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A NEW OPTIMIZED RUNGE-KUTTA METHOD FOR SOLVING OSCILLATORY PROBLEMS

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Abstract: A new explicit Runge-Kutta method of fifth algebraic order is developed in this paper, for solving second-order ordinary differential equations with oscillatory solutions. The new method has zero phase-lag, zero amplification error and zero first derivative of the phase-lag. Numerical results show that the new proposed method is more efficient as compared with other Runge-Kutta methods in the scientific literature, for the numerical integration of oscillatory problems.

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Key Words: Runge-Kutta method, phase lag, amplification error, oscillatory problems

1. Introduction

In this paper, we focus our interest in developing an optimized Runge-Kutta

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method, for the numerical integration of second-order ordinary differential equations (ODEs) with oscillatory solutions of the form

$$y''(x) = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \tag{1}$$

This type of problem occurs in various of applied fields such as quantum mechanics, electronics, physical chemistry, molecular dynamics, astronomy, chemical physics and control engineering. The equation (1) can be transformed into an equivalent system of first-order ordinary differential equations as follows

$$y'(x) = f(x, y), \quad y(x_0) = y_0, \tag{2}$$

where $f : R \times R \to R$ is a sufficiently smooth function. Problem (2) can be solved using Runge-Kutta (RK) methods or multistep methods. The solution of (2) often shows a pronounced oscillatory behaviour. Several researchers such as [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11] improved numerical methods for solving oscillatory problems based on the phase-fitted and amplification fitted properties. Phase-lag (dispersion error) is the angle between the true and the approximated solutions and amplification error (dissipation error) is the distance of the computed solution from the standard cyclic solution. Anastassi and Simos [14] proposed a phase fitted and amplification fitted Runge-Kutta method for solving orbital problems. Van de Vyver [15] developed two step hybrid methods based on phase-fitted and amplification-fitted properties. Hybrid method with zero dissipative for solving oscillatory problems constructed by Ahmad et al. [12]. Jikantoro et al. [13] derived semi-implicit hybrid method with minimized phase-lag for solving oscillatory problems. Simos and Aguiar [16] proposed a modified Runge-Kutta-Nyström method with phase lag of order infinity for solving the Schrödinger equation and related problems.

In this paper, the new method will be constructed by combining the nullification of phase-lag, amplification factor and phase-lag's derivative, based on the coefficients of Runge-Kutta RK method of algebraic order five as presented in Butcher [17].

The paper is organized as follows: In Section 2, the phase-lag properties of explicit RK method is presented. Derivation of the optimized RK method is given in Section 3. In section 4, we present numerical experiments to show the effectiveness and competency of the new optimized RK method as compared with the well known Runge-Kutta methods from the scientific literature. Conclusions are given in Section 5.

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ c_3 & a_{31} & a_{32} & & \\ \vdots & \vdots & \vdots & & \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss-1} \\ \hline & b_1 & b_2 & \dots & b_s \end{array}$$

2. Phase Lag Analysis of Runge-Kutta Method

In this section, an $s-$stage explicit Runge-Kutta method for solving ODEs (2) can be written as follows

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i, \tag{3}$$

$$k_i = f(x_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j). \quad i = 2, 3, \dots, s. \tag{4}$$

where the coefficients $a_{ij}, c_i, b_i, i = 1, \dots, s$ are constants, h is the step size The scheme (3)-(4) can be expressed in Butcher tableau as follows where the coefficients $c_2, c_3, \dots, c_s$ must satisfy the following row sum condition

$$c_i = \sum_{j=1}^{i-1} a_{ij}, \quad i = 2, 3, \dots, s \tag{5}$$

To derive the new method based on phase lag analysis, we consider the following test equation

$$y' = iwy, \quad w \in R \tag{6}$$

when the expression (3) is applied to test equation (6), we obtain the numerical solution as follows

$$y_{n+1} = a_*^n \, y_n, \qquad a_* = A(z^2) + iz\, B(z^2). \tag{7}$$

where $z = wh$ and A, B are polynomials in z^2 totally determined by the parameters a_{ij}, c_i and b_i of Runge-Kutta method (3)-(4). when we compare the exact solution with the numerical solution, it yields to the following definition of phase-lag and amplification error according to Houwen and Sommeijer [1].

