Fifth Order Two Derivative Runge-Kutta Method with Reduced Function Evaluations for Solving IVPs

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Abstract: In this paper, the First Same As Last (FSAL) technique is implemented to Two Derivative Runge-Kutta method (TDRK) for the numerical integration of first order Initial Value Problems (IVPs). Using the FSAL property, a four stages fifth algebraic order TDRK method is constructed. Hence, the new method has three effective stages meaning that it has three function evaluations per step. It has two stages less compared with the classical Runge-Kutta for the same order. The stability of the method derived is analyzed. The numerical experiments are carried out to show the accuracy and efficiency of the method by comparing the derived method with other existing Runge-Kutta methods (RK).

Key–Words: TDRK method, FSAL technique, IVPs, Explicit methods

1 Introduction

Consider the numerical solution of the Initial Value Problems (IVPs) for the first order Ordinary Differential Equations (ODEs) given in the following form

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

A numerous number of researchers have proposed several efficient TDRK methods with constant step-size as well as implementing the FSAL technique in the derivation of their methods. In the evolution of TDRK methods, Chan and Tsai[1] introduced special explicit TDRK methods by including the second derivative which involves one evaluation of f and a few evaluations of g per step with stages up to five and of order up to seven as well as some embedded pairs. Chan et al.[2] then presented their study related to stiff ODEs problems on explicit and implicit TDRK methods and extend the applications of the TDRK methods to various Partial Differential Equations (PDEs).

Zhang et al.[3] developed a new Trigonometrically Fitted TDRK method of algebraic order five, analyze the linear stability and phase properties of the new method. Chen et al.[4] constructed three practical exponentially fitted TDRK (EFTDRK) methods where the numerical experiments show the efficiency and accuracy of the developed methods compared to their prototype TDRK methods or RK methods of the same order and the traditional exponentially fitted RK method in the literature. In the previous year, Yakubu and Kwami[5] introduced a new class of implicit TDRK collocation methods especially for the numerical solution of systems of equations and their implementation in an efficient parallel computing environment.

By implementing FSAL technique, Dormand and Prince[6] derived a family of embedded RK formulae RK5(4) with an extended region of absolute stability and a “small” principal truncation terms in the fifth order formulae. Franco[7] designed an explicit Exponentially Fitted Runge-Kutta Nyström method (EFRKN) with two and three stages and algebraic order three and four as well as a 4(3) embedded pair based on the FSAL technique for the numerical integration of second order IVPs with oscillatory solutions.

Fang et al. in [8] and [9] proposed extended RKN method with fixed step-size and embedded pairs for numerical integration of perturbed oscillators and higher order RK (pair) method of order five and four as well as new fifth order RK method specially adapted to the numerical integration of IVPs with oscillatory solutions respectively. Meanwhile, Van de Vyver[10] constructed a new way for constructing efficient embedded modified RK methods based on the FSAL technique which has algebraic order four and five for the numerical solution of the Schrödinger equation.

The main objective of the paper is that we want to reduce the number function evaluations per step.

Hence, in this paper, a fifth order four stages TDRK method with FSAL property is constructed. The advantage of the TDRK method is that it has one less number of stage than the classical RK method for the same order of the method. Furthermore by using FSAL technique another one more less number of stage and the total of two number of function evaluation per step less compared with the classical RK method for the same order of the method will be developed. In Section 2, an overview of TDRK method is given. The new FSAL TDRK method is constructed and the stability of the new method is analyzed in Section 3. The numerical results, discussion and conclusion are dealt in Section 4, Section 5 and Section 6 respectively.

2 Two Derivative Runge-Kutta Methods

Consider the scalar ODEs (1) with $f : \Re^N \to \Re^N$. For this case, we assume that the second derivative is also known where

$$y^{''} = g(y) := f'(y)f(y), \quad g : \Re^N \to \Re^N. \tag{2}$$

An explicit TDRK method for the numerical integration of IVPs (1) is given by

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f(y_j) + h^2 \sum_{j=1}^{s} \hat{a}_{ij} g(Y_j), \tag{3}$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(y_i) + h^2 \sum_{i=1}^{s} \hat{b}_i g(Y_i), \tag{4}$$

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

We present the explicit TDRK method with the coefficients in (3) and (4) using the Butcher tableau as follows

c	A	$\hat{A}$
	b^T	$\hat{b}^T$

Explicit methods with minimal number of function evaluations can be developed by considering the methods in the form

$$Y_i = y_n + hc_i f(x_n, y_n) + h^2 \sum_{j=1}^{i-1} \hat{a}_{ij} g(x_n + hc_j, Y_j), \tag{5}$$

$$y_{n+1} = y_n + hf(x_n, y_n) + h^2 \sum_{i=1}^{s} \hat{b}_i g(x_n + hc_i, Y_i), \tag{6}$$

where $i = 2, \ldots, s$.

The above method is called special explicit TDRK methods. The unique part of this method is that it involves only one evaluation of f per step compared to many evaluation of f per step in traditional explicit RK methods. Its Butcher tableau is given as follows

c	$\hat{A}$
	$\hat{b}^T$

The TDRK parameters $\hat{a}_{ij}, \hat{b}_i$ and c_i are assumed to be real and s is the number of stages of the method. We introduce the s-dimensional vectors $\hat{b}, c$ and $s \times s$ matrix, $\hat{A}$ where $\hat{b} = \left[\hat{b}_1, \hat{b}_2, \ldots, \hat{b}_s\right]^T, c = [c_1, c_2, \ldots, c_s]^T$ and $\hat{A} = [\hat{a}_{ij}]$ respectively.

The order conditions for special explicit TDRK methods are given in the following Table 1.

Table 1: Order conditions for special explicit TDRK methods.

Order	Conditions		
1	$b^T e = 1$		
2	$\hat{b}^T e = \frac{1}{2}$		
3	$\hat{b}^T c = \frac{1}{6}$		
4	$\hat{b}^T c^2 = \frac{1}{12}$		
5	$\hat{b}^T c^3 = \frac{1}{20}$	$\hat{b}^T \hat{A} c = \frac{1}{120}$	
6	$\hat{b}^T c^4 = \frac{1}{30}$	$\hat{b}^T c\hat{A} c = \frac{1}{180}$	$\hat{b}^T \hat{A} c^2 = \frac{1}{360}$
7	$\hat{b}^T c^5 = \frac{1}{42}$	$\hat{b}^T c^2\hat{A} c = \frac{1}{252}$	$\hat{b}^T c\hat{A} c^2 = \frac{1}{504}$
	$\hat{b}^T \hat{A} c^3 = \frac{1}{840}$	$\hat{b}^T \hat{A}^2 c = \frac{1}{5040}$	

The following simplifying assumption is used in practice

$$\sum_{i=1}^{s} \hat{a}_{ij} = \frac{1}{2}{c_i}^2, \tag{7}$$

for $i = 2, \ldots, s$.

3 A Fifth-order TDRK Method with FSAL property

An interesting special class of explicit RK methods for which the coefficients have a special structure known as First Same As Last (FSAL) where

$$\hat{b}_i = \hat{a}_{si}, \quad i = 1, \dots, s-1, \quad and \quad \hat{b}_s = 0. \quad (8)$$

The function value k_s at the end of one integration step is the same as the first function value k_1 at the next integration step.

The FSAL technique is implemented into the TDRK methods. The order conditions given in Table 1 as well as the simplifying assumption (7) need to be satisfied in order for a method to be a TDRK method. In this paper, a four stages explicit TDRK method given by the following Butcher tableau with FSAL property is considered.

$$\begin{array}{c||cccc} 0 & 0 & & & \\ c_2 & \hat{a}_{21} & 0 & & \\ c_3 & \hat{a}_{31} & \hat{a}_{32} & 0 & \\ 1 & \hat{a}_{41} & \hat{a}_{42} & \hat{a}_{43} & 0 \\ \hline & \hat{a}_{41} & \hat{a}_{42} & \hat{a}_{43} & 0 \end{array} \quad (9)$$

