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A NOTE ON EXPLICIT THREE-DERIVATIVE RUNGE-KUTTA METHODS (ThDRK)

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Abstract. Recently, the Runge-Kutta methods, obtained via Taylor's expansion is exist in the literature. In this study, we have derived explicit methods for problems of the form $y' = f(y)$ including second and third derivatives , by considering available Two-Derivative Runge-Kutta methods (TDRK). The methods use one evaluation of first derivative, one evaluation of second derivative and many evaluations of third derivative per step. The methods can be named as Three- Derivative Runge-Kutta methods, ThDRK shortly. We present methods with stages up to three and order up to seven. Comparisons is made with other some existing methods on some standard problems. The stability region of the methods are given.

1. Introduction

We consider initial value problems expressed in following form

$$y' = f(y), \qquad y(x_0) = y_0 \tag{1.1}$$

where $f : \mathbb{R}^n \to \mathbb{R}^n$ and assuming that second and third derivative are known,

$$\begin{aligned} y'' &= g(y) := f'(y)f(y), \qquad f : \mathbb{R}^n \to \mathbb{R}^n \\ y''' &= \hat{g}(y) := f''(y)(f(y), f(y)) + f'(y)f'(y)f(y), \qquad \hat{g} : \mathbb{R}^n \to \mathbb{R}^n \end{aligned} \tag{1.2}$$

where bi-linear operator is introduced, and we use these terms in formulation of the method.

Most efforts have been made to improve the order of Runge- Kutta methods via increasing the number of terms in Taylor's expansion. The use of higher order derivative terms has been proposed for stiff problems by many authors [**2, 4, 5,**

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6, 12]. Goeken and Johnson [**3**], presented third, fourth and fifth order method using second derivative in internal stages. Wu and Xia [**13**] proposed methods including second derivative in external stages. Akanbi et al. [**9**] and Wusu et al. [**1**] , developed Multiderivative Explicit Runge-Kutta method utilizing both second and third derivative in internal stages. Recently, Chan and Tsai [**10**] constructed Two-Derivative Runge-Kutta methods (TDRK) incorporating second derivative in the formulation of the methods, which use second derivative in both internal stages and external stages.

In section 2 we presented the derivation of Three-Derivative Runge-Kutta methods (ThDRK) with minimal number of function evaluation. In section 3 stability analysis was made. In section 4 numerical examples were given for comparing presented methods with other existing methods on some standard problems.

2. Derivation of the methods

We consider s stage explicit methods in the following form

$$\begin{aligned} Y_1 &= y_n \\ Y_i &= y_n + hc_i f(y_n) + \frac{1}{2}h^2 c_i^2 g(y_n) + h^3 \sum_{j=1}^{i-1} a_{ij}\hat{g}(Y_j), \quad i = 2, \ldots, s \qquad (2.1) \\ y_{n+1} &= y_n + hf(y_n) + \frac{1}{2}h^2 g(y_n) + h^3 \sum_{i=1}^{s} b_i \hat{g}(Y_i). \end{aligned}$$

It is important to note that in addition to the computation of the f values at the internal stages in standart Runge-Kutta methods, the proposed method involves computing g and $\hat{g}$ values. Therefore, the method would be handier if the cost considered in evaluating g and $\hat{g}$ are compatible to those in evaluating f in classical methods.

So, by taking above considerations, we seek to determine the coefficients of the methods presented in (2.1). Hence, utilizing the Taylor series expansion and comparing coefficients of the powers of h are obtained s stage explicit ThDRK methods.

Butcher [**7**] proposed a way of deriving the coefficients that arise in the Taylor series expansions of approximate solutions for $y' = f(y)$. The idea in Butcher's formulation is that one to one correspondence between the derivatives in the expansion and Butcher's tableau which simplifies the determination of the coefficients of the expansion.

Thus, for our approach, the coefficients of the ThDRK method can be expressed by using Butcher notation in the tableau as follows:

$$\begin{array}{c||cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ \vdots & \vdots & \ddots & & \\ c_s & a_{s1} & & a_{ss-1} & \\ \hline & b_1 & \ldots & b_{s-1} & b_s \end{array}$$

Assumptions in Butcher's tableau readily simplify the order conditions to those presented in Table 1. On the other hand, the list given in Table 2, summaries the various counts of interest for these special explicit methods.

2.1. One stage method. With $b_1 = 1/6$ we obtain

$$y_{n+1} = y_n + hf(y_n) + \frac{1}{2}h^2 g(y_n) + \frac{1}{6}h^3 \hat{g}(y_n).$$

This method requires one evaluation f, one evaluation g and one evaluation $\hat{g}$. This has the same stability polynomial as three stage explicit Runge-Kutta methods with same order (see [**8**]).