Definition 1. (see [1]) In the explicit $s-$stage Runge-Kutta method defined in (3)-(4), the quantities

Table 1: Runge-Kutta method of order five

0						
$\frac{1}{3}$	$\frac{1}{3}$					
$\frac{2}{5}$	$\frac{4}{25}$	$\frac{6}{25}$				
1	$\frac{1}{4}$	-3	$\frac{15}{4}$			
$\frac{2}{3}$	$\frac{2}{27}$	$\frac{10}{9}$	$-\frac{50}{81}$	$\frac{8}{81}$		
$\frac{4}{5}$	$\frac{2}{25}$	$\frac{12}{25}$	$\frac{2}{15}$	$\frac{8}{75}$	0	
	$\frac{23}{192}$	0	$\frac{125}{192}$	0	$-\frac{27}{64}$	$\frac{125}{192}$

(i) $P(z) = z - arg[a_*(z)] \ = z - \arctan\left(z\frac{B(z^2)}{A(z^2)}\right),$

(ii) $D(z) = 1 - |a_*(z)| \ = 1 - \sqrt{(A(z^2))^2 + z^2(B(z^2))^2}.$

are called the phase lag (or dispersion error) and the amplification error (or dissipation error) of the method, respectively.

The method is said to be dispersive of order q and dissipative of order p if $P(z) = \mathrm{O}(z^{q+1})$ and $D(z) = \mathrm{O}(z^{p+1})$ respectively.
The method is called phase fitted (zero dispersive) and amplification fitted (zero dissipative) respectively, if $P(z) = 0$ and $D(z) = 0$.

3. Construction of the New Runge-Kutta Methods

In this section, an optimized Runge-Kutta method will be derived, based on the fifth-order Runge-Kutta method with six stage derived by Butcher [17], which is given in the tableau as follows (see Table 1): To achieve this, we set a_{62}, a_{63} and a_{64} as free coefficients while all other coefficients are the same as in Table 1, first we compute the polynomials $A(z^2)$ and $B(z^2)$ in terms of Runge-Kutta coefficients in Table 1. Then from these polynomials we obtain the quantities $P(z)$ and $D(z)$ and by nullification of the phase-lag, amplification error and phase- lag's derivative. Hence, we obtain a system of three equations as follows:

$$P(z) = \tan(z)\Big(1 + \Big(- \frac{1}{32} - \frac{125}{192}\,a_{62} - \frac{125}{192}\,a_{63} - \frac{125}{192}\,a_{64}\Big)z^2 + \Big(\frac{125}{384}\,a_{64} + \frac{5}{96}\,a_{63}\Big)z^4\Big) - z - \Big(- \frac{125}{192}\,a_{64} + \frac{1}{24} - \frac{25}{96}\,a_{63} - \frac{125}{576}\,a_{62}\Big)z^3 - \Big(- \frac{1}{80} + \frac{25}{128}\,a_{64}\Big)z^5 = 0, \tag{8}$$

$$\begin{aligned} D(z) = {} & \Big(\frac{1}{6400} - \frac{5}{1024}\,a_{64} + \frac{625}{16384}\,a_{64}^2\Big)z^{10} + \Big(- \frac{3125}{36864}\,a_{64}a_{62} \\ & - \frac{625}{9216}\,a_{63}a_{64} + \frac{25}{9216}\,a_{63}^2 + \frac{25}{768}\,a_{64} - \frac{21875}{147456}\,a_{64}^2 + \frac{25}{4608}\,a_{62} \\ & + \frac{5}{768}\,a_{63} - \frac{1}{960}\Big)z^8 + \Big(- \frac{67}{2880} + \frac{15625}{331776}\,a_{62}^2 - \frac{125}{6912}\,a_{62} \\ & - \frac{115}{4608}\,a_{63} + \frac{5825}{18432}\,a_{64} - \frac{15625}{110592}\,a_{64}a_{62} + \frac{625}{13824}\,a_{63}a_{62} \\ & - \frac{625}{4096}\,a_{63}a_{64}\Big)z^6 + \Big(\frac{15625}{36864}\,a_{64}^2 + \frac{15625}{36864}\,a_{63}^2 - \frac{3625}{9216}\,a_{62} \\ & - \frac{625}{1024}\,a_{64} + \frac{15625}{36864}\,a_{62}^2 + \frac{15625}{18432}\,a_{63}a_{64} + \frac{259}{3072} \\ & + \frac{15625}{18432}\,a_{64}a_{62} - \frac{385}{1024}\,a_{63} + \frac{15625}{18432}\,a_{63}a_{62}\Big)z^4 \\ & + \Big(- \frac{125}{96}\,a_{64} - \frac{125}{96}\,a_{62} - \frac{125}{96}\,a_{63} + \frac{15}{16}\Big)z^2 = 0, \end{aligned} \tag{9}$$

