into matrix finite difference equation as follow

$$IU_{n+1} = AU_n + h^3(B \cdot F_n) + h^4(C \cdot G_n), \tag{4.46}$$

where
$U_{n+1} = \left[u_{n+1}, hu'_{n+1}, h^2u''_{n+1}\right]^T, U_n =$-
$\left[u_n, hu'_n, h^2u''_n\right]^T, F_n = [f_n, f_n, f_n]^T, G_n = [g_n, g_n, g_n]^T, A, B$ and C are matrices 3×3. In STDRKT methods, knowing that

$$A = \begin{pmatrix} 1 & 1 & \frac{1}{2} \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then,

$$I\xi - A = \begin{pmatrix} \xi - 1 & 1 & \frac{1}{2} \\ 0 & \xi - 1 & 1 \\ 0 & 0 & \xi - 1 \end{pmatrix}.$$

First characteristic polynomial can be defined as

$$p(\xi) = det[I\xi - A] = (\xi - 1)^3. \tag{4.47}$$

Thus, STDRKT method is zero stable by reason of the roots, $\xi_i = 1, i = 1, 2, 3$, are less than or equal to one.

Definition 4.2. The method is consistent with the order at least p if and only if local truncational error, $T_{p+1} = O\left(h^{p+1}\right)$ as $h \to 0$ (see Suli [14]).

We considered explicit STDRKT methods in the class as follow:

$$\sum_{j=0}^{r}\alpha_j u_{n+j} = \sum_{j=0}^{r-1}\left(h\beta_j u'_{n+j} + h^2\gamma_j u''_{n+j} + h^3\delta_j f_{n+j}\right) + \sum_{j=0}^{r-1}h^4\left(\phi_g\left(u_{n+r-1}, \ldots, u_n, u'_{n+r-1}, \ldots, u'_n, u''_{n+r-1}, \ldots, u''_n\right)\right. \tag{4.48}$$

On putting $r = 1$, then

$$\alpha_1 = 1, \quad \alpha_0 = -1, \quad \beta_0 = 1, \quad \gamma_0 = \tfrac{1}{2}, \quad \delta_0 = \tfrac{1}{6}, \qquad \phi_g(u''_n, u'_n, u_n, x_n; h) = \sum_{i=1}^{s} b_i k_i, \quad i = 1, 2, 3, \ldots, s \tag{4.49}$$

Table 3 The STDRKT2(5) method.

0	0		0		0	
$\frac{1}{2}$	$\frac{1}{384}$	0	$\frac{1}{40}$	0	$\frac{1}{8}$	0
	$\frac{1}{40}$	$\frac{1}{60}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{6}$	$\frac{1}{3}$

Table 4 The STDRKT3(6) method.

0	0			0			0		
c_2	$A_{2,1}$	0		$\widehat{A}_{2,1}$	0		$\overline{A}_{2,1}$	0	
c_3	$A_{3,1}$	$A_{3,2}$	0	$\widehat{A}_{3,1}$	$\widehat{A}_{3,2}$	0	$\overline{A}_{3,1}$	$\overline{A}_{3,2}$	0
	b_1	b_2	b_3	b'_1	b'_2	b'_3	b''_1	b''_2	b''_3

where $A_{2,1} = \frac{1609}{6616950}, A_{3,1} = \frac{6764}{734409}, A_{3,2} = \frac{253}{114305}, \widehat{A}_{2,1} = \frac{6503}{1847919}, \widehat{A}_{3,1} = \frac{18869}{298808}, \widehat{A}_{3,2} = 0, \overline{A}_{2,1} = \frac{15066}{394433}, \overline{A}_{3,1} = -\frac{22733}{421493}, \overline{A}_{3,2} = \frac{109801}{347760},$

$b_1 = \frac{1}{72}, b_2 = \frac{94667}{3597934}, b_3 = \frac{2092}{1426731}, b'_1 = \frac{1}{24}, b'_2 = \frac{67297}{616924}, b'_3 = \frac{5473}{343884}, b''_1 = \frac{1}{12}, b''_2 = \frac{109801}{364179}, b''_3 = \frac{43796}{380293}, c_2 = \frac{28657}{103682}, c_3 = \frac{75025}{103682}.$

where $k_i = f\left(x_n + c_i h, u_n + hu'_n + \frac{h^2}{2}u''_n + \frac{h^3}{6}f_n + h^4\sum_{j=1}^{s} a_{i,j}k_j\right)$.