3.1 Construction of the new method

Evaluate the simplifying assumption (7) leads to

$$\hat{a}_{21} = \frac{c_2^2}{2}, \quad \hat{a}_{31} = \frac{c_3^2}{2} - \hat{a}_{32}, \quad \hat{a}_{41} = \frac{c_4^2}{2} - \hat{a}_{42} - \hat{a}_{43}. \quad (10)$$

According to order conditions up to order five in Table 1, we have

$$\hat{a}_{42}c_2 + \hat{a}_{43}c_3 - \frac{1}{6} = 0, \quad (11)$$

$$\hat{a}_{42}{c_2}^2 + \hat{a}_{43}{c_3}^2 - \frac{1}{12} = 0, \quad (12)$$

$$\hat{a}_{42}{c_2}^3 + \hat{a}_{43}{c_3}^3 - \frac{1}{20} = 0, \quad (13)$$

$$\hat{a}_{43}\hat{a}_{32}c_2 - \frac{1}{120} = 0. \quad (14)$$

Solving equation (11)–(14) will lead to a solution of $\hat{a}_{32}, \hat{a}_{42}, \hat{a}_{43}$ and c_3 in term of c_2

$$\hat{a}_{32} = -\frac{-50\,{c_2}^3 + 80\,{c_2}^2 - 45\,c_2 + 9}{-3000\,{c_2}^3 + 1500\,{c_2}^2 + 2000\,{c_2}^4 - 250\,c_2}, \quad (15)$$

$$\hat{a}_{42} = \frac{1}{120\,{c_2}^3 - 120\,{c_2}^2 + 36\,c_2}, \quad (16)$$

$$\hat{a}_{43} = -\frac{300\,{c_2}^2 - 150\,c_2 - 200\,{c_2}^3 + 25}{-108 + 600\,{c_2}^3 - 960\,{c_2}^2 + 540\,c_2}, \quad (17)$$

$$c_3 = -\frac{-5\,c_2 + 3}{10\,c_2 - 5}. \quad (18)$$

Our aim is to choose c_2 such that the principal local truncation error coefficient, $\left\|\tau^{(6)}\right\|_2$ have a very small value. Wrong choices of c_2 may cause a huge global error difference. By plotting the graph of $\left\|\tau^{(6)}\right\|_2$ against c_2, a small value of c_2 is chosen in the range of $[0.0, 1.0]$ and hence, the value of c_2 lies between $[0.2, 0.4]$. We choose $c_2 = \frac{329}{1000}$ for an optimized pair. All the coefficients are showed in the following Butcher tableau and it is denoted as FSALTDRK4(5).

Table 2: Butcher Tableau for FSALTDRK4(5) method

$$\begin{array}{c||cccc} 0 & 0 & & & \\ \frac{329}{1000} & \frac{108241}{2000000} & 0 & & \\ \frac{271}{342} & -\frac{163144981}{13160555352} & \frac{536857775}{1645069419} & 0 & \\ 1 & \frac{54959}{534954} & \frac{25000000}{78210867} & \frac{1666737}{21474311} & 0 \\ \hline & \frac{54959}{534954} & \frac{25000000}{78210867} & \frac{1666737}{21474311} & 0 \end{array}$$

The norms of the principal local truncation error coefficients for FSALTDRK4(5) method is given by

$$\left\|\tau^{(6)}\right\|_2 = 1.456891018 \times 10^{-3}. \quad (19)$$

3.2 Stability of the new method

The stability function of explicit TDRK method is given as follows

$$\begin{aligned} R(z) =& 1 + zb^T\left(I - zA - z^2\hat{A}\right)^{-1}e + \\ & z^2b^T\left(I - zA - z^2\hat{A}\right)^{-1}e. \end{aligned} \quad (20)$$

Meanwhile for special explicit TDRK method, the following test equation is considered

$$y' = i\lambda y \quad \text{where} \quad \lambda > 0. \quad (21)$$

Apply equation (21) to the special explicit TDRK method produces the difference equation

$$y_{n+1} = H(z)y_n \quad \text{and} \quad z = iv, \quad v = \lambda h, \quad (22)$$

where

$$H(z) = \left(1 + z^2 \hat{b}\left(I - v^2 \hat{A}\right)^{-1} e\right) + i\left(v + v^3 \hat{b}\left(I - v^2 \hat{A}\right)^{-1} c\right). \tag{23}$$

$\hat{A}, c$ and $\hat{b}$ are the coefficient given in Table 2 with

$$I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad e = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}. \tag{24}$$

The stability function of FSALTDRK4(5) method is

$$H(z) = 1 + v + \frac{1}{2}v^2 + \frac{1}{6}v^3 + \frac{1}{24}v^4 + \frac{1}{120}v^5 + \frac{329}{240000}v^6. \tag{25}$$

The stability region of FSALTDRK4(5) method is plotted in Figure 1.