2.2. Two stage method. Simplifying assumption is given by

$$\sum_{j=1}^{i-1} a_{ij} = \frac{c_i^3}{6}, \qquad i = 2, \dots, s \tag{2.2}$$

is useful determine order conditions in Table 1. For fourth order method we obtain with three unknowns two equations

$$b_1 + b_2 = \frac{1}{6}, \qquad b_2 c_2 = \frac{1}{24}.$$

These have one parameter family of methods. Selecting free parameter c_2 we obtain

$$b_1 = \frac{1}{24}\frac{4c_2 - 1}{c_2}, \qquad b_2 = \frac{1}{24c_2}.$$

For fifth order method is obtained with three unknowns three equations, we have unique solution

$$c_2 = \frac{2}{5}, \qquad b_1 = \frac{1}{16}, \qquad b_2 = \frac{5}{48}$$

which gives a unique method of order five. This method requires one evaluation f, one evaluation g and two evaluations $\hat{g}$.

2.3. Three stage methods. It is easy to see that there are six unknowns in the tableau

$$\begin{array}{c||ccc} 0 & & & \\ c_2 & \frac{c_2^3}{6} & & \\ c_3 & \frac{c_3^3}{6} - a_{32} & a_{32} & \\ \hline & b_1 & b_2 & b_3 \end{array}$$

There are four equation of order six. This gives

$$\begin{aligned} b_1 &= \frac{1}{120}\frac{15c_2^2 - 10c_2 + 1}{c_2(2c_2 - 1)}, \qquad b_2 = \frac{1}{120}\frac{1}{5c_2^2 - 4c_2 + 1}, \\ b_3 &= \frac{1}{120}\frac{(5c_2 - 2)(25c_2^2 - 20c_2 + 4)}{(2c_2 - 1)(5c_2^2 - 4c_2 + 1)}, \qquad c_3 = \frac{2c_2 - 1}{5c_2 - 2} \end{aligned}$$

where c_2 is free parameter and a_{32} is independent from order conditions. Also, there are six equation of order seven. Then there are two solutions which is conjugated with each other. One of this solution is obtained by the following parameters:

$$b_1 = \frac{1}{30}, \qquad b_2 = \frac{1}{15} + \frac{13\sqrt{2}}{480}, \qquad b_3 = \frac{1}{15} - \frac{13\sqrt{2}}{480},$$
$$c_2 = \frac{3}{7} - \frac{\sqrt{2}}{7}, \qquad c_3 = \frac{3}{7} + \frac{\sqrt{2}}{7}, \qquad a_{32} = \frac{122}{7203} + \frac{71\sqrt{2}}{7203}.$$

This method requires one evaluation f, one evaluation g and three evaluations $\hat{g}$.

3. Stability analysis

The stability region of the method is defined using standard test problem, $y' = \lambda y$, where λ is a complex constant. Then stability polynomial of fifth order three-derivative Runge-Kutta method, ThDRK5, is

$$R(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 + \frac{1}{120}z^5 + \frac{1}{900}z^6,$$

where $z = \lambda h$. Stability polynomial of seventh order three-derivative Runge-Kutta method, ThDRK7, is

$$\begin{aligned} R(z) &= 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 + \frac{1}{120}z^5 + \frac{1}{720}z^6 + \frac{1}{5040}z^7 + \left(\frac{1}{23520} - \frac{\sqrt{2}}{70560}\right)z^8 \\ &+ \left(\frac{11}{1481760} - \frac{\sqrt{2}}{246960}\right)z^9, \end{aligned}$$

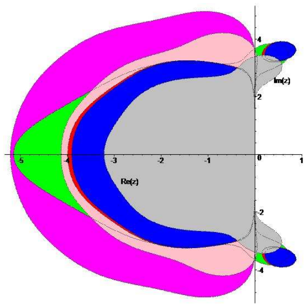

FIGURE 1. Stability Regions for RK5, TDRK5e, TDRK5f, ThDRK5, ThDRK7, TDRK7 methods

In Figure 1 gray region is of RK5, blue region is of TDRK5f, red region is of ThDRK5, pink region is of TDRK7, green region is of TDRK5e and magenta region is of ThDRK7.

TABLE 1. Order conditions for explicit ThDRK methods

Order	Conditions	
3	$\sum_{i=1}^{s} b_i = \frac{1}{6}$	
4	$\sum_{i=2}^{s} b_i c_i = \frac{1}{24}$	
5	$\sum_{i=2}^{s} b_i c_i^2 = \frac{1}{60}$	
6	$\sum_{i=2}^{s} b_i c_i^3 = \frac{1}{120}$	
7	$\sum_{i=2}^{s} b_i c_i^4 = \frac{1}{210}$	$\sum_{i=3}^{s} b_i a_{ij} c_j = \frac{1}{5040}$

TABLE 2. Counts for special explicit ThDRK methods assuming (2.2)

s	order	unknowns	conditions
1	3	1	1
2	4	3	2
2	5	3	3
3	6	6	4
3	7	6	6

4. Numerical Examples

In this section we applied methods of order five and seven on the some standard problems for comparisons. In these implementations we use L_∞ norm for errors. The methods used for comparison are given in the following.