$$\begin{aligned} P'(z) = {} & \Big(1 + \tan^2(z)\Big)\Big(1 + \Big(- \frac{1}{32} - \frac{125}{192}\,a_{62} - \frac{125}{192}\,a_{63} \\ & - \frac{125}{192}\,a_{64}\Big)z^2 + \Big(\frac{125}{384}\,a_{64} + \frac{5}{96}\,a_{63}\Big)z^4\Big) + \tan(z)\Big(\Big(- \frac{1}{16} \\ & - \frac{125}{96}\,a_{62} - \frac{125}{96}\,a_{63} - \frac{125}{96}\,a_{64}\Big)z + \Big(\frac{125}{96}\,a_{64} + \frac{5}{24}\,a_{63}\Big)z^3\Big) \\ & - 1 - \Big(- \frac{125}{192}\,a_{64} + \frac{1}{24} - \frac{25}{96}\,a_{63} - \frac{125}{576}\,a_{62}\Big) - z^2\Big(- \frac{1}{80} \end{aligned}$$

$$+\frac{25}{128}a_{64}\Big)z^4 - z\Big(\Big(-\frac{125}{96}a_{64} + \frac{1}{12} - \frac{25}{48}a_{63} - \frac{125}{288}a_{62}\Big)z + \Big(-\frac{1}{20} + \frac{25}{32}a_{64}\Big)z^3\Big) = 0. \quad (10)$$

Solving simultaneously the system of equations (8),(9) and (10) we obtain the coefficients a_{62}, a_{63} and a_{64} which are completely depend on z when z is the product of the step-size h and the frequency w. The expressions for a_{62}, a_{63} and a_{64} are too complicated, hence we replaced by their Taylor series expansion to obtain the following expressions

$$a_{62} = \frac{12}{25} + \frac{48}{875}z^2 + \frac{32}{1875}z^4 + \frac{1157}{86625}z^6 + \frac{10785259}{1182431250}z^8 + \frac{8156483}{1289925000}z^{10} + \frac{31676135809}{7236479250000}z^{12} + \dots$$

$$a_{63} = \frac{2}{15} - \frac{32}{525}z^2 - \frac{104}{4725}z^4 - \frac{12538}{779625}z^6 - \frac{472273}{42567525}z^8 - \frac{4906436}{638512875}z^{10} - \frac{4949705143}{930404475000}z^{12} + \dots$$

$$a_{64} = \frac{8}{75} + \frac{16}{2625}z^2 + \frac{124}{23625}z^4 + \frac{791}{222750}z^6 + \frac{2620894}{1064188125}z^8 + \frac{435406187}{255405150000}z^{10} + \frac{5913223843}{5009870250000}z^{12} + \dots$$

4. Numerical Results

To evaluate the efficiency of the new optimized Runge-Kutta methods derived in this paper, we apply them to five oscillatory problems and then compared the results with some efficient methods, which are chosen from the scientific literature. In the numerical comparisons the criteria used are based on the maximum error in the solution (Max Error$=\max(|\, y(t_n) - y_n\,|)$) which is equal to the maximum between absolute errors of the true solutions and the computed solutions. Figures 1-5 show the efficiency curves of Log_{10}(Max Error) against the computational effort measured by (CPU Time Second) which is required by each method. The interval of integration for all problems is $[0, 1000]$. The following methods are used in the comparison.

- ORK5: The new optimized six-stage fifth-order Runge-Kutta method with phase-lag, the first derivative of phase-lag and amplification error of order infinity derived in Section 3 in this paper.
- RK5: The six-stage fifth-order Runge-Kutta method given in Butcher [17].
- RK5TS: The phase fitted fifth-order Runge-Kutta method proposed by Tsitouras and Simos [22].
- RK5AS: The optimized fifth-order Runge-Kutta method derived by Anastassi and Simos [10].
- RK5V: The higher order method of the phase fitted embedded RK5(4) pair proposed by Van de Vyver [23].

Problem 1: (Homogeneous problem studied by Chakravarti and Worland [18]).

$$y'' = -y, \quad y(0) = 0, \quad y'(0) = 1.$$

The exact solution is $y(x) = \sin(x)$, and the frequency is $w = 1$.

Problem 2: (Inhomogeneous equation studied by Simos [21]).

$$y'' = -100y + 99\sin(x), \quad y(0) = 1, \quad y'(0) = 11.$$

The exact solution is $y(x) = \cos(10x) + \sin(10x) + \sin(x)$, and the frequency is $w = 10$.