The condition for (4.47) to be consistent are

$$\sum_{j=0}^{r}\alpha_j = 0,\quad \sum_{j=0}^{r} j\alpha_j - \sum_{j=0}^{r-1}\beta_j = 0,\quad \sum_{j=0}^{r}\frac{j^2}{2}\alpha_j - \sum_{j=0}^{r-1}\gamma_j = 0,$$
$$\sum_{j=0}^{r}\frac{j^3}{3!}\alpha_j - \sum_{j=0}^{r-1}\delta_j = 0, \frac{\phi_g(u''(x_n),\ldots,u''(x_n),u'(x_n),\ldots,u'(x_n,u(x_n),\ldots,u(x_n),x_n;0))}{\sum_{j=0}^{r}\frac{j^4}{4!}\alpha_j}$$
$$= g(x_n, u(x_n), u'(x_n), u''(x_n)). \tag{4.50}$$

Applying the conditions (4.49), the necessary and sufficient condition for STDRKT methods to acquire consistency is

$$\phi_g(y''(x_n), y'(x_n), y(x_n), x_n; 0) = g\left(x_n, y_n, y'_n, y''_n\right) \Longleftrightarrow \sum_{i=1}^{s} b_i = \frac{1}{24}. \tag{4.51}$$

Here, local truncation error, T_{n+1} at x_{n+1} is expressed as the residual when $u_{n+j},\ u'_n,\ u''_n$ is replaced by $u(x_{n+j}),\ u'(x_n),\ u''(x_n),\ j = 0, 1,$which is

$$\begin{aligned} T_{n+1} &= u(x_{n+1}) + hu'(x_{n+1}) + \tfrac{h^2}{2}u''(x_{n+1}) \\ &\quad + \tfrac{h^3}{6}f(x_{n+1}, y(x_{n+1}), y'(x_{n+1}), y''(x_{n+1})) \\ &\quad - \left[u(x_n) + hu'(x_n) + \tfrac{h^2}{2}u''(x_n) + \tfrac{h^3}{6}f(x_n, u(x_n), u'(x_n), u''(x_n))\right] \\ &\quad - h^4\phi_g(u''(x_n), u'(x_n), u(x_n), x_n; h), \end{aligned} \tag{4.52}$$

where ϕ_g is defined in (4.49). Assuming that p is the largest integer whereby $T_{n+1} = O\left(h^{p+1}\right)$, then the method has order p (see Lambert [16]). We denote by $\tilde{u}_{n+1}$ the value at x_{n+1} generated by STDRKT methods when the localising assumption, $u_n = u(x_n)$ is made. Since

$$\tilde{u}_{n+1} = u_n + hu'_n + \frac{h^2}{2}u''_n + \frac{h^3}{6}f\left(x_n, u_n, u'_n, u''_n\right) + h^4\phi_g\left(u''_n, u'_n, u_n, x_n; h\right). \tag{4.53}$$

Then we have

$$u(x_{n+1}) + hu'(x_{n+1}) + \tfrac{h^2}{2}u''(x_{n+1}) + \tfrac{h^3}{6}f(x_{n+1}, u(x_{n+1}), u'(x_{n+1}), u''(x_{n+1})) - \tilde{u}_{n+1} = T_{n+1}. \tag{4.54}$$

STDRKT methods are consistent if they follow (4.49) that

$$\begin{aligned} &u(x_{n+1}) + hu'(x_{n+1}) + \tfrac{h^2}{2}u''(x_{n+1}) + \tfrac{h^3}{6}f(x_{n+1}, u(x_{n+1}), u'(x_{n+1}), \\ &u''(x_{n+1}) - \left[u(x_n) + hu'(x_n) + \tfrac{h^2}{2}u''(x_n) + \tfrac{h^3}{6}f(x_n, u(x_n), u'(x_n), u''(x_n))\right] \\ &\qquad = \tfrac{h^4}{24}f'\left(x_n, u_n, u'_n, u''_n\right) - \tfrac{h^4}{24}g\left(x_n, u_n, u'_n, u''_n\right) + O\left(h^5\right). \end{aligned} \tag{4.55}$$

By reason of $f'(x_n, u(x_n), u'(x_n), u''(x_n)) = g\left(x_n, u_n, u'_n, u''_n\right)$, T_{n+1} for STDRKT methods is equal to $O\left(h^5\right)$, it shows that STDRKT methods are consistent if their order is at least 4, which is in line with our definitions of order for linear multistep methods. Since the order of STDRKT methods is at least 4, and hence, this method is consistent.

Convergence is a property of numerical method related to truncation errors that ensures the numerical solution converges onto the exact solution and the global truncation error goes to zero at all step size indices in the limit $\triangle h \to 0$ (see Atkinson [15]). Maximum absolute global truncation error between the analytical solution and numerical solution the gets smaller as the step size becomes lesser.

Definition 4.3. The numerical method is convergent iff acquiring the properties of zero stability and consistency. (see Lambert [16])

Since STDRKT methods are zero-stable and consistent, implies that STDRKT methods are convergent.

5. Problem testing and numerical result

Efficiency of the new methods with order five and six are examined on selected numerical problems for comparison purpose. Below are the numerical methods utilised to be compared:

- **STDRKT3(6)** - Newly proposed special explicit two-derivative Runge-Kutta type method of six algebraic order proposed.
- **STDRKT2(5)** - Newly proposed special explicit two-derivative Runge-Kutta type method of five algebraic order proposed.
- **RK5** - Runge-Kutta fifth-order method (proposed by Butcher) (Source: Goeken [17])
- **RKDP45** - Runge-Kutta Dormand-Prince method (proposed by Dormand [18])
- **RK6** - Rung-Kutta sixth-order method (proposed by Luther [19]) e
- **RK6S** - Runge-Kutta sixth-order method (proposed by Al-Shimmary [20])

Problem 1 Consider the linear homogeneous problem

$$u''' = -u', u(0) = 0, u'(0) = 1, u''(0) = 2, \quad x \in [0, 20]$$

whose analytic solution is $u(x) = 2(1 - \cos x) + \sin x$.Source: Yap et al. [6].

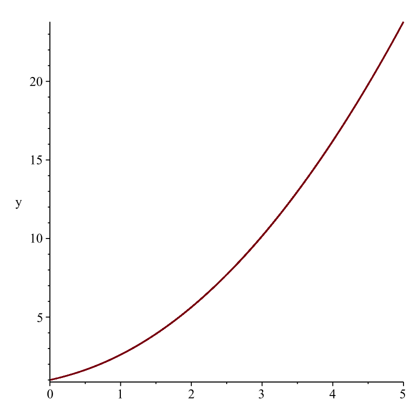


Fig. 1 Illustration of thin films flow of viscous fluid with $u''' = u^{-2}$.

Problem 2 Consider the linear nonhomogeneous problem

$$u''' = u^2 + (\cos x)^2 - \cos x - 1, u(0) = 0, u'(0) = 1, u''(0) = 0,$$
$$x \in [0, 10]$$

whose analytic solution is $u(x) = 2u(x)u'(x) - 2\cos x\ \sin x + \sin x$.Source: Mechee et al. [21].

Problem 3 Consider the linear nonhomogeneous problem

$$u''' = u'' - u' + u + e^x, u(0) = 1, u'(0) = 1, u''(0) = 0, x \in [0, 2]$$

whose analytic solution is $u(x) = \frac{1}{2}xe^x + \cos(x) + \frac{1}{2}\sin(x)$.

Problem 4 Consider nonlinear nonhomogeneous system

$$u_1''' = \frac{1}{2}e^{4x}u_3u_2', \quad u_2''' = \frac{8}{3}e^{2x}u_1u_3', \quad u_2''' = 27u_2u_1',$$

$$u_1(0) = 1, u_1'(0) = -1, u_1''(0) = 1,$$

$$u_2(0) = 1, u_2'(0) = -2, u_2''(0) = 4,$$

$$u_3(0) = 1, u_3'(0) = -3, u_3''(0) = 9, x \in [0, 1]$$

whose analytic solution is $u_1(x) = e^{-x}, u_2(x) = e^{-2x}$, $u_3(x) = e^{-3x}$.

Source: Fawzi et al. [22].

Problem 5 Consider linear homogeneous system

$$u_1''' = u_2'', \quad u_2''' = u_3'', \quad u_2''' = u_1'',$$

$$u_1(0) = 1, u_1'(0) = 1, u_1''(0) = 1,$$

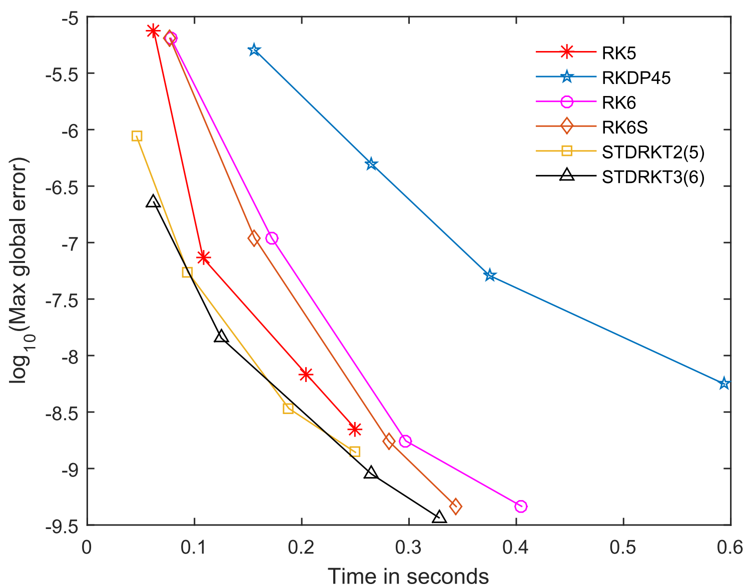


Fig. 2 Maximum global error versus time of computation curves for Problem 1.

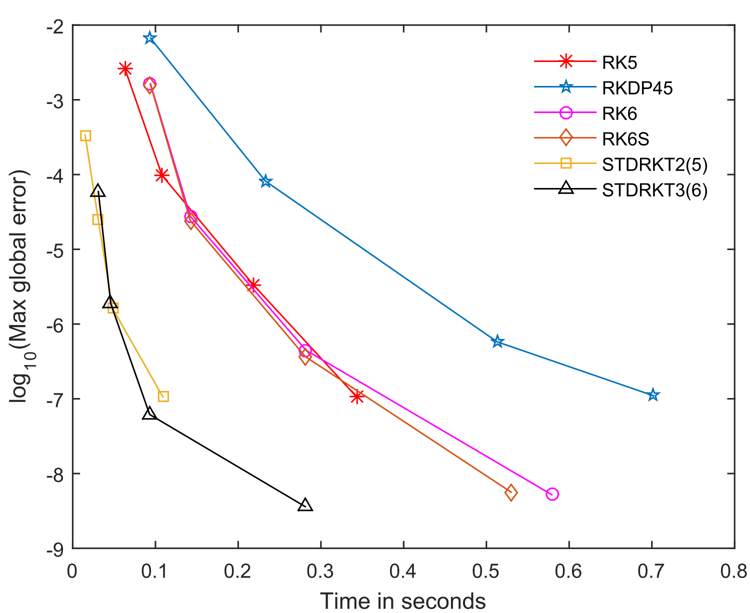


Fig. 3 Maximum global error versus time of computation curves for Problem 2.

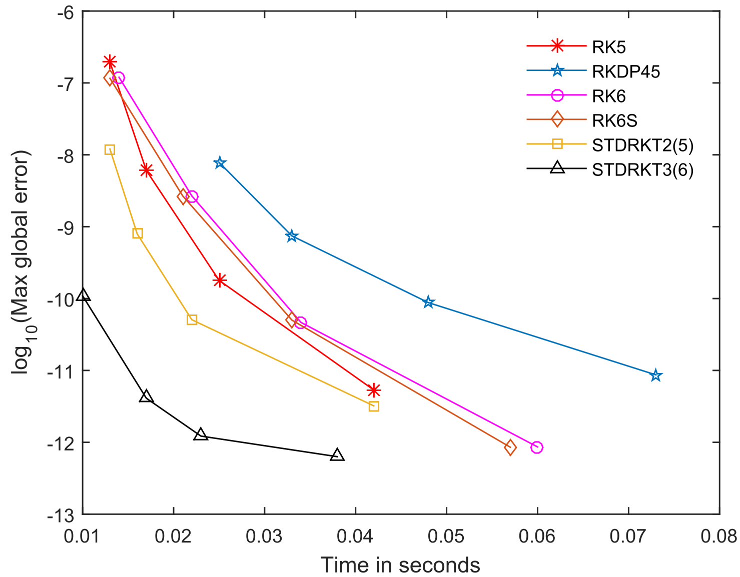


Fig. 4 Maximum global error versus time of computation curves for Problem 3.

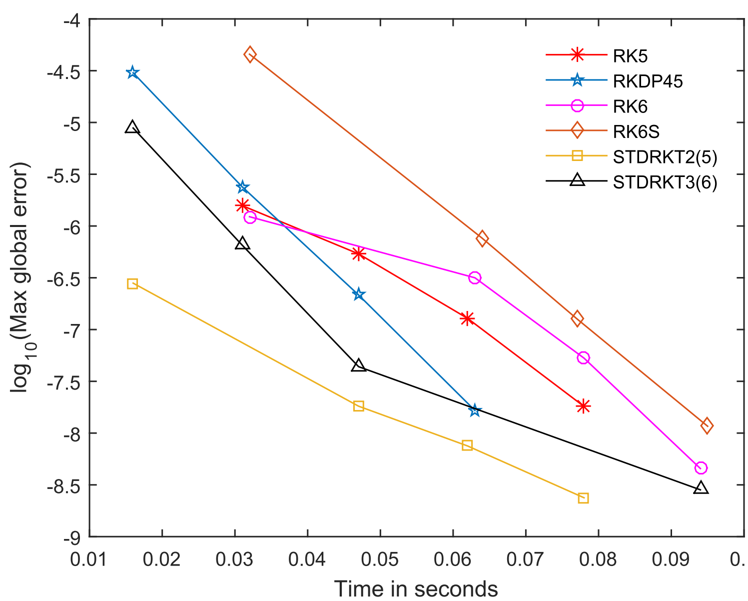


Fig. 5 Maximum global error versus time of computation curves for Problem 4.

$$u_2(0) = 1, u_2'(0) = 2, u_2''(0) = 4,$$

$$u_3(0) = 1, u_3'(0) = 3, u_3''(0) = 9, x \in [0, 1]$$

whose analytic solutions are follow:

$$u_1(x) = -3 - 8x + \frac{14}{3}e^x + \frac{8}{3}e^{-\frac{1}{2}}\sin\left(\frac{\sqrt{3x}}{2}\right) - \frac{2}{3}e^{-\frac{x}{2}}\cos\left(\frac{\sqrt{3x}}{2}\right),$$

$$u_2(x) = -8 + \frac{14}{3}e^x - \sqrt{3e^{-\frac{x}{2}}}\sin\left(\frac{\sqrt{3x}}{2}\right) + \frac{13}{3}e^{-\frac{x}{2}}\cos\left(\frac{\sqrt{3x}}{2}\right) + x,$$

$$u_3(x) = \frac{14}{3}e^x - \frac{5}{3}\sqrt{3e^{-\frac{x}{2}}}\sin\left(\frac{\sqrt{3x}}{2}\right) - \frac{11}{3}e^{-\frac{x}{2}}\cos\left(\frac{\sqrt{3x}}{2}\right) - x.$$

Problem 6 Consider the nonlinear, homogeneous and dynamic chaotic system, Genesio equation. (see Yap [6])

$$u''' + Au'' + Bu' - f(u(t)) = 0,$$

where

$$f(u(t)) = -Cu(t) + (u(t))^2,$$

with A, B and C are constants and contingent on the following initial conditions:

$$u(0) = 0.2, \quad u'(0) = -0.3, \quad u''(0) = 0.1$$

Genesio equation is used widely as jerk equation that exhibit various features of the regular and chaotic motion. (see Umut [5]) The problem is integrated on the interval $[0, 5]$ with positive constants, $A = 1.2, B = 2.92$ and $C = 6$ that satisfy

$AB < C$ for the existence of solution.There is no exact solution of of this problem, and hence, the numerical approximations obtained from selected methods compare with the numerical approximations obtained by Runge Kutta order 4 method with $h = 0.001$.

Problem 7 Consider the nonlinear nonhomogeneous system of thin film flow equations of liquids. In fluid dyamics, this system can be used to represent the motion of the fluid on plane surface and dynamic balance between surface tension and viscous forces in the fluid layer with the absence of gravity. (see Tuck [23])Thin film flow equation can be generalised into

$$u''' = f(u), \tag{5.56}$$

where

$$\begin{aligned} f(u) &= -1 + u^{-2}, \\ f(u) &= -1 + \left(1 + \delta + \delta^2\right)u^{-2} - \left(\delta + \delta^2\right)u^{-3}, \\ f(u) &= u^{-2} - u^{-3}, \\ f(u) &= u^{-2}. \end{aligned} \tag{5.57}$$

In this study, we consider nondimensionalised equation of thin film flow equations, written as follow:

$$u''' = u^{-2}. \tag{5.58}$$

The problem is integrated on the interval $[0, 5]$ with the initial conditions $u(0) = u'(0) = u''(0) = 1$. There is no analytical solution for Eq. (5.58). Numerical approximations obtained

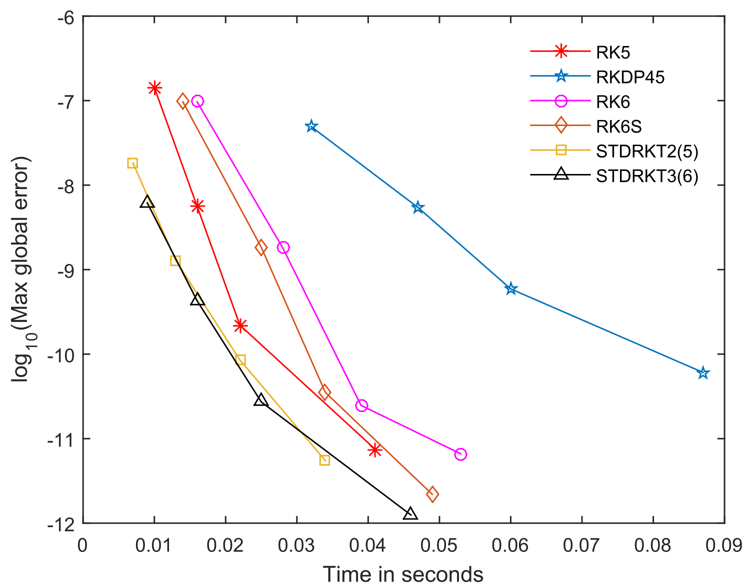


Fig. 6 Maximum global error versus time of computation curves for Problem 5.

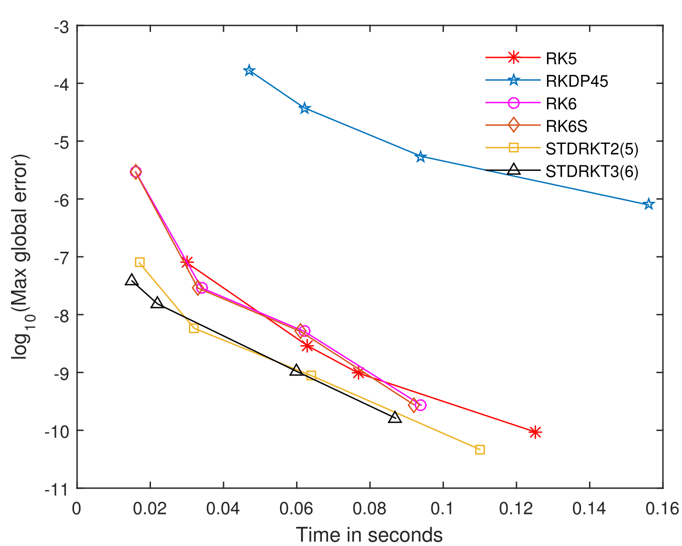


Fig. 7 Maximum global error versus time of computation curves for Problem 6.

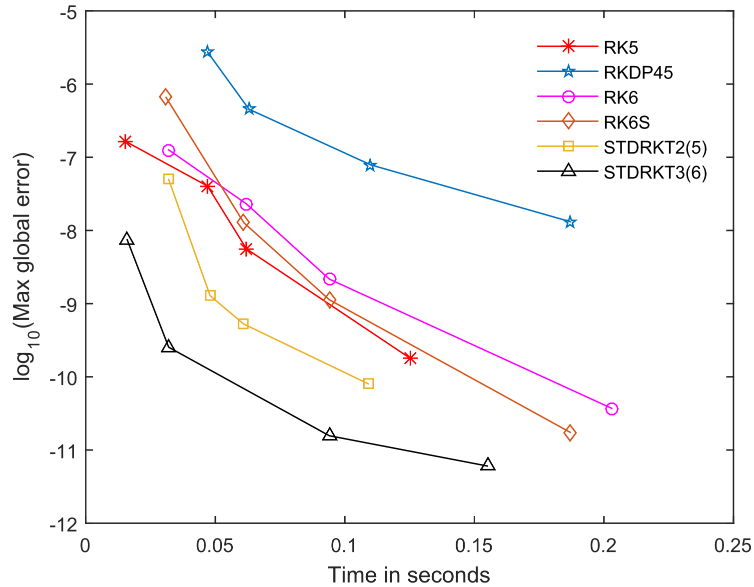


Fig. 8 Maximum global error versus time of computation curves for Problem 7.

from selected methods compared with the numerical approximations obtained by Runge-Kutta order 4 method with $h = 0.0001$. The illustration of thin films flow of viscous fluid with a free surface with Eq. (5.58) are shown below:

6. Numerical results

Figures below show the numerical results of selected methods in term of maximum global truncation error versus cost of computation measured using time. The model of computer used in computing the numerical results is Lenovo G50-70 Intel Core i3-4030U (1.9 GHz).

7. Conclusions

In summary, the special class of explicit two-derivative Runge-Kutta type methods that comprises one f-evaluation and multiple g-evaluations for solving third order ODEs with initial value conditions provided were derived. Many researchers have proposed improved Kutta methods with definitions and algebraic theories of rooted trees and B-series theory depending on the theories and concepts presented by Butcher ([24–26]) and Chen et al. ([9]) to solve first-order and second-order ODEs (see [11,27]).

In this work, essential aspects of B-series, comprised of integer function, fundamental differential, real function, density and elementary weights are derived and formulated to construct B-series specifically for STDRKT methods depending on algebraic order conditions in the form of $u^{(4)} = g(x, u, u', u'')$ to solve general third order ODEs directly. In this paper, we developed two-stages of order five and three-stages of order six, denoted as STDRKT2(5) and STDRKT3 (6) methods respectively. STDRKT methods are proved as efficient direct methods with the properties of zero stability, consistency and convergence. (see Fig. 1).

The numerical results are sketched in Figs. 2–8*** and these figures display the proficiency curves in which the new proposed methods, STDRKT2(5) and STDRKT3(6) are compared with RK5, DOPRI45, RK6 and RK6S in term of maximum global truncation error and computational cost in term of time using the same computational machine. STDRKT2(5) method is more efficient than RK5 and DOPRI45 while STDRKT3(6) method is more efficient compared to RK6 and RK6S methods in solving numerical linear problems in Figs. 2 and 3. Next, STDRKT2(5) method outperforms RK5, DOPRI45 and similar to STDRKT3(6) method surpasses RK6 and RK6S in solving both nonlinear homogeneous system and linear homogeneous system with analytical solutions provided as shown in Figs. 4 and 6. In Figs. 7 and 8, we notice that STDRKT2(5) method is more potent compared to RK5 and DOPRI5 methods and on the other hand, STDRKT3(6) method is shown better than RK6 and RK6S in solving application problems with no analytical solution and the numerical approximations are compared to RK4 methods with $h = 0.001$.

From the figures above, it is evident that these new Runge-Kutta methods are more proficient than traditional Runge-Kutta methods in term of maximum global error versus time of computation. STDRKT methods with same amount of stages acquired higher accuracy rate due to their ability to reach higher algebraic order compared to traditional Runge-Kutta methods with the inclusion of higher derivative, g-evaluations. Numerical results showed that STDRKT methods are well performed methods generating less maximum global truncation error while requiring less cost of evaluations compared to existing Runge-Kutta methods.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

The authors declare that there is no partiality of interest related to the publication of this paper. This research work was financially supported by Malaysia Ministry of Education under FRGS grant (No.: FRGS/1/2018/STG06/UPM/02/2) and Universiti Putra Malaysia.