- RK6: the classical sixth order Runge-Kutta method requires seven evaluations of f per step in [**10, 11**].
- TDRK5e: the classical fifth order TDRK method requires one evaluation of f and three evaluations of g per step (in page 180) in [**10**].
- TDRK7: the classical seventh order TDRK method requires one evaluation of f and five evaluations of g per step (the one in the left in page 182) in [**10**].
- ThDRK5: the fifth order ThDRK method derived in section 2.2, which requires one evaluation of f and one evaluation of g and two evaluations $\hat{g}$ per step.
- ThDRK7: the seventh order ThDRK method derived in section 2.3, which requires one evaluation of f and one evaluation of g and three evaluations $\hat{g}$ per step.

Problem 1: We consider Prothero-Robinson Problem (see [**10**]) is given by

$$y'(x) = \lambda(y(x) - \varphi(x)) + \varphi'(x), \qquad y(0) = \varphi(0), \qquad Re(\lambda) < 0,$$

with $\varphi(x) = sinx$. Its exact solution is $y(x) = \varphi(x)$. We solve this problem for two different λ values, -1 and -200, and integrate to 2.8π. The results are shown in Figure 2 and Figure3.

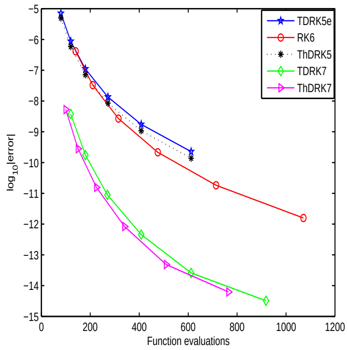

FIGURE 2. Errors versus function evaluations for Prothero-Robinson, $\lambda = -1$, $x_{end} = 2.8\pi$

In Figure 2 number of steps is experimented with 20, 30, 45, 68, 102, 153.

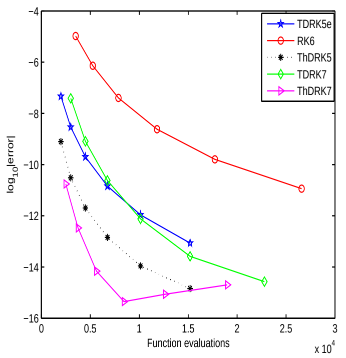

FIGURE 3. Errors versus function evaluations for Prothero-Robinson $\lambda = -200$, $x_{end} = 2.8\pi$

In Figure 3 number of steps is experimented with 500, 750, 1125, 1688, 2532, 3798.
Problem 2:We consider Kaps Problem (see [**10**]) is given by

$$y'(x) = \begin{bmatrix} -y_1(1+y_1) + y_2 \\ \lambda(y_1^2 - y_2) - 2y_2 \end{bmatrix}, \qquad y(0) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

where λ is a positive parameter. Its exact solution is

$$y(x) = \begin{bmatrix} e^{-x} \\ e^{-2x} \end{bmatrix}.$$

We take $\lambda = 1$ and $\lambda = 200$ and integrate to $x = 5$. The results are shown in Figure 4 and Figure 5.

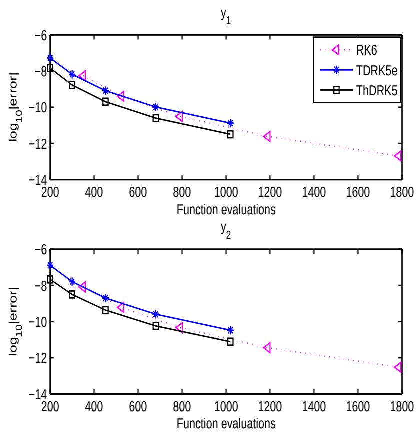

FIGURE 4. Errors versus function evaluation for Kaps Problem, $\lambda = 1$, $x_{end} = 5$

In Figure 4 number of steps is experimented with 50, 75, 113, 170, 255.

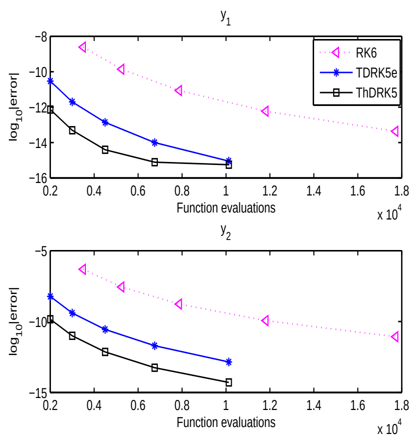

FIGURE 5. Errors versus function evaluation for Kaps Problem, $\lambda = 200$, $x_{end} = 5$

In Figure 5 number of steps is experimented with 500, 750, 1125, 1688, 2532.

5. Conclusion

In this study we presented a special class of explicit three-derivative Runge-Kutta methods up to order seven. The present approach was constructed by containing fewer function evaluations comparing to classical Runge-Kutta methods. Comparing with TDRK methods ([**10**]) in the literature, present approach attain higher order using for fewer stages.

Also, the numerical examples propose that the ThDRK methods can be efficient as TDRK methods, comparing classical RK methods, for certain types of mildly stiff problems.

As a further study, we will attempt to study higher order ThDRK methods for diverse applications.

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