Problem 3: (Almost periodic orbit problem given in Stiefel and Bettis [19]).

$$y_1'' + y_1 = 0.001\cos(x), \quad y(0) = 1, \quad y'(0) = 0,$$

$$y_2'' + y_2 = 0.001\sin(x), \quad y(0) = 0, \quad y'(0) = 0.9995.$$

The exact solutions are $y_1(x) = \cos(x) + 0.0005x\sin(x)$ and $y_2(x) = \sin(x) - 0.0005x\cos(x)$. The frequency is $w = 1$.

Problem 4: (Inhomogeneous linear system studied by Franco [20]).

$$y'' + \begin{pmatrix} \frac{101}{2} & -\frac{99}{2} \\ -\frac{99}{2} & \frac{101}{2} \end{pmatrix} y = \begin{pmatrix} \frac{93}{2}\cos(2x) & -\frac{99}{2}\sin(2x) \\ \frac{93}{2}\sin(2x) & -\frac{99}{2}\cos(2x) \end{pmatrix},$$

$$y(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} -10 \\ 12 \end{pmatrix}.$$

The frequency is $w = 10$, and the exact solution is

$$y(x) = \begin{pmatrix} -\cos(10x) - \sin(10x) + \cos(2x) \\ \cos(10x) + \sin(10x) + \sin(2x) \end{pmatrix}$$

Problem 5: (The oscillatory system studied by Franco [24]).

$$y'' + \begin{pmatrix} 13 & -12 \\ -12 & 13 \end{pmatrix} y = \begin{pmatrix} 9\cos(2x) - 12\sin(2x) \\ -12\cos(2x) + 9\sin(2x) \end{pmatrix},$$

$$y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} -4 \\ 8 \end{pmatrix}$$

The frequency is $w = 5$, and the exact solution is

$$y(x) = \begin{pmatrix} \sin(x) - \sin(5x) + \cos(2x) \\ \sin(x) + \sin(5x) + \sin(2x) \end{pmatrix}$$

5. Conclusion

A new fifth-order Runge-Kutta method with phase-lag and amplification error of order infinity, also the first derivative of the phase-lag is of order infinity is developed in this paper. The method is then used to solve second-order ordinary differential equations whose solutions have oscillatory properties by reducing it first to a system of first-order ODEs. Numerical results illustrate that the new method is more efficient in solving special second-order ODEs with oscillatory solution as compared with other methods of the same order.

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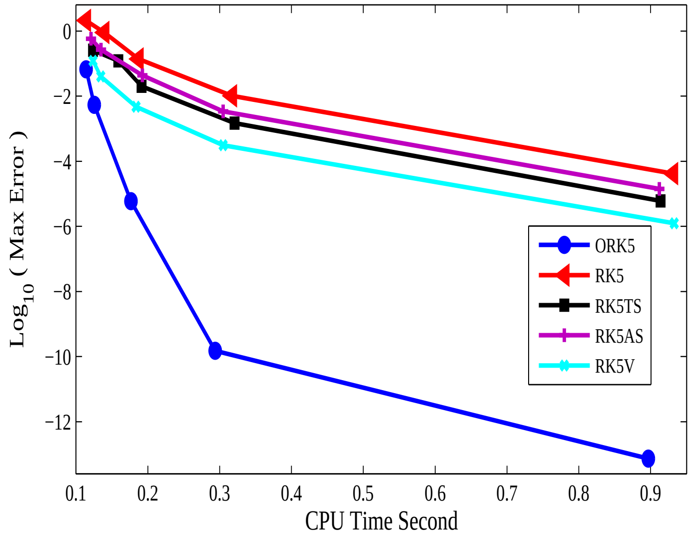

Figure 1: The efficiency curves for Problem 1 with $h = 1, 0.875, 0.625, 0.375, 0.125$.

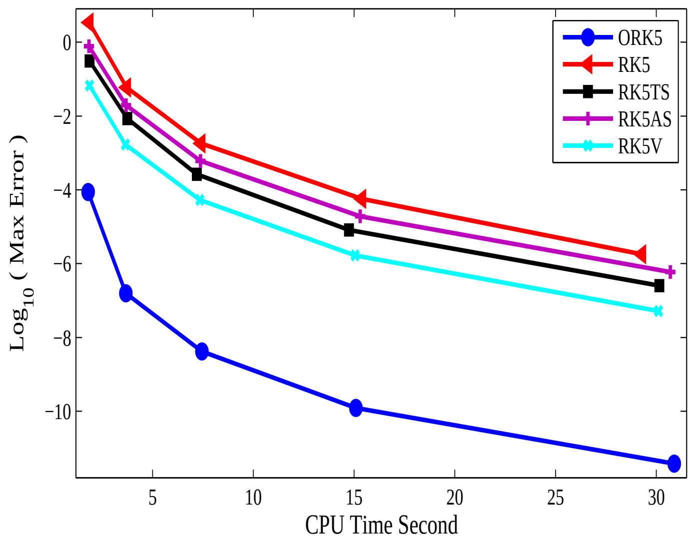

Figure 2: The efficiency curves for Problem 2 with $h = 1/2^i, i = 4, \ldots, 8$.

