An Embedded 5(4) Pair of Optimized Runge-Kutta Method for the Numerical Solution of Periodic Initial Value Problems

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Abstract
This paper presents an alternative method for developing effective embedded optimized Runge-Kutta (RK) algorithms to solve oscillatory problems numerically. The embedded scheme approach has algebraic orders of 5 and 4. By transforming second-order ordinary differential equations (ODEs) into their first-order counterpart, the suggested approach solves first-order ODEs. The amplification error, phase-lag, and first derivative of the phase-lag are all nil in the embedded pair. The alternative method’s absolute stability is demonstrated. The numerical tests are conducted to demonstrate the effectiveness of the developed approach in comparison to other RK approaches. The alternative approach outperforms the current RK methods.

Keywords: Runge-Kutta Methods, Amplification error, Phase-lag, Ordinary Differential Equations, Oscillatory problems, Initial Value Problems (IVPs).

1. Introduction
Consider the initial value problem of first-order ordinary differential equation as follows:

\[ y' = f(x,y), \quad y(x_0) = y_0 \]  

(1)

whose solutions show a periodical behavior. This type of issue can be seen in a variety of
applied scientific domains, such as orbital mechanics, mechanics and electronics [1,2]. Most periodic behavior disorders are second-order or higher-order in nature. To solve the ODEs, it is critical to reducing higher-order issues to the first-order problem (1). Several numerical methods for the approximate solution of the general ordinary differential equations with oscillating solutions have been developed in recent decades, the most common methