algorithms

Communication

Construction of Two-Derivative Runge–Kutta Methods of Order Six

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Abstract: Two-Derivative Runge–Kutta methods have been proposed by Chan and Tsai in 2010 and order conditions up to the fifth order are given. In this work, for the first time, we derive order conditions for order six. Simplifying assumptions that reduce the number of order conditions are also given. The procedure for constructing sixth-order methods is presented. A specific method is derived in order to illustrate the procedure; this method is of the sixth algebraic order with a reduced phase-lag and amplification error. For numerical comparison, five well-known test problems have been solved using a seventh-order Two-Derivative Runge–Kutta method developed by Chan and Tsai and several Runge–Kutta methods of orders 6 and 8. Diagrams of the maximum absolute error vs. computation time show the efficiency of the new method.

Keywords: numerical integration; two-derivative Runge–Kutta methods; phase-lag error; amplification error; order conditions

MSC: 65L05; 65L06

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1. Introduction

We consider systems of first-order ODEs of the form

$$y'(x) = f(x, y(x)), \quad x \in [x_0, X], \quad y(x_0) = y_0. \tag{1}$$

These problems can be solved efficiently using Runge–Kutta (RK) or multi-step methods. Numerical methods of a high algebraic order are efficient integrators. The computational cost increases with the order, for example, for the RK methods, it is well known that seven, nine, and eleven stages are needed for orders six, seven, and eight, respectively. To reduce the computational cost, research has been devoted to methods with special properties suitable for specific problems. Special methods for the integration of problems with oscillatory behavior of the solution have been considered by several authors from the early stages of research on ODE solvers. There are two general classes of numerical methods for the integration of oscillatory problems. One class consists of methods with frequency-dependent coefficients, while the other includes constant coefficients. In the first class are exponentially, trigonometrically, or phase-fitted methods (see [1–3]); for these methods, a good estimate of the frequency of the specific problem is needed. The advantage of these methods in the second general class is that they can be applied to every oscillatory problem since the coefficients are constant. Among these are methods with low dissipation and low dispersion, (see [4–6]). The dispersion (or phase-lag) property was introduced in the pioneer paper of Brusa and Nigro [7].

In this work, we consider Two-Derivative RK methods with special properties and constant coefficients. These methods originate in the work of Kastlunger and Wanner [8,9], of which they introduced methods where the values of the derivatives of $f(x, y(x))$, with respect to x, as well as the values of the function $f(x,y)$ at some intermediate points, are used. Chan and Tsai [10] considered the case where only the first derivative of $f(x,y(x))$, with respect to x ($g(x,y(x)) := y'' = f' f$), as well as the function $f(x,y)$ are evaluated at each step of the method. They call these methods Two-Derivative Runge–Kutta (TDRK) methods. The TDRK method are of the form

$$\begin{aligned} Y_i &= y_n + h\sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j) + h^2 \sum_{j=1}^{s} \hat{a}_{ij} g(x_n + c_j h, Y_j) \\ y_{n+1} &= y_n + h\sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i) + h^2 \sum_{i=1}^{s} \hat{b}_i g(x_n + c_i h, Y_i) \end{aligned}$$

the associated Butcher tableau is

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

where A and $\hat{A}$ are $s \times s$ matrices, and b and $\hat{b}$, c are $s \times 1$ vectors. Chan and Tsai derived order conditions for the TDRK methods based on Butcher's algebraic theory of trees [11] in a different way than the conditions were derived in [8,9]. They considered explicit TDRK methods and gave algebraic order conditions up to order five.

Specifically in [10], the special class of explicit TDRK (ETDRK) methods was introduced, where only the first derivative of $f(x,y(x))$, with respect to x, is evaluated at intermediate points at each step. In this case, the matrix A has non-zero elements only in the first column i.e., the function f is evaluated only at x_n; these methods are called special ETDRK methods. We shall refer to methods where non-zero entries are allowed into the matrix A at any column as general ETDRK methods. In [10], conditions are given up to order seven for special ETDRK methods. Since then, research has focused on special ETDRK methods only, where several authors have constructed minimum phase-lag, trigonometrically fitted, phase-fitted methods (see [12–14]).

The authors were the first to consider the general case; in [15], they presented methods of an algebraic order up to five, and in [14], they derived order conditions for trigonometrically fitted methods. As mentioned above, algebraic order conditions for the general ETDRK methods up to order five were given. In this work, we consider general ETDRK methods and algebraic order conditions and, following the ideas of [10], derive the algebraic order conditions for order six. Conditions generalizing the simplifying assumptions given by Fehlberg in [16] are also derived, which leads to a significant reduction in the number of order conditions. The theory is illustrated with the construction of a sixth-order general ETDRK method. The paper is organized as follows. Section 2 is of an introductory nature, where we review the TDRK methods. In Section 3, we consider methods of order six, derive algebraic conditions and simplifying assumptions, and the framework for constructing sixth-order methods is given. In order to illustrate the procedure, we construct a method of the sixth algebraic order with a reduced phase-lag and amplification error. In Section 4, we present numerical results using five well-known test problems. A discussion of the results is given in Section 5.

2. TDRK Methods

2.1. Algebraic Order Conditions

We shall give a brief summary of the derivation of the order conditions in [10]. A method is of order p if $\alpha(t) = 1/\gamma(t)$ for all trees of an order that is less or equal to p, where $\alpha(t)$ is the elementary weight. The elementary weights $\alpha(t)$ are defined in terms of the vector of the elementary weight functions for the internal stages

$$\alpha(t) = b^T \eta(t \backslash \bullet) + \hat{b}^T \eta(\, t \backslash :\,)$$

for $r(t) > 1$ and $\alpha(\bullet) = b^T e$. The elementary weight vector is determined by the recursive formula

$$\eta(t) = A\eta(t\backslash \bullet) + \hat{A}\eta(t\backslash \overset{\bullet}{\bullet})$$

for $r(t) > 1$ and $\eta(\bullet) = c$, $\eta(\emptyset) = e$. The elementary weight vectors for trees up to order 4 and the elementary weights up to order 5 are also given in [10]. As in the case of Runge–Kutta methods, simplifying assumptions can be used

$$A\,c^{k-1} + (k-1)\hat{A}\,c^{k-2} \;=\; \frac{c^k}{k}, \quad k = 1, 2, \ldots, q.$$

We note here that the assumption corresponding to ($k = 2$) for the RK methods $A\,c = c^2/2$ cannot be satisfied for explicit methods.

The authors in [15] presented a fifth-order method with four stages. They used the first two simplifying assumptions ($k = 1$ and $k = 2$):

$$A\,e = c, \qquad A\,c + \hat{A}\,e = \frac{c^2}{2} \tag{2}$$

It is obvious that the quadrature conditions

$$b^T c^{k-1} + (k-1)\hat{b}^T c^{k-2} e \;=\; \frac{1}{k}, \quad k = 1, \ldots, 5 \tag{3}$$

are not affected. Under the second assumption, the conditions corresponding to trees

$$[[\tau], t_2, t_3, \ldots, t_m] \quad \text{and} \quad [\tau, \tau, t_2, t_3, \ldots, t_m]$$

are equivalent; consequently, we can disregard some order conditions. For order 3, there are three conditions; the extra conditions for order 4 are two; and four more conditions are needed for order 5. In [15], apart from quadrature conditions (3), the additional condition for order 4 is

$$b^T A\,c^2 + 2b^T \hat{A}\,c + \hat{b}^T c^2 = \frac{1}{12} \tag{4}$$

and the additional conditions for order 5 are

$$b^T c\,A\,c^2 + 2b^T c\,\hat{A}\,c + \hat{b}^T c^3 + \hat{b}^T A\,c^2 + 2\hat{b}^T \hat{A}\,c = \frac{1}{15} \tag{5}$$

$$b^T A\,c^3 + 3b^T \hat{A}\,c^2 + \hat{b}^T c^3 = \frac{1}{20} \tag{6}$$

$$b^T A^2 c^2 + 2b^T A\,\hat{A}\,c + b^T \hat{A}\,c^2 + \hat{b}^T A\,c^2 + 2\hat{b}^T \hat{A}\,c = \frac{1}{60}. \tag{7}$$

2.2. Stability, Dispersion, and Dissipation

The stability function of a TDRK method is

$$R(z) = 1 + zb^T\left(I - zA - z^2\hat{A}\right)^{-1} e + z^2\hat{b}^T\left(I - zA - z^2\hat{A}\right)^{-1} e.$$

Van der Houwen and Sommeijer [17] give the definition of dispersion (or phase-lag) error $\phi(v)$

$$\phi(v) = v - \arg R(iv)$$

and the dissipation (or amplification) error $\alpha(v)$

$$\alpha(v) = 1 - \mid R(iv) \mid$$

where $v = wh$. A TDRK method is said to have a dispersion order p and dissipative order q if

$$\phi(v) = c_\phi v^{p+1} + O(v^{p+3}) \quad \text{and} \quad \alpha(v) = c_\alpha v^{q+1} + O(v^{q+3})$$

For explicit TDRK methods, we can write

$$R(iv) = A_s(v^2) + ivB_s(v^2),$$

where A_s and B_s are polynomials in v^2 of degree s. It follows that

$$\phi(v) = v - \arctan\left(v\frac{B_s(v^2)}{A_s(v^2)}\right) \quad \text{and} \quad \alpha(v) = 1 - \sqrt{A_s^2(v^2) + v^2B_s^2(v^2)}.$$

3. Sixth-Order Methods

Here we present the conditions of order six. There are 20 trees of order 6. By applying the first and second simplifying assumptions (2), the number of order conditions reduces to eight, of which these conditions are given in Table 1. The elementary weight vectors for trees of order 5 are given in Table 2.

To further reduce the number of order conditions, we shall use the third simplifying assumption

$$A\,c^2 + \hat{A}\,c = \frac{c^3}{3} \tag{8}$$

together with

$$b_2 = \hat{b}_2 = 0$$

This assumption cannot be fulfilled for explicit methods, since we can ask for this assumption except for the second component. Condition (8) and $b_2 = \hat{b}_2 = 0$ have the effect that the conditions corresponding to the trees

$$[[\tau,\tau], t_2, t_3, \ldots, t_m] \quad \text{and} \quad [\tau,\tau,\tau, t_2, t_3, \ldots, t_m]$$

are equivalent. This allows us to disregard condition (4) of order 4, condition (5) of order 5, and the condition corresponding to tree t_{62}. The number of order conditions reduces to 3, 4, and 7 for orders 3, 4, and 5 respectively.

Following the idea of Fehlberg [16], we impose the following conditions

$$\sum_{i=3}^{s} b_i a_{i2} = 0, \quad \sum_{i=3}^{s} b_i a_{i2} c_i = 0, \quad \sum_{i=4}^{s}\sum_{j=3}^{s-1} b_i a_{ij} a_{j2} = 0, \tag{9}$$

as well as

$$\sum_{i=3}^{s} \hat{b}_i a_{i2} = 0, \qquad \sum_{i=3}^{s} b_i \hat{a}_{i2} = 0. \tag{10}$$

Then

- from the first of (9), the conditions corresponding to t_{53} and t_{54} are equivalent,
- from the second of (9) and the first of (10), the conditions corresponding to t_{63} and t_{64} are equivalent,
- from the first of (9) and the second of (10), the conditions corresponding to t_{65} and t_{66} are equivalent,
- from the third of (9), the conditions corresponding to t_{67} and t_{68} are equivalent.

Finally, the number of order conditions reduces to 6 and 10 for orders 5 and 6, respectively, i.e., the quadrature conditions and

$$b^T A\, c^3 + 3b^T \hat{A}\, c^2 + \hat{b}\, c^3 = \frac{1}{20} \tag{11}$$

$$b^T c\left(A\, c^3 + 3\hat{A}\, c^2\right) + \hat{b}^T\left(A\, c^3 + 3\hat{A}\, c^2 + c^4\right) = \frac{1}{24} \tag{12}$$

$$b^T\left(A\, c^4 + 4\,\hat{A}\, c^3\right) + \hat{b}^T c^4 = \frac{1}{30} \tag{13}$$

$$b^T\left(A\,(A\, c^3 + 3\hat{A}\, c^2) + \hat{A}\, c^3\right) + \hat{b}(A\, c^3 + 3\hat{A}\, c^2) = \frac{1}{120} \tag{14}$$

A sixth-order method can be constructed following the next steps (Algorithm 1).

Table 1. Trees of order 6 and conditions.

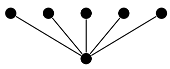
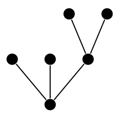
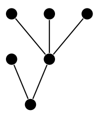
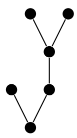
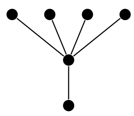
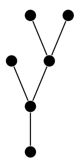
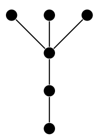
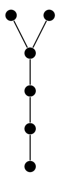
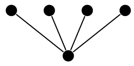
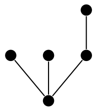
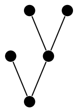
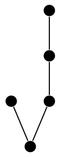
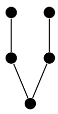
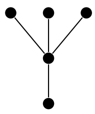
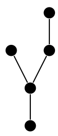
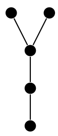
Tree		**Order Condition**
t_{61}		$b^T c^5 + 5\hat{b}^T c^4 = \frac{1}{6}$
t_{62}		$b^T c^2\, \eta(t_{31}) + 2\hat{b}^T c\, \eta(t_{31}) + \hat{b}^T c^4 = \frac{1}{18}$
t_{63}		$b^T c\, \eta(t_{41}) + \hat{b}^T \eta(t_{41}) + \hat{b}^T c^4 = \frac{1}{24}$
t_{64}		$b^T c\, \eta(t_{43}) + \hat{b}^T \eta(t_{43}) + \hat{b}^T c\, \eta(t_{31}) = \frac{1}{72}$
t_{65}		$b^T \eta(t_{51}) + \hat{b}^T c^4 = \frac{1}{30}$
t_{66}		$b^T \eta(t_{53}) + \hat{b}\, c\, \eta(t_{31}) = \frac{1}{90}$
t_{67}		$b^T \eta(t_{56}) + \hat{b}\eta(t_{41}) = \frac{1}{120}$
t_{68}		$b^T \eta(t_{58}) + \hat{b}^T \eta(t_{43}) = \frac{1}{360}$

Table 2. Elementary weight vectors of order 5.

Tree (t)		**Elementary Weight Vector $\eta(t)$**
t_{51}		$A\,c^4 + 4\,\hat{A}\,c^3$
t_{52}		$A\,c^2\,A\,c + A\,c^2\,\hat{c} + 2\,\hat{A}\,c\,A\,c + 2\,\hat{A}\,c\,\hat{c} + \hat{A}\,c^3$
t_{53}		$A\,c\,A\,c^2 + 2\,A\,c\,\hat{A}\,c + \hat{A}\,A\,c^2 + 2\,\hat{A}^2\,c + \hat{A}\,c^3$
t_{54}		$A\,c\,A^2\,c + A\,c\,A\,\hat{c} + A\,c\,\hat{A}\,c + \hat{A}\,A^2\,c + \hat{A}\,A\,\hat{c} +$ $\hat{A}^2\,c + \hat{A}\,c\,A\,c + \hat{A}\,c\,\hat{c}$
t_{55}		$A\,((A\,c + \hat{c}) * (A\,c + \hat{c})) + 2\,\hat{A}\,c\,A\,c + 2\,\hat{A}\,c\,\hat{c}$
t_{56}		$A^2\,c^3 + 3\,A\,\hat{A}\,c^2 + \hat{A}\,c^3$
t_{57}		$A^2\,c\,A\,c + A^2\,c\,\hat{c} + A\,\hat{A}\,A\,c + A\,\hat{A}\,\hat{c} + A\,\hat{A}\,c^2 + \hat{A}\,c\,A\,c + \hat{A}\,c\,\hat{c}$
t_{58}		$A^3\,c^2 + 2\,A^2\,\hat{A}\,c + A\,\hat{A}\,c^2 + \hat{A}\,A\,c^2 + 2\hat{A}^2\,c$
t_{59}		$A^4\,c + A^3\,\hat{c} + A^2\,\hat{A}\,c + A\,\hat{A}\,A\,c + A\,\hat{A}\,\hat{c} + \hat{A}\,A^2\,c + \hat{A}\,A\,\hat{c} + \hat{A}^2\,c$

Algorithm 1 Construction of sixth order explicit TDRK method.

1. $c_1 = 0$ and $c_5 = 1$
2. c_i for $i = 2, 3, 4$ can be chosen as free parameters
3. $b_2 = \hat{b}_2 = 0$
4. b_i and $\hat{b}_i$ from the linear system of Equation (3)
5. a_{21}, a_{31}, a_{43}, a_{54} from the first of (2)
6. $\hat{a}_{21}$, $\hat{a}_{32}$, $\hat{a}_{43}$, $\hat{a}_{54}$ from the second of (2)
7. $\hat{a}_{31}$, a_{41}, a_{51} from (8)
8. $\hat{a}_{42}$ from the second of (10)
9. $\hat{a}_{41}$, $\hat{a}_{51}$, $\hat{a}_{52}$, $\hat{a}_{53}$ from (11)–(14)
10. a_{32}, a_{42}, a_{52} from (9)

As an application, we shall demonstrate the construction of a specific method. Since the c_is are free parameters, we chose the equidistant grid $c_2 = \frac{1}{4}$, $c_3 = \frac{1}{2}$, $c_4 = \frac{3}{4}$. From the quadrature conditions (3), we derive

$$b_1 = \tfrac{1}{405}\left(101 - 345\,b_5 - 4440\,\hat{b}_5\right), \qquad b_3 = \frac{16}{15} - 12\,b_5 - 136\,\hat{b}_5,$$
$$b_4 = \tfrac{64}{405}\left(-2 + 75\,b_5 + 930\,\hat{b}_5\right), \qquad \hat{b}_1 = \frac{1}{54}\left(1 - 6\,b_5 + 78\,\hat{b}_5\right),$$
$$\hat{b}_3 = \tfrac{1}{15} - 2\,b_5 - 24\,\hat{b}_5, \qquad \hat{b}_4 = -\frac{16}{135}\left(-1 + 15\,b_5 + 150\,\hat{b}_5\right).$$

Assumptions (9) and the first of (10) are satisfied by setting $a_{32} = a_{42} = a_{52} = 0$. From the choice of c_i, we have $\hat{a}_{41} = \hat{a}_{43}$. Let $\hat{a}_{41} = 0$. From the second of (10)

$$\hat{a}_{42} = \frac{-9(4 - 45b_5 + 45\hat{a}_{52}b_5 - 510\hat{b}_5)}{64(-2 + 75b_5 + 930\hat{b}_5)}.$$

From (11)–(14)

$$\begin{aligned} \hat{a}_{51} &= \frac{1}{180b_5}\left(-8 + 5(26 + a_{53})b_5 + 1560\hat{b}_5\right) \\ \hat{a}_{52} &= -\frac{-2}{15b_5}\left(-1 + 20b_5 + 240\hat{b}_5\right) \\ \hat{a}_{53} &= \frac{1}{6 - b_5}\left(-8 + 15(8 + a_{53})b_5 + 1560\hat{b}_5\right). \end{aligned}$$

At this point, all order conditions are satisfied. Still, coefficients a_{53}, b_5 and $\hat{b}_5$ are not determined. We choose these coefficients so that the next two terms of the phase-lag error and one term of the amplification error are eliminated

$$a_{53} = \frac{1}{315b_5^2}\left(-2520b_5^2 + b_5(110 - 35{,}280\hat{b}_5) + 224(1 - 195\hat{b}_5)\hat{b}_5\right)$$

and

$$\hat{b}_5 = \frac{28{,}721 + 31\sqrt{723{,}121}}{642{,}600}, \quad b_5 = \frac{-1{,}396{,}559 - 1669\sqrt{723{,}121}}{3{,}901{,}500}$$

For this method, the stability function is

$$R(z) = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \frac{z^4}{4!} + \frac{z^5}{5!} + \frac{z^6}{6!} + \frac{z^7}{7!} + \frac{z^8}{8!} + \frac{z^9}{9!}$$

and the phase-lag and amplification errors are

$$\phi(v) = -\frac{1}{3{,}991{,}680}v^{11} + O(v^{13}) \quad \text{and} \quad \alpha(v) = -\frac{1}{3{,}628{,}800}v^{10} + O(v^{12})$$

In Figure 1, we have plotted the stability region both for this method (*new*) and for the seventh-order special TDRK method (*CT*) in [10].

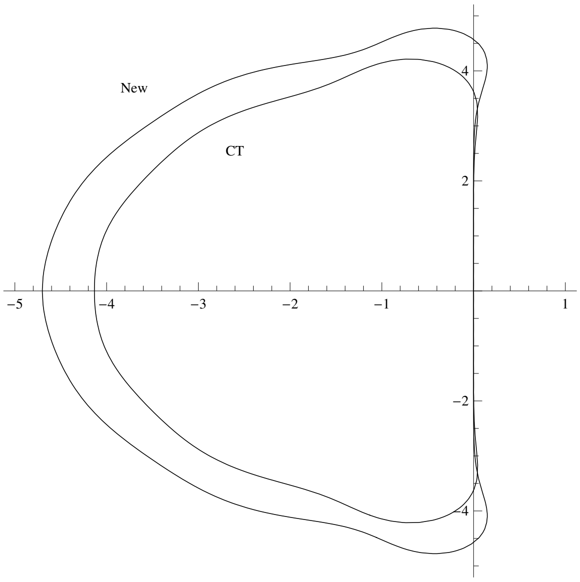


Figure 1. Stability regions for methods *new* and *CT*.

4. Numerical Results

In order to illustrate the efficiency of the new method, we have chosen several well-known RK methods of the sixth and eighth order with 7, 8, and 13 stages. Also, we compare the new method with a special TDRK method of the sixth order with five stages. The methods are:

- The method constructed in this work (*New*)
- Chan–Tsai's seventh-order method with five stages (*CT*) [10]
- Butcher's sixth-order method with seven stages (*Butcher*) [11]
- Dormand–Prince's eighth-order method with 13 stages (*DP*) [18]
- Fehlberg's eighth-order method with 13 stages (*Fehlberg*) [19]
- Verner's sixth-order method with eight stages (*Verner*) [20]

4.1. Problem 1

An inhomogeneous equation studied by van der Houwen and Sommeijer [17]

$$y'' = -\omega^2 y + (\omega^2 - 1)\sin(x), \quad y(0) = 1, \quad y'(0) = \omega + 1$$

where $x \geq 0$. The exact solution is $y(x) = \cos(\omega x) + \sin(\omega x) + \sin(x)$. We choose $\omega = 10$ and an integration interval $[0, 100]$. In Figure 2, we see the efficiency of the methods vs. CPU time for the inhomogeneous equation. Specifically for this problem, the maximum error of the solution is presented. As we can see, the method *New* requires 0.1 s in the order to give an accuracy of 10^{-4}, while at the same time, the other methods either have an accuracy of 10^{-2} or fail. Furthermore, in 0.4 s, the method *New* has a maximum absolute error less than 10^{-10}; meanwhile, at the same time, methods *CT* and *DP* give a maximum absolute error that is almost 10^{-7}. The rest of the methods need much more time to accomplish an accuracy of 10^{-6}.

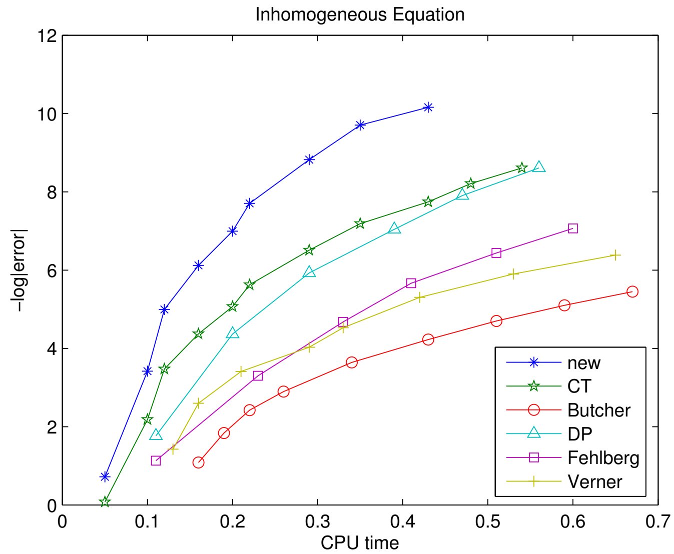


Figure 2. Problem 1: Efficiency curves.

4.2. Problem 2

We consider the oscillatory linear system studied by Franco in [21]

$$\begin{aligned} y_1'' + 13y_1 - 12y_2 &= 9\cos(2x) - 12\sin(2x), \quad y_1(0) = 1, \quad y_1'(0) = -4 \\ y_2'' - 12y_1 + 13y_2 &= -12\cos(2x) + 9\sin(2x), \quad y_2(0) = 0, \quad y_2'(0) = 8. \end{aligned}$$

The exact solution is

$$\begin{aligned} y_1(x) &= \sin(x) - \sin(5x) + \cos(2x), \\ y_2(x) &= \sin(x) + \sin(5x) + \sin(2x). \end{aligned}$$

In Figure 3, the maximum error of the solution is presented in the interval $[0, 100]$.

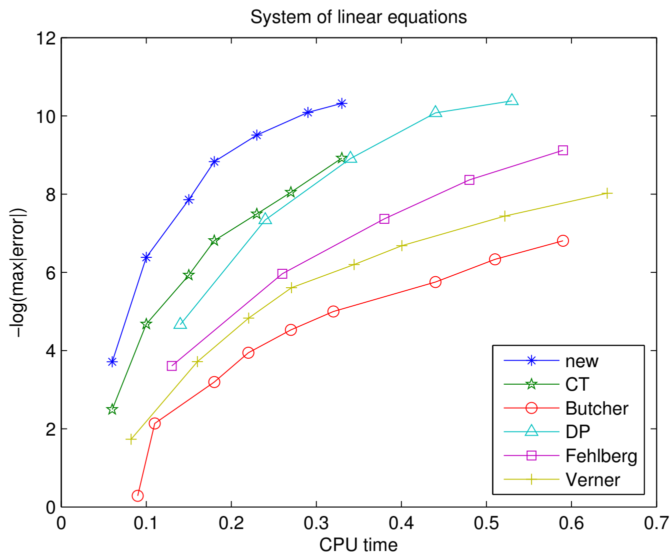


Figure 3. Problem 2: Efficiency curves.

We see the efficiency of the methods vs. CPU time for this system of linear equations. We see that the most efficient methods are *New* and *DP*, where the first requires 0.3 s in order to give a maximum absolute error less that 10^{-10}, while the second needs 0.5 s to reach the same accuracy.

4.3. Problem 3

We consider the following almost periodic orbit problem studied by Stiefel and Bettis [22]:

$$\begin{aligned} y_1'' &= -y_1 + 0.001\cos(x), \quad y_1(0) = 1, \quad y_1'(0) = 0 \\ y_2'' &= -y_2 + 0.001\sin(x), \quad y_2(0) = 0, \quad y_2'(0) = 0.9995 \end{aligned}$$

The exact solution is

$$y_1(x) = \cos(x) + 0.0005x\sin(x), \qquad y_2(x) = \sin(x) - 0.0005x\cos(x).$$

In Figure 4, the maximum error of the solution is presented $[0, 1000]$.

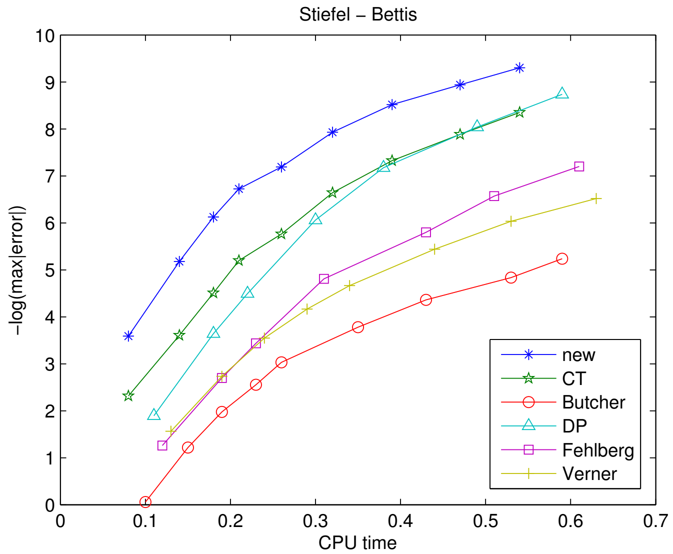


Figure 4. Problem 3: Efficiency curves.

We see the efficiency of the methods vs. CPU time for this problem and notice a similar performance with problem 2. Again, the TDRK methods and *DP* are the most efficient: for 0.54 s, methods *New* and *CT* give errors of 5 $\times 10^{-10}$ and 5 $\times 10^{-9}$, while *DP* gives an error of 2 $\times 10^{-9}$.

4.4. Problem 4

The Prothero–Robinson problem has been studied in [10].

$$y'(x) \quad = \quad k(y - \phi(x)) + \phi'(x), \quad y(0) = \phi(0),$$

where k is a negative parameter and $\phi(x)$ is a smooth function. The exact solution is $y(x) = \phi(x)$. In this work, we choose $\phi(x) = \sin x$. In Figure 5, the maximum error of the solution is presented in $[0, 100]$ for $k = -200$ when the problem is mildly stiff.

We see the efficiency of the methods vs. CPU time for this problem. The TDRK methods have a superior performance, where at time 0.5 s, methods *New* and *CT* give errors of 3 $\times 10^{-9}$ and 2 $\times 10^{-8}$. The classical RK methods fail to give as accurate results even in triple time, where more than 1.5 s are needed to give errors in the range 10^{-7} and 10^{-8}.

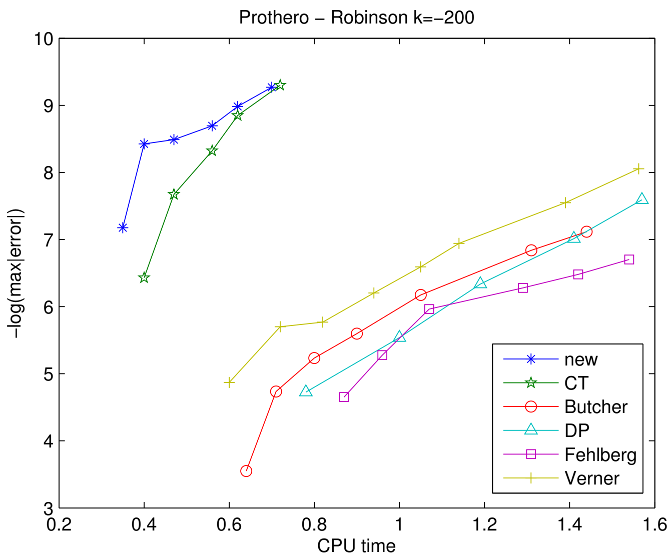


Figure 5. Problem 4: Efficiency curves.

4.5. Problem 5

We consider a Van der Pol oscillator

$$y'' = -y + \delta(1 - y^2)y', \quad y(0) = y_0, \quad y'(0) = 0$$

where $\delta > 0$

$$y_0 = 2 + \frac{1}{96}\delta^2 + \frac{1033}{552960}\delta^4 + \frac{1019689}{55738368000}\frac{1}{2}\delta^6.$$

For this problem, the integration interval considered is $[0, 100]$ for $\delta = 5$, when the problem is mildly stiff. In Figure 6, the maximum error of the solution is presented in $[0, 100]$.

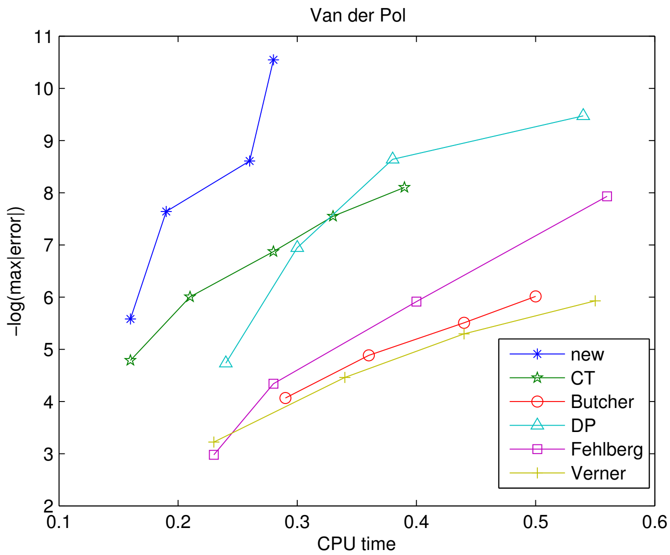


Figure 6. Problem 5: Efficiency curves.

We see the efficiency of the methods vs. CPU time for the Van der Pol oscillator. The TDRK methods and *DP* are the most efficient. The method derived in this study reaches an accuracy of 3×10^{-11} in 0.3 s, where methods *CT* and *DP* give errors of 10^{-7} at the same time.

4.6. Numerical Rate of Convergence

We shall examine the rate of convergence given by

$$p_N = \log_2\left(\frac{E_N}{E_{2N}}\right)$$

where E_N is the maximum absolute error

$$E_N = \max_{1 \le i \le N} \|y_i - y(x_i)\|.$$

We give p_N for several values of N for the Prothero–Robinson problem for $k = -10, -50, -100$.

$k = -10$	$N = 1000$	$N = 2000$	$N = 3000$	$N = 4000$
p_N	6.19	6.11	6.03	5.97
$k = -50$	$N = 3000$	$N = 4000$	$N = 5000$	$N = 6000$
p_N	6.21	6.21	6.19	6.16
$k = -100$	$N = 4000$	$N = 5000$	$N = 6000$	$N = 7000$
p_N	6.02	6.18	6.21	6.22

5. Discussion and Conclusions

In this work, for the first time, sixth-order conditions for an explicit TDRK method of the general case has been derived. Also, a new method with five stages of algebraic order 6, phase-lag order 10, and amplification order 9 has been constructed. In order to demonstrate the efficiency of the new method, we have chosen four well-known RK methods of order 6 and 8 with 7, 8, and 13 stages (Butcher, Verner, Dormand–Prince, and Fehlberg) and a special two-derivative Runge–Kutta method of order 6 with five stages. Generally, the new method performs better than all RK methods tested, including the special TDRK method. The plot of the maximum absolute error with the CPU time are given for all problems studied. For Problem 1 of CPU time less than 0.4 s, the new method gives an error less than 10^{-10}, whereas *CT* and *DP* give errors less than 10^{-8} in 0.5 s and the other methods reach an error of 10^{-6} in 0.6 s. Similar results are produced for Problems 2 and 3. Then, we have used two stiff problems to test the efficiency of the method derived in this work concerning the famous Prothero–Robinson problem ($k = -200$) and the Van der Pol oscillator ($\delta = 5$). For the first stiff problem (Problem 4), the TDRK methods have a superior performance compared to the RK methods. The TDRK methods give an error less than 10^{-9} in 0.6 s, while the RK methods need 1.6 s to give an error of 10^{-8}. For the second stiff problem (Problem 5), the new method clearly has a superior performance of 10^{-11} in 0.3 s, while methods *CT* and *DP* give errors of 10^{-7} at the same time.

The advantage of the TDRK methods is that the number of stages needed for a specific order is much fewer than those for the RK methods. Method *CT* in [10] has order 7 and five stages, and the method constructed in this study has order 6 and five stages. Concerning sixth-order methods *Butcher* and *Verner* use seven and eight stages, respectively, while the eighth-order methods *DP* and *Fehlberg* use 13 stages.

In this work, we have given the framework of constructing methods of the general type of order 6. In order to illustrate the construction of such methods, we give an example with a reduced phase-lag and amplification error. Certainly, methods can be derived with other characteristics. In future work, we will focus on TDRK methods of the general type and construct embedded methods to be used for variable step size. Also, we shall consider symmetric methods and methods with frequency-dependent coefficients.

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