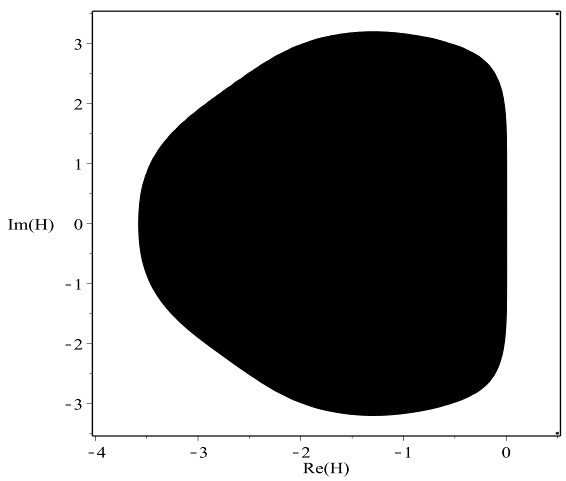

Figure 1: Stability region of FSALTDRK4(5) method.

The stability interval of this new method is $(-3.57, 0.00)$.

4 Problems Tested and Numerical Results

In this section, we compare the performance of the proposed method FSALTDRK4(5) with existing RK methods by considering the following problems. All problems below are tested using C code for solving first order ODEs.

Problem 1(Harmonic Oscillator[11])

$$\begin{aligned} y_1{}' &= y_2, & y_1(0) &= 1, & x &\in [0, 10], \\ y_2{}' &= -64y_1, & y_2(0) &= -2. \end{aligned}$$

Exact solution is

$$\begin{aligned} y_1(x) &= -\frac{1}{4}\sin(8x) + \cos(8x), \\ y_2(x) &= -2\cos(8x) - 8\sin(8x). \end{aligned}$$

Problem 2(Inhomogeneous problem[10])

$$\begin{aligned} y_1{}' &= y_2, & y_1(0) &= 1, & x &\in [0, 10], \\ y_2{}' &= -100y_1 + 99\sin(x), & y_2(0) &= 11. \end{aligned}$$

Exact solution is

$$\begin{aligned} y_1(x) &= \cos(10x) + \sin(10x) + \sin(x), \\ y_2(x) &= -10\sin(x) + 10\cos(10x) + \cos(x). \end{aligned}$$

Problem 3(An “almost” Periodic Orbit problem[12])

$$\begin{aligned} y_1{}' &= y_2, & y_1(0) &= 1, & x &\in [0, 10], \\ y_2{}' &= -y_1 + 0.001\cos(x), & y_2(0) &= 1, \\ y_3{}' &= y_4, & y_3(0) &= 0, \\ y_4{}' &= -y_3 + 0.001\sin(x), & y_4(0) &= 0.995. \end{aligned}$$

Exact solution is

$$\begin{aligned} y_1(t) &= \cos(x) + 0.0005x\sin(x), \\ y_2(x) &= -\sin(x) + 0.0005x\cos(x) + 0.0005x\sin(x), \\ y_3(t) &= \sin(x) - 0.0005x\cos(x), \\ y_4(x) &= \cos(x) + 0.0005x\sin(x) - 0.0005\cos(x). \end{aligned}$$

Problem 4(Allen and Wing[13])

$$\begin{aligned} y_1{}' &= y_2, & y_1(0) &= 1, & x &\in [0, 10], \\ y_2{}' &= -y_1 + x, & y_2(0) &= 2. \end{aligned}$$

Exact solution is

$$\begin{aligned} y_1(x) &= \sin(x) + \cos(x) + x, \\ y_2(x) &= \cos(x) - \sin(x) + 1. \end{aligned}$$

