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An Optimized Runge-Kutta Method for the Numerical Solution of the Oscillatory Problems

[1]Firas A. Fawzi, [1]A.M. Gaftan, [2]P.E. Oguntunde and [3]N. Senu
[1]Department of Mathematics, Faculty of Computer Science and Mathematics, Tikrit University, Tikrit, Iraq
[2]Department of Mathematics, Covenant University, Ota, Nigeria
[3]Department of Mathematics and Institute for Mathematical Research, Universiti Putra Malaysia (UPM) 43400 Serdang, Selangor, Malaysia, firasadil01@gmail.com

Abstract: In this study, an optimized explicit Runge-Kutta (RK) method which is based on a method of Dormand with six-stage and fifth algebraic order with FSAL property denoted as the ORK5 method is constructed. The proposed method solves first-order Ordinary Differential Equations (ODEs) by first converting the second order ODEs to an equivalent first order. The new method has zero phase-lag, zero amplification error and zero first derivative of the phase-lag. Absolute stability of the new method is as well shown. The numerical experiments are carried out to show the efficiency of the derived method in comparison with other existing RK methods.

Key words: Amplification error, numerical analysis, ordinary differential equation, oscillatory problems, phase lag, Runge-Kutta method

INTRODUCTION

In this study, we are dealing with the Initial Value Problems (IVPs) of the form:

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

Where:

$$y(x) = [y_1(x), y_2(x), ..., y_s(x)]^T$$
$$f(x,y) = [f_1(x,y), f_2(x,y), ..., f_s(x,y)]^T$$

y_0 is a given vector of initial conditions and their solution is oscillatory. This type of problem occurs in various applied fields such as quantum mechanics, electronics, physical chemistry, molecular dynamics astronomy, chemical physics and control engineering.

In effect, Eq. 1 can be solved using Runge-Kutta methods or multi-step methods. The solution of Eq. 1 often shows a pronounced oscillatory behavior. In general, most problems with oscillatory or periodical behavior are a second order or higher order. Hence, it is important to reduce the higher order problems to first-order problems in order to solve the ODEs in Eq. 1. Several researchers have improved numerical methods for solving oscillatory problems based on the phase-fitted and amplification fitted properties. Simos and Aguiar (2001) constructed a modified phase-fitted RK method with phase-lag of order infinity for the numerical solution of periodic IVPs based on the fifth algebraic-order RK method of Dormand and Prince.

Chen *et al*. (2012) improved traditional RK methods by introducing frequency-depending weights in the update. With the phase-fitting and amplification-fitting conditions and algebraic order conditions, new practical RK integrators are obtained and two of the new methods have updates that are also phase-fitted and amplification-fitted. With the evolution of RK methods, Papadopoulos *et al*. (2010) developed a new Runge-Kutta Nystrom (RKN) method for the numerical solution of the Schrodinger equation with phase-lag and amplification error of order infinity based on the fourth-order RKN method by Dormand, El-Mikkawy and Prince. Meanwhile, Moo *et al*. (2013) derived two new RKN methods for solving second-order differential equations with oscillatory solutions based on two existing RKN methods, a fourth-order three-stage Garcias RKN method and fifth-order four-stage Hairers RKN method.

The derived methods both have two variable coefficients with zero amplification error (zero dissipative) and phase-lag of order infinity. In the last few years, Senu *et al*. (2014) constructed zero dissipative explicit RK

Corresponding Author: Firas A. Fawzi, Department of Mathematics, Faculty of Computer Science and Mathematics, Tikrit University, Tikrit, Iraq, firasadil01@gmail.com

method for solving second-order ODEs with periodical solutions which have algebraic order three with the dissipation of order infinity. Fawzi *et al*. (2016a, b) developed fourth-algebraic-order phase-fitted and amplification-fitted modified RK method and fourth-order seven-stage phase-fitted and amplification-fitted RK methods, respectively. Hussain *et al*. (2016) proposed a new optimized RK method for solving oscillatory problems. Recently, Ahmad *et al*. (2017) constructed a phase-fitted and amplification-fitted two-derivative RK method of high algebraic order for the numerical solution of first-order Initial Value Problems (IVPs) which possesses oscillatory solutions.

