Solving Oscillatory Problems Using An Optimized Runge–Kutta Method

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Abstract: New explicit Runge–Kutta method with zero phase-lag, zero first derivative of the phase-lag and zero amplification error is derived for the effective numerical integration of second-order initial-value problems with oscillatory solutions in this paper. The new method is based on the sixth-stage fifth-order Runge–Kutta method. Numerical illustrations show that the new proposed method is much efficient as compared with other Runge–Kutta methods in the scientific literature, for the numerical integration of oscillatory problems.

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 method, for the numerical integration of second order initial value problems IVPs with oscillatory solutions of the form

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

This type of problem occurs in a various of applied fields such as quantum mechanics, electronics physical chemistry, molecular dynamics, astronomy, chemical physics and control engineering. Which can transform into the form of an equivalent system of first-order ordinary differential equations as follows

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

where $f : R \times R \to R$ is a sufficiently smooth function. The problem (2) can be solved using Runge–Kutta (RK) methods or multistep methods. Often the solution of (2) shows a pronounced oscillatory behaviour. Several researchers improved numerical methods based on the phase fitted and amplification fitted properties (see for instance [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]). 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 [18] proposed a phase fitted and amplification fitted Runge–Kutta method for solving orbital problems. Van de Vyver [19] developed two step hybrid methods based on phase-fitted and amplification-fitted properties. hybrid method with zero dissipative for solving oscillatory problems constructed by Ahmed et. al. [16]. Jikantoro et. al [17] derived semi-implicit hybrid method with minimized phase-lag for solving oscillatory problems. Simos and Aguiar [20] proposed a modified Runge-Kutta-Nystrom method with phase lag of order infinity for solving the Schrödinger equation and related problems.

In this paper, we will construct a new explicit Runge–Kutta methods using the technique of phase-lag and the first derivative of phase-lag of order infinity,also the amplification error is of order infinity, based on the coefficients of Runge–Kutta method of algebraic order five as presented in Butcher [21]. The paper is organized as follows: In section 2, we present the phase lag properties of explicit Runge–Kutta RK method. In section 3, we introduce the construction of the new explicit Runge-Kutta methods with zero phase-lag, phase lag's derivative and amplification error. In section 4, we give numerical experiments to show the effectiveness and competence of the new optimized Runge–Kutta method as compared with the well known Runge–Kutta methods from the scientific literature. Conclusions is given in section 5.

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

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

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

where the coefficients $a_{ij}, c_i, b_i, i = 1, \ldots, s$ are constants, h is the step size The scheme (3)-(4) can be expressed in Butcher tableau as follows

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

where the coefficients $c_2, c_3, \ldots, c_s$ must satisfy the following row sum condition

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

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 method 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.

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

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

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

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 $D(z) = \mathrm{O}(z^{p+1})$.
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 by nullifying the phase lag, the first derivative of phase lag and amplification error which is based on the five algebraic order Runge–Kutta method of six stage, which is given in Butcher tableau (see Table 1).

Table 1: Runge–Kutta method of order five

$$\begin{array}{c|cccccc} 0 & & & & & & \\ \frac{1}{3} & \frac{1}{3} & & & & & \\ \frac{2}{5} & \frac{4}{25} & \frac{6}{25} & & & & \\ 1 & \frac{1}{4} & -3 & \frac{15}{4} & & & \\ \frac{2}{3} & \frac{2}{27} & \frac{10}{9} & -\frac{50}{81} & \frac{8}{81} & & \\ \frac{4}{5} & \frac{2}{25} & \frac{12}{25} & \frac{2}{15} & \frac{8}{75} & 0 & \\ \hline & \frac{23}{192} & 0 & \frac{125}{192} & 0 & -\frac{27}{64} & \frac{125}{192} \end{array}$$

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, firstly we compute the polynomials $A(z^2)$ and $B(z^2)$ in terms of Runge–Kutta method parameters in Table 1. Then from these polynomials we obtain the quantities $P(z)$ and $D(z)$, and by requiring of vanishing the phase lag, amplification error and phase lag's derivative.

Through that we obtain a system of three equations as follows:

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

$$P'(z)=\Big(1+\tan^2(z)\Big)\Big(1+\Big(-\frac{1}{32}-\frac{125}{192}a_{62}-\frac{125}{192}a_{63}-\frac{125}{192}a_{64}\Big)z^2+\Big(\frac{125}{384}a_{64}+\frac{5}{96}a_{63}\Big)z^4\Big)+\tan(z)\Big(2\Big(-\frac{1}{32}-\frac{125}{192}a_{62}-\frac{125}{192}a_{63}-\frac{125}{192}a_{64}\Big)z+4\Big(\frac{125}{384}a_{64}+\frac{5}{96}a_{63}\Big)z^3\Big)-1-\Big(-\frac{125}{192}a_{64}+\frac{1}{24}-\frac{25}{96}a_{63}-\frac{125}{576}a_{62}\Big)z^2-\Big(-\frac{1}{80}+\frac{25}{128}a_{64}\Big)z^4-z\Big(2\Big(-\frac{125}{192}a_{64}+\frac{1}{24}-\frac{25}{96}a_{63}-\frac{125}{576}a_{62}\Big)z+4\Big(-\frac{1}{80}+\frac{25}{128}a_{64}\Big)z^3\Big)=0. \quad (9)$$

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

Solving simultaneously the system of equations (8),(10) and (9) we obtain the coefficients a_{62}, a_{63} and a_{64} which are completely depend on z, where z is the product of the step-size h and the frequency of the method w. The expressions for a_{62}, a_{63} and a_{64} are too complicated. As $z\to 0$, they have the Taylor series expressions as follows:

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

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

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

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. We use in the numerical comparisons the criteria based on computing 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 five-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 five-order Runge–Kutta method given in Butcher [21].
- RK5TS: The phase fitted five-order Runge–Kutta method proposed by Tsitouras and Simos [27].
- RK5AS: The optimized fifth-order Runge–Kutta method derived by Anastassi and Simos [26].
- RK5V: The higher order method of the phase fitted embedded RK5(4) pair proposed by Van de Vyver [28].