Problem 5(Jawias et al.[14])

$$y' = y - x^2 + 1, \quad y(0) = 0.5, \quad x \in [0, 10].$$

Exact solution is

$$y(x) = (x + 1)^2 - 0.5e^x.$$

Problem 6(Radzi et al.[15])

$$y' = y, \qquad y(0) = 1, \qquad x \in [0, 10].$$

Exact solution is

$$y(x) = e^x.$$

Problem 7(Radzi et al.[15])

$$y_1' = y_2, \qquad y_1(0) = 0, \quad x \in [0, 10],$$
$$y_2' = 2y_2 - y_1, \quad y_2(0) = 1.$$

Exact solution is

$$y_1(x) = xe^x, \qquad y_2(x) = (1 + x)e^x.$$

Problem 8(Ismail and Salih[16])

$$y' = 15 - 3y, \quad y(0) = 0, \quad x \in [0, 10].$$

Exact solution is

$$y(x) = 5(1 - e^{-3x}).$$

The following notations are used in Figures 2–9 :

- **FSALTDRK4(5):** New TDRK method with FSAL property of fifth order four stages derived in this paper
- **TDRK3(5):** Existing fifth order three stage TDRK method developed by Chan and Tsai[1].
- **RKE**: Existing fifth order six stage RK method given in Lambert[17].
- **RKDP**: Existing fifth order seven stage RK method derived by Wanner and Hairer[18].
- **RKF**: Existing fifth order six stage RK method developed by Fehlberg[19].
- **RKCK**: Existing fifth order six stage RK method derived by Cash and Karp[20].

We represent the performance of these numerical results graphically in the following Figures 2–9:

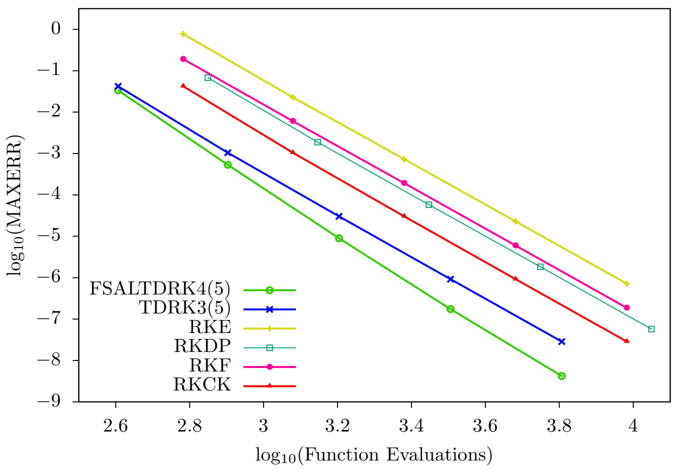

Figure 2: The efficiency curve for the harmonic oscillator (Problem 1) with $h = 0.1/2^i, i = 0, \ldots, 4$.

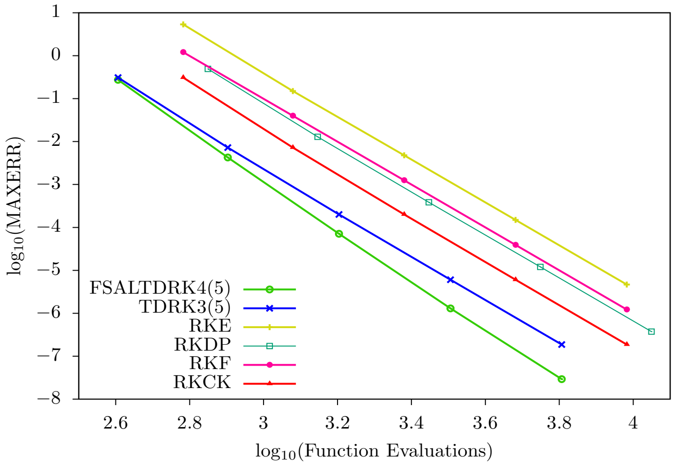

Figure 3: The efficiency curve for the inhomogeneous problem (Problem 2) with $h = 0.1/2^i, i = 0, \ldots, 4$.