In this research, the new technique will be constructed by combining the nullification of phase-lag amplification factor and phase-lags derivative, based on a method of Dormand with six-stage and fifth algebraic order (Butcher and Wanner, 1996).

MATERIALS AND METHODS

Phase lag analysis of Runge-Kutta method: We consider the m-stage explicit RK method of the form:

$$y_{n+1} = y_n + h\sum_{i=1}^{m} b_i k_i \tag{2}$$

$$k_i = f\left(x_n + c_i h,\ y_n + h\sum_{j=1}^{i-1} a_{ij} k_j\right);\ i = 1,\ \ldots,\ m \tag{3}$$

The method is said to be explicit when $a_{ij} = 0$ for $i \leq j$ and implicit otherwise. The method in Eq. 2 and 3 can be reduced into Butcher tableau form (Fig. 1).

To derive the new method based on phase lag analysis, we consider the following test equation based on Moo *et al*. (2013):

$$y' = ivy \tag{4}$$

where, v is real. Then, we compare the theoretical solution and the numerical solution for this equation. By requiring that the solutions are in phase with a maximal order in the step-size h, we derive the so-called dispersion relation. Applying the above method in Eq. 2 and 3 to the test Eq. 4, we obtain:

$$y_n = a_*^n y_0$$

with:

$$a_* = A_m\left(H^2\right) + iHB_m H^2 \tag{5}$$

where, H = vh. The amplification factor is, $a_* = a_*(H)$ and denotes the approximation to $y(x_n)$. A comparison of

0					
c_2	a_{21}				
.	.				
.	.				
.	.				
c_m	a_{m1}	.	.	.	$a_{m,\ m-1}$
	b_1	.	.	.	b_m

Fig. 1: m-stage explicit Runge-Kutta method

Eq. 5 with the solution of Eq. 4 leads to the following definition of the dispersion or phase error or phase-lag and the amplification error.

Definition 2.1: An explicit m-stage RK, presented in Fig. 1 the quantities:

$$\begin{aligned} t(H) &= H - \arg\left[a_*(H)\right] \\ a(H) &= 1 - |a_*(H)| \end{aligned} \tag{6}$$

are called the dispersion or phase error or phase-lag and the amplification error, respectively. If $t(H) = O(H^{r+1})$ and $a(H) = O(H^{s+1})$ then the method is said to be phase-lag order r and dissipative orders (Fawzi *et al*., 2016a, b). From Eq. 6, it follows that:

$$a(H) = 1 - \sqrt{\left[A_m^2\left(H^2\right) + H^2 B_m^2\left(H^2\right)\right]} \tag{7}$$

Meanwhile, for the Runge-Kutta method given in Fig. 1, the following formula is used for the direct calculation of the phase-lag order r and the phase-lag constant q:

$$\tan(H) - H\left[\frac{B_m\left(H^2\right)}{A_m\left(H^2\right)}\right] = qH^{r+1} + O\left(H^{s+3}\right) \tag{8}$$

The analysis of phase-fitted (dispersion of order infinity) and amplification-fitted (dissipation of order infinity) are based on dispersion and dissipation quantities that have discussed above. The RK method is phase-fitted and amplification-fitted, if the following conditions hold:

$$t(H) = 0 \text{ and } a(H) = 0 \tag{9}$$

Table 1: Runge-Kutta method of order five

0							
$\frac{1}{5}$	$\frac{1}{5}$						
$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$					
$\frac{4}{5}$	$\frac{44}{45}$	$-\frac{56}{15}$	$\frac{32}{9}$				
$\frac{8}{9}$	$\frac{19372}{6561}$	$-\frac{25360}{2187}$	$\frac{64448}{6561}$	$-\frac{212}{729}$			
1	$\frac{9017}{3168}$	$-\frac{355}{33}$	$\frac{46732}{5247}$	$\frac{49}{176}$	$-\frac{5103}{18656}$		
1	b_1	b_2	b_3	b_4	b_5	b_6	
	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	0