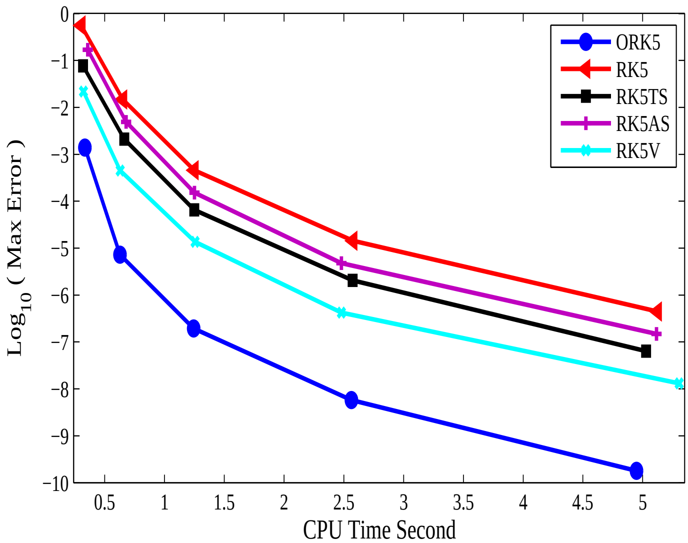

Figure 3: The efficiency curves for Problem 3 with $h = 0.8/2^i, i = 0, \ldots, 4$.

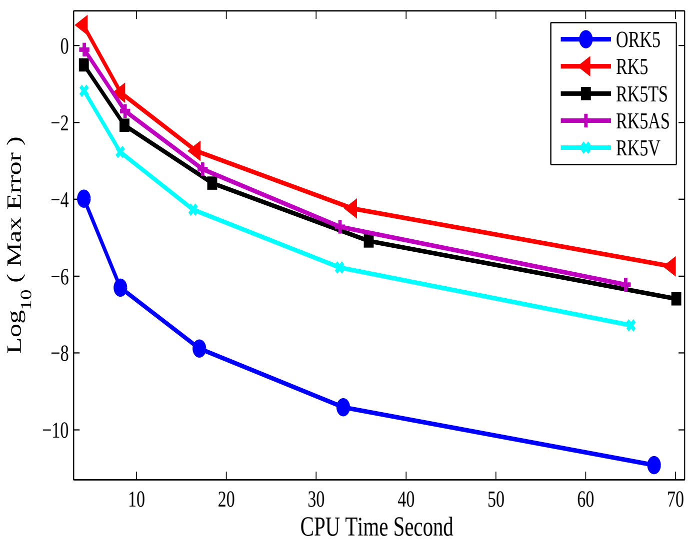

Figure 4: The efficiency curves for Problem 4 with $h = 1/2^i, i = 4, \ldots, 8$.

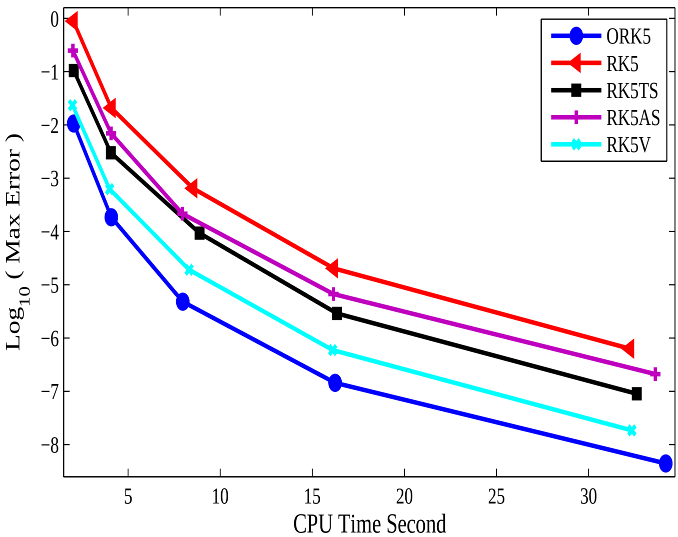

Figure 5: The efficiency curves for Problem 5 with $h = 1/2^i, i = 3, \ldots, 7$.

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