References

[1] C. Chun, T. Kim, Several new third-order iterative methods for solving nonlinear equations, Acta Appl. Math. (2010) 1053–1063.
[2] J.R. Sharma, R. Sharma, Some third order methods for solving system of nonlinear equations, J. Math. Comput. Sci. 5 (2011) 1865–1871.
[3] A.A. Omar, A. Zaer, A. Ramzi, M. Shaher, A reliable analytical method for solving higher-order initial value problems, Discrete Dyn. Nat. Soc. 2013, Article ID 673829, 12p..
[4] S. Mehrkanoon, A direct variable step block multistep method for solving general third-order ODEs, Numer. Algorithms 57 (2011) 53–66.
[5] O. Umut, S. Yasar, A simple jerky dynamics, genesio system, Int. J. Mod. Nonlinear Theory Appl. 2 (2013) 66–68.
[6] L.K. Yap, F. Ismail, N. Senu, An accurate block hybrid collocation method for third order ordinary differential equations, J. Appl. Math. 2014, Article ID 673829, 12p..
[7] X. You, Z.X. Chen, Direct integrators of Runge-Kutta type for special third-order ordinary differential equations, Appl. Numer. Math. 74 (2013) 128–150.
[8] Y.L. Fang, X. You, Q.H. Ming, Trigonometrically fitted two-derivative Runge-Kutta methods for solving oscillatory differential equations, Numer. Algorithms 63 (2014) 651–667.
[9] Z. Chen, Z. Qiu, J. Li, X. You, Two-derivative Runge-Kutta-Nyström methods for second-order ordinary differential equations, Numer. Algorithms 70 (2015) 897–927.
[10] J.O. Ehigie, M.M. Zou, X.L. Hou, X. You, On modified TDRKN methods for second-order systems of differential equations, Int. J. Comput. Math. 95 (2017) 1–15.
[11] T.S. Mohamed, N. Senu, Z.B. Ibrahim, N.M.A. Nik Long, Efficient two-derivative Runge-Kutta-Nyström for solving general second-order ordinary differential equations, Discrete Dyn. Nat. Soc., 2018, Article ID 2393015, 10p..
[12] E. Hairer, C. Lubich, G. Wanner (Eds.), Geometry Numerical Integration, Structure Preserving Algorithms for Ordinary Differential Equations, vol. 31, Springer, Berlin, 2006.
[13] P. Henrici, Discrete Variable Methods in Ordinary Differential Equations, John Wiley & Sons, New York, 1962.
[14] E. Suli, D.F. Mayers, An Introduction to Numerical Analysis, Cambridge University Press, Cambridge, United Kingdom, 2003.
[15] K. Atkinson, W.M. Han, D. Stewart, Numerical Solution of Ordinary Differential Qquations: Convergence, Stability and Symptotic Error, John Wiley & Sons, New Jersey, 2009.
[16] J.D. Lambert, Numerical Methods for Ordinary Differential Systems: the Initial Value Problem, John Wiley & Sons, New Jersey, 2009.
[17] D. Goeken, O. Johnson, Fifth-order Runge-Kutta with higher order derivation approximations, Electron. J. Differ. Equ. 95 (1999) 1–9.
[18] J.R. Dormand, P.J. Prince, A family of embedded Runge-Kutta formulae, J. Comput. Appl. Math. 6 (1980) 19–26.
[19] M. Hatun, Differential equation solver simulator for Runge-Kutta methods, J. Faculty Eng. 21 (2016), https://doi.org/10.17482/uujfe.70981.
[20] A.F.A. Al-Shimmary, Solving initial value problem using Runge-Kutta 6-th order method, ARPN J. Eng. Appl. Sci. 12 (2017) 3953–3961.
[21] M. Mechee, N. Senu, F. Ismail, B. Nikouravan, Z. Siri, Three-stage fifth-order Runge-Kutta method for directly solving special third-order differential equation with application to thin film flow problem, Math. Probl. Eng. 2013, Article ID 795397, 7p..
[22] F.A. Fawzi, N. Senu, F. Ismail, Z.A. Majid, An efficient of integrator of Runge-Kutta type method for solving $y''' = f(x, y, y')$ with application to thin film flow problem, Int. J. Pure Appl. Math. 120 (2018) 27–50.
[23] E.O. Tuck, L.W. Schwartz, A numerical and asymptotic study of some third-order ordinary differential equatios relevant to draining and coating flows, SIAM Rev. 32 (1990) 453–469.
[24] J.C. Butcher, Numerical methods for ordinary differential methods in the 20th century, J. Comput. Appl. Math. 125 (2000) 1–29.
[25] J.C. Butcher, Numerical Methods for Ordinary Differential Equations, John Wiley & Sons, Chichester, 2008.
[26] J.C. Butcher, Trees, stumps, and applications, Axioms 7 (2018), https://doi.org/10.3390/Axioms 7030052.
[27] N. Ghawadri, N. Senu, F. Ismail, F.A. Fawzi, Z.B. Ibrahim, Explicit integrator of Runge-Kutta type for direct solution of $u^4 = f(x, u, u', u'')$, Symmetry 11 (2019), https://doi.org/10.3390/1102024.