RESULTS AND DISCUSSION

Construction of the new Runge-Kutta methods: In this study, an optimized Runge-Kutta method will be derived, based on the fifth-order Runge-Kutta method with six-stage derived by Butcher and Wanner (1996) which is given in the tableau in Table 1. To achieve this, we set b_1, b_2 and b_3 as free coefficients while all other coefficients are the same as in Table 1, first, we compute the polynomials A^2_m and B^2_m in terms of Runge-Kutta coefficients in Table 1. Then from these polynomials, we obtain the quantities t(H) and a(H) and by the nullification of the phase-lag amplification error and phase-lag's derivative. Hence, we obtain a system of three equations as follows:

$$\begin{gathered}
a(H)=\left(1-\frac{1}{600}H^4+QH^2\right)+\\
H^2\left(\frac{1}{120}H^4+PH^2+b_3+b_1+\frac{65479}{142464}+b_2\right)^2-1=0\\
t(H)=\tan(H)-H\left(\frac{1}{120}H^4+PH^2+b_3+b_1+\frac{65479}{142464}+b_2\right)\\
\left(1-\frac{1}{600}h^6+\frac{1}{24}h^4+Qh^2\right)^{-1}=0
\end{gathered} \tag{10}$$

$$\begin{gathered}
t'(H)=1+\left[\tan(H)\right]-\\
\left(\frac{1}{120}H^4+PH^2+b_3+b_1+\frac{65479}{142464}+b_2\right)\\
\left(1-\frac{1}{600}H^6+\frac{1}{24}H^4+QH^2\right)^{-1}-H\left(\frac{1}{30}H^3+2PH\right)\\
\left(1-\frac{1}{600}H^6+\frac{1}{24}H^4+QH^2\right)^{-1}+\\
H\left(\frac{1}{120}H^4+PH^2+b_3+b_1+\frac{65479}{142464}+b_2\right)\\
\left(-\frac{1}{100}H^5+\frac{1}{6}H^3+2QH\right)\left(1-\frac{1}{600}H^6+\frac{1}{24}H^4+QH^2\right)^{-2}
\end{gathered} \tag{11}$$

where:

$$P=-\frac{163}{1113}-\frac{9}{200}b_3$$

and:

$$Q=-\frac{3}{10}b_3-\frac{1}{5}b_2-\frac{271}{742}$$

Solving simultaneously the system of Eq. 10-12, we obtain the coefficients b_1, b_2 and b_3 which are completely dependent on H where, H is the product of the step-size h and the frequency v. The expressions for b_1, b_2 and b_3 are too complicated, hence, we replaced by their Taylor series expansion and obtained the following expressions:

$$\begin{gathered}
b_1=\frac{35}{384}+\frac{643}{45360}H^4+\frac{62677}{16329600}H^6+\frac{5933}{4435200}H^8+\\
\frac{50184187}{9340531200}H^{10}+\frac{2560520257}{11769069312000}H^{12}+\\
b_2=-\frac{601}{15120}H^4-\frac{1831}{217728}H^6-\frac{26041}{798330}H^8-\\
\frac{328333}{249080832}H^{10}-\frac{83804419}{156920924160}H^{12}+,...,\\
b_3=\frac{500}{1113}+\frac{29}{1134}H^4+\frac{451}{81648}H^6+\frac{2171}{997920}H^8+\\
\frac{410413}{467026560}H^{10}+\frac{20951107}{58845346560}H^{12}+,....
\end{gathered} \tag{12}$$

Stability of the new method: Here, the linear stability of the method developed is analyzed. Consider to the test Eq. 4 where ν>0, the exact solution of this equation with initial value $y(x_0) = y_0$ satisfies:

$$y(x_0+h)=R(H)y_0 \tag{13}$$

When applying Eq. 2-4:

$$y_{n+1}=R(H)y_0 \tag{14}$$

$$R(H)=1+Hb^T(I-HA)^{-1}e \tag{15}$$

where, $e = (1, ..., 1)^T$, $A = [a_{ij}]$ and $b^T = [b_1, b_2, b_3, ..., b_m]$. R(H) is called the stability function of the method in Eq. 3.

Definition 3.1: A Runge-Kutta method is said to be absolutely stable if ∀H∈(-h, 0), |R(H^)|<1 (Fawzi *et al*., 2016a, b). The stability polynomial of the ORK5 method is given as follows:

$$R(H)=1+H+\frac{1}{2}H^2+\frac{1}{6}H^3+\frac{1}{24}H^4+\frac{1}{120}H^5+\frac{1}{720}H^6+\frac{53}{25200}H^7-\frac{1}{40320}H^8+\frac{907}{1814400}H^9+\frac{1}{3628800}H^{10}+\frac{39073}{199584000}H^{11}-\frac{1}{479001600}H^{12}+\frac{2462483}{31135104000}H^{13}+\frac{1}{87178291200}H^{14}+\frac{9164119691}{57164050944000}H^{15}+\frac{11547559819}{266765571072000}H^{16}+\frac{11547559819}{1778437140480000}H^{17} \quad (16)$$

The comparison of the stability region of the ORK5 method up to H^I where, I = 8, 10, 12 and its original method is plotted in Fig. 2. The stability interval of the original method is -306567892 and the stability interval of this method with the coefficients of H^8, H^{10}, H^{12} is -3.306570336. Observing from the stability regions plotted in Fig. 2, our new method is absolutely stable, since,

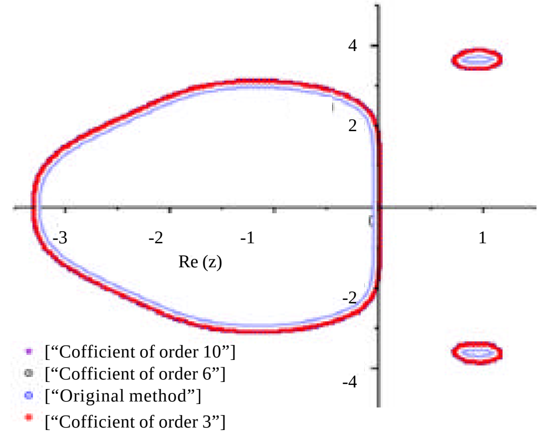

Fig. 2: Stability region of ORK5 method for different order

∀H∈(-3.3, 0)|R(H)|<1. We, however, obtained the result using maple package. Figure 2 shows the stability region of ORK5 method for different order.

Error analysis: The Local Truncation Error (LTE) of the new method is based on the Taylor series expansion of the differences y_{n+1} and $y(x_n+h)$:

$$LTE = y_{n+1}+y(x_n+h) \quad (17)$$

$$\begin{aligned}
LTE = {} & h^6\left[\frac{1}{3600}w^4f_yf+\frac{2417}{381600}f_{xxxyy}f^2+\frac{21361}{3052800}f_{xxxy}f_x+\frac{1517}{381600}f_{xxyyy}f^3\right]+\\
& h^6\left[\frac{35747}{6105600}f_{yxx}f_{xx}+\frac{239}{254400}f_{xyyyy}f^4+\frac{30045211}{6328115200}f_{xyy}f_{xx}+\frac{17563}{9158400}f_{xy}f_{xxx}\right]+\\
& h^6\left[\frac{31}{8480}f_{xyy}f_x+\frac{1}{648000}f_{yyyyy}f^5+\frac{2251}{4070400}f_yf_{xxxx}-\frac{1}{3600}f_{yyyy}f_x-\frac{1}{3600}f_{yyyyy}f\right]+\\
& h^6\left[\frac{61187}{3052800}ff_{xyy}f_yf_x+\frac{213825583}{32036083200}f_{xy}ff_{yy}f_x+\frac{22403}{3434400}f_{xy}f_{yy}f_yf^2\right]+\\
& h^6\left[\frac{17641}{10074240}ff_{yy}f_{yy}f_x+\frac{27}{13568}f^2f_{yyy}f_yf_x+\frac{6859}{1526400}f_{xxxxy}f\right]+\\
& h^6\left[\frac{14161}{1017600}ff_{xxyy}f_x+\frac{94}{11925}f_{xxxy}f_yf+\frac{17}{1272}f_{xxyy}f_yf^2+\frac{343}{25440}f_{yxx}f_{xy}f\right]+\\
& h^6\left[\frac{349}{47700}f_{yxx}f_{yy}f^2+\frac{2527}{190800}f_{yxx}f_yf_x+\frac{2527}{190800}f_{yxx}f_{yy}f+\frac{2317}{381600}f_{xyyy}f_yf^3\right]+\\
& h^6\left[\frac{7649}{1017600}ff_{xyy}f_{xx}+\frac{4979}{381600}f_{xyy}f_{xy}f^2+\frac{113}{21200}f_{xyy}f_{yy}f^3+\frac{11627}{763200}f_{xyy}f_{yy}f^2\right]+\\
& h^6\left[\frac{2257}{381600}f_{xyy}f_yf+\frac{833}{429300}f_{xy}f_{yyy}f^3+\frac{431}{381600}f_{xy}f_yf_{xx}+\frac{333627097}{17085911040}ff_{yyy}f_{xx}\right]+\\
& h^6\left[\frac{217}{122112}ff_{yy}f_{xxx}+\frac{18649}{27475200}f^3f_{yyy}f_x+\frac{1}{129600}f_{yyyy}f_yf^4+\frac{104123}{54950400}f^2f_{yyy}f_{xx}\right]+\\
& h^6\left[\frac{1}{64800}f_{yyy}f_{yy}f^4-\frac{1}{43200}f_{yyy}f_{yy}f^3+\frac{18649}{27475200}f^2f_{yyy}f_x+\frac{1}{64800}f_{yyy}f_yf^3\right]+
\end{aligned}$$

$$h^6\left[\frac{11}{43200}f_{yy}f_{yyy}f^2+\frac{1252708019}{512577331200}f_{yy}f_{xx}f_x+\frac{75379}{50371200}f_{yy}f_yf_{xx}+\frac{73097}{6105600}f_{xxxxx}\right]+$$
$$h^6\left[\frac{1}{3600}w^4f_x+\frac{102427}{54950400}ff_{yy}f_yf_{xx}+\frac{2587}{339200}f^2f_{xyyy}f_x\right]+O(h^7) \quad (18)$$

From Eq. 18, it is clear that the order of the new method is five because all the terms of h lower than h^6 are vanished.

Tested problems and numerical results: In this study, the performance of the proposed method ORK5 is compared with existing RK methods by considering the following problems. All problems below are tested using C code for solving differential equations where the solutions are periodic:

ORK5: An optimized fifth-order RK method derived in this study.

MODRK5PLDPLAM: The phase-fitted six-stage fifth-order RK method derived by Ming *et al*. (2012).

MODPHARK5S: The modified phase-fitted fifth-order RK method given in Simos and Aguiar (2001a, b).

PHRK54: The higher order method of the phase-fitted embedded RK5(4) proposed by Van de Vyver (2006).

RK-Fehlberg5th: An optimized fifth-order RK method derived by Kosti *et al*. (2010).

Problem 1: Homogeneous problem, Chawla and Rao (1985):

$$y_1 = y_2, \qquad y_1(x) = 1$$
$$y_2 = -64y_1, \quad y_2(x) = -2$$

Theoretical solution:

$$y_1(x) = -\frac{1}{4}\sin(8x)+\cos(8x)$$
$$y_2(x) = -2\cos(8x)-8\sin(8x)$$

Problem 2: In homogeneous problem, Van der Houwen and Sommeijer (1987):

$$y_1 = y_2$$
$$y_1(x) = 1$$
$$y_2 = -v^2y_1+(v^2-1)\sin(x)$$
$$y_2(x) = v+1$$

Estimated frequency: $v = 10$.
Theoretical solution:

$$y_1(x) = \cos(vx)+\sin(vx)+\sin(x)$$
$$y_2(x) = -v\sin(vx)+v\cos(vx)+\cos(x)$$

Problem 3: Almost periodic orbit problem (Stiefel and Bettis, 1969):

$$y_1 = y_3, \quad y_1(x) = 1$$
$$y_3 = -y_1+0.001\cos(x), \quad y_3(x) = 0$$
$$y_2 = y_4, \quad y_2(x) = 0$$
$$y_4 = -y_2+0.001\sin(x), \quad y_4(x) = 0.9995$$