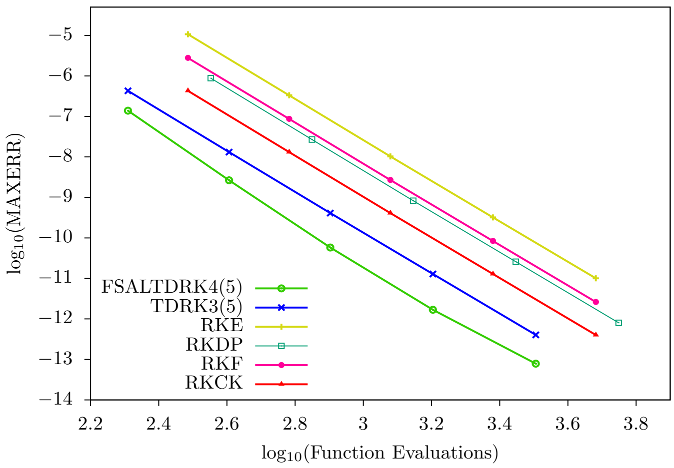

Figure 4: The efficiency curve for the "almost" periodic problem (Problem 3) with $h = 0.1/2^i, i = -1, \ldots, 3$.

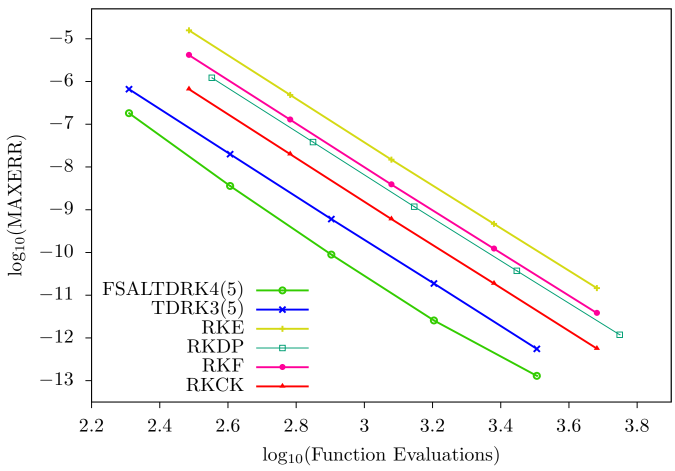

Figure 5: The efficiency curve for Problem 4 with $h = 0.1/2^i, i = -1, \ldots, 3$.

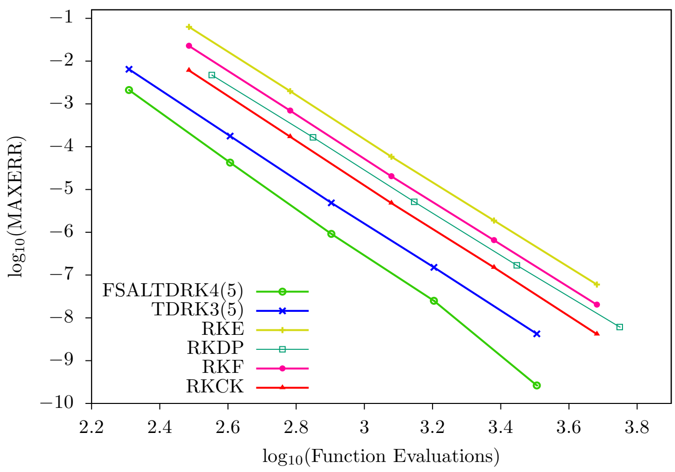

Figure 6: The efficiency curve for Problem 5 with $h = 0.1/2^i, i = -1, \ldots, 3$.

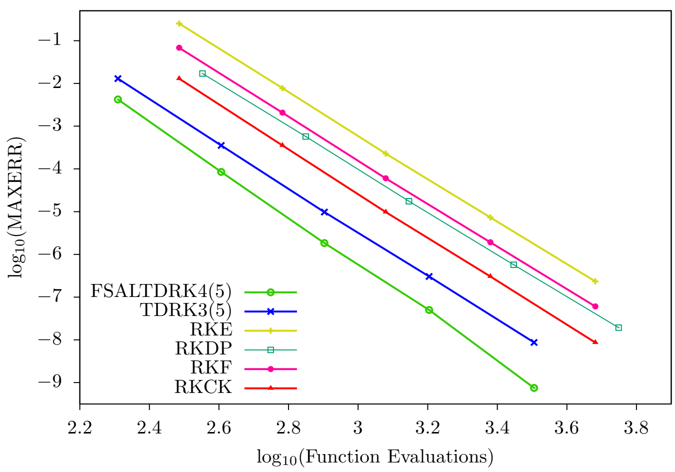

Figure 7: The efficiency curve for Problem 6 with $h = 0.1/2^i, i = -1, \ldots, 3$.

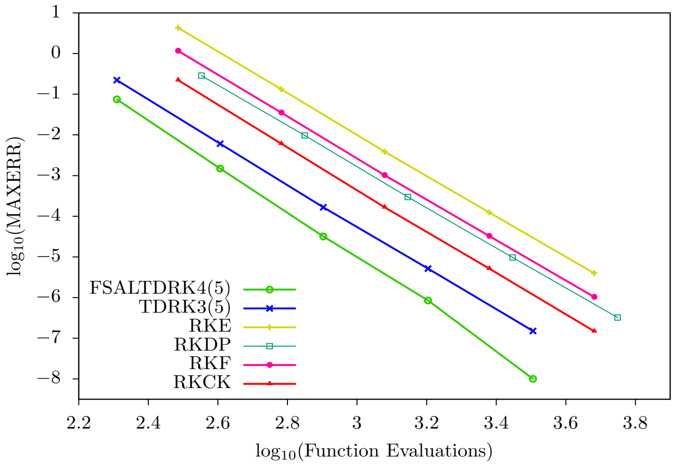

Figure 8: The efficiency curve for Problem 7 with $h = 0.1/2^i, i = -1, \ldots, 3$.

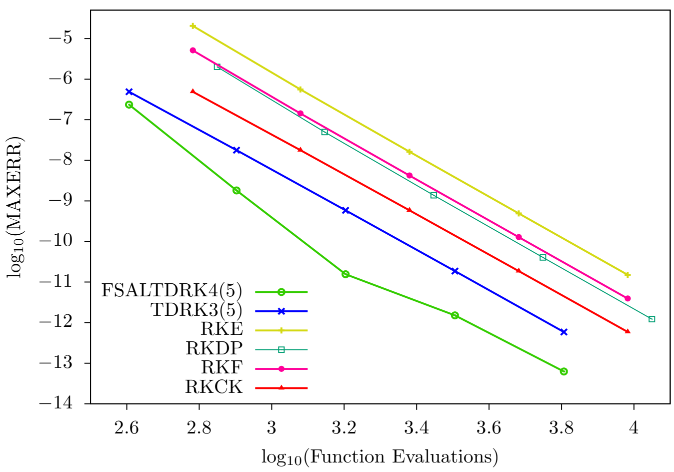

Figure 9: The efficiency curve for Problem 8 with $h = 0.1/2^i, i = 0, \ldots, 4$.

5 Discussion

The results show the typical properties of the new TDRK method with FSAL property, FSALTDRK4(5) which have been derived earlier. The derived method are compared with some well-known existing RK methods. Figures 2-9 represent the efficiency and accuracy of the method developed by plotting the graph of the logarithm of the maximum global error against the logarithm number of function evaluations. From Figures 2–9, the global error produced by the FSALTDRK4(5) method has smaller global error compared to TDRK3(5), RKE, RKDP, RKF and RKCK. Moreover, from the same figures, FSALTDRK4(5) has the least number of function evaluations per step compared to other existing RK methods of the same order.

6 Conclusion

In this research, a fifth algebraic order TDRK method with FSAL property has been developed. The advantage of the TDRK together with FSAL property make the new method more efficient in term of function evaluations and also more accurate compared with the classical RK methods. Based on the numerical results obtained, it can be concluded that the new FSALTDRK4(5) method is more promising compared to other well-known existing explicit RK and TDRK methods in terms of accuracy and the number of function evaluations per step.

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