Problem 1: (Homogeneous problem studied by Chakravarti and Worland [22]).

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

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

Problem 2: (Inhomogeneous equation studied by Simos [25]).

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

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

Problem 3: (Almost periodic orbit problem given in Stiefel and Bettis [23]).

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

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

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 [24]).

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

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

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 [29]).

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

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

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

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

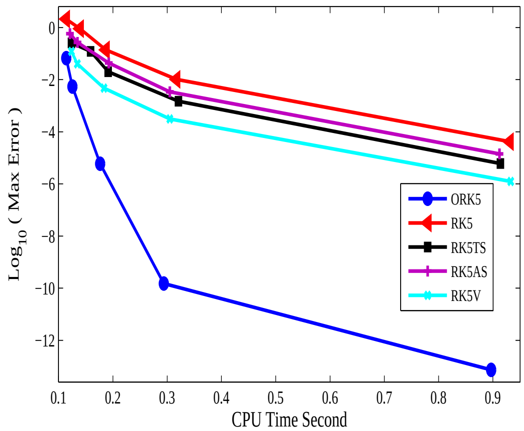

Figure 1: The efficiency curves for Problem 1 with $h = 1, 0.875, 0.625, 0.375, 0.125$.

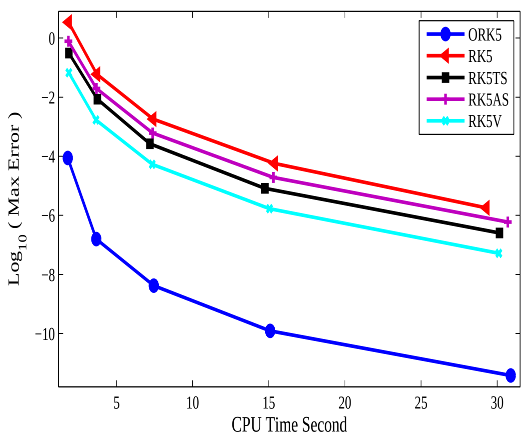

Figure 2: The efficiency curves for Problem 2 with $h = 1/2^i, i = 4, \ldots, 8$.

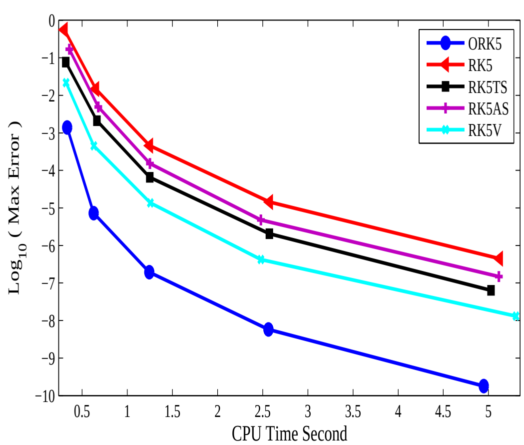

Figure 3: The efficiency curves for Problem 3 with $h = 0.8/2^i, i = 0, \ldots, 4$.

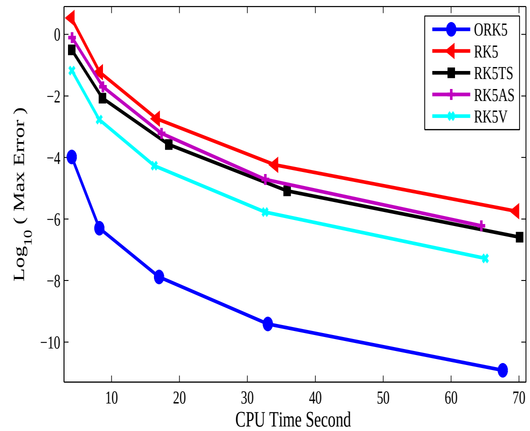

Figure 4: The efficiency curves for Problem 4 with $h = 1/2^i, i = 4, \ldots, 8$.

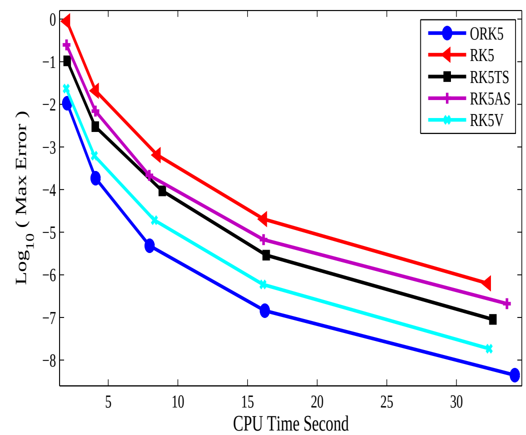

Figure 5: The efficiency curves for Problem 4 with $h = 1/2^i, i = 3, \ldots, 7$.

5 Conclusion

In the present paper, zero phase lag and the first derivative of phase lag Runge–Kutta method of order six with amplification error of order infinity is constructed for solving second order ordinary differential equations whose solutions have oscillatory properties. The numerical tests illustrate that the new method is much efficient for solving special second order IVPs with oscillatory solution as compared with other methods of the same order.

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