Theoretical solution:

$$y_1(x) = \cos(x)+0.0005x\sin(x)$$
$$y_2(x) = \sin(x)-0.0005x\cos(x)$$
$$y_3(x) = -\sin(x)+0.0005x\cos(x)$$
$$y_4(x) = \cos(x)+0.0005x\sin(x)$$

Problem 4: Inhomogeneous system (Franco, 2006):

$$y_1 = y_3, \quad y_1(x) = 1$$
$$y_2 = -13y_1+12y_2+9\cos(2x)-12\sin(2x),$$
$$y_3(x) = -4$$
$$y_3 = y_4, \quad y_2(x) = 0$$
$$y_4 = 12y_1-13y_2-12\cos(2x)+9\sin(2x),$$
$$y_4(x) = 8$$

Estimated frequency: $v = 5$
Theoretical solution:

$$y_1(x) = \sin(x)-\sin(5x)+\cos(2x)$$
$$y_2(x) = \sin(x)+\sin(5x)+\sin(2x)$$
$$y_3(x) = \cos(x)-5\cos(5x)-2\sin(2x)$$
$$y_4(x) = \cos(x)+5\cos(5x)+2\cos(2x)$$

Problem 5: Inhomogeneous system, Salih *et al*. (2015):

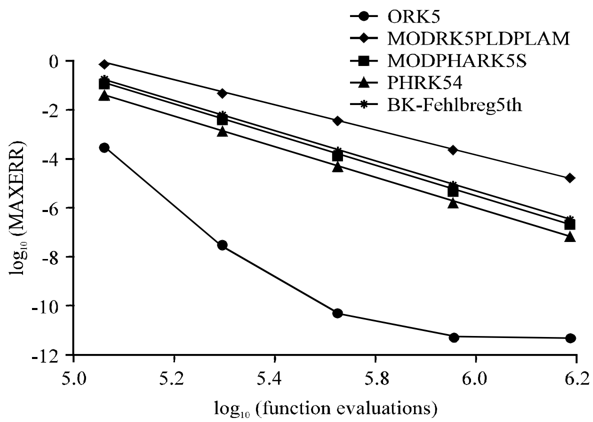

Fig. 3: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg 5th problem 1 with b = 10000

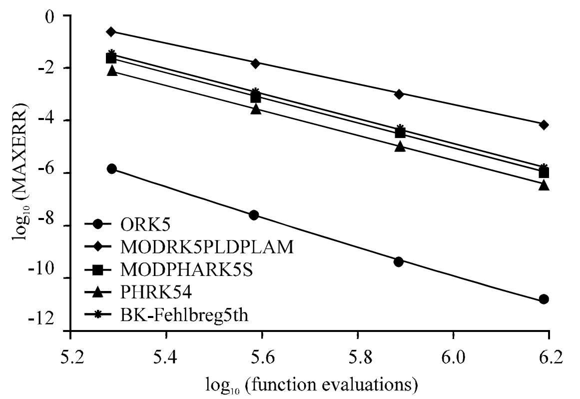

Fig. 4: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg 5th problem 2 with b = 10000

$$y_1' = y_3, \quad y_1(x) = 0$$

$$y_2' = \frac{-101}{2}y_1 + \frac{99}{2}y_2 + \frac{93}{2}\cos(2x) - \frac{99}{2}\sin(2x),$$

$$y_3(x) = -10$$

$$y_3' = y_4, \quad y_2(x) = 1$$

$$y_4' = \frac{99}{2}y_1 - \frac{101}{2}y_2 + \frac{93}{2}\sin(2x) - \frac{99}{2}\cos(2x),$$

$$y_3(x) = 12$$

Estimated frequency: $\nu = 10$

Theoretical solution:

$$y_1(x) = -\cos(10x) - \sin(10x) + \cos(2x)$$

$$y_2(x) = \cos(10x) + \sin(10x) + \cos(2x)$$

$$y_3(x) = 10\sin(10x) - 10\cos(10x) - 2\sin(2x)$$

$$y_4(x) = -10\sin(10x) + 10\cos(10x) + 2\cos(2x)$$

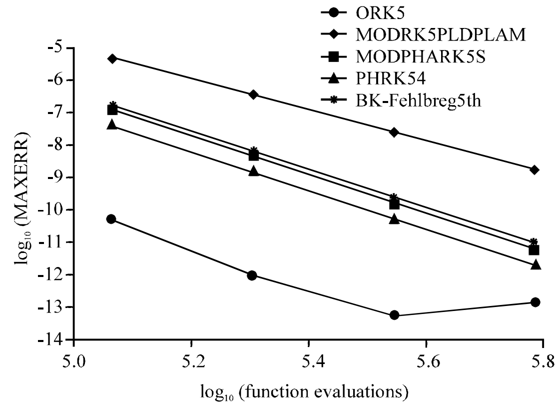

Fig. 5: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg 5th problem 3 with b = 10000

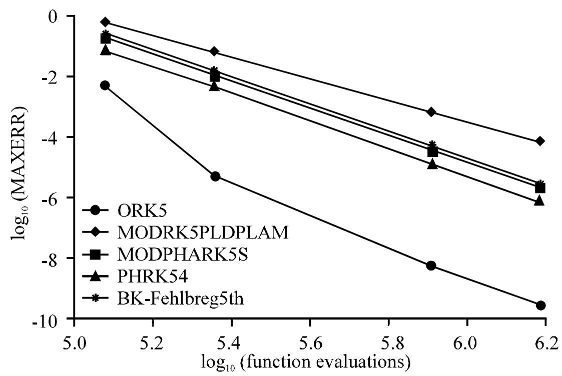

Fig. 6: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg 5th problem 4 with b = 10000

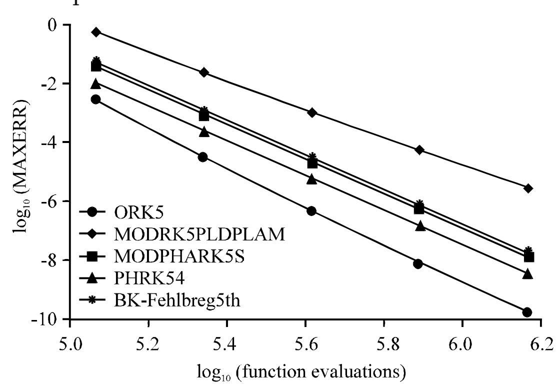

Fig. 7: Comparison for ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg 5th problem 5 with b = 10000

Figure 3-7 show the various comparisons between ORK5, MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg5th problems 1-5, respectively with b = 10000.

CONCLUSION

In this study, a six-stage fifth-order RK method denoted as ORK5 for solving first-order ODEs by first converting the second order ODEs to an equivalent first order with phase-lag and amplification error of order infinity and the first derivative of phase-lag is of order infinity is developed. The comparison is made with other well-known existing explicit RK methods that have same algebraic order which are found in Van der Houwen and Sommeijer (1987), Ming *et al.* (2012), Simos and Aguiar (2001a, b) and Van de Vyver (2006). In the numerical comparisons, we used the criteria based on computing the maximum error in the solution [Max error = max $(|y(t_n\text{-}y_n)|)$] which is equal to the maximum between absolute errors of the true solutions and the computed solutions. Figure 3-7 show the efficiency curves of Log10 (max error) against the computational effort measured by Log10 (function evaluations) required by each method and we observed that the new ORK5 method is more efficient for integration first-order differential equations possessing an oscillatory solution compared with other methods which are MODRK5PLDPLAM, MODPHARK5S, PHRK54 and RK-Fehlberg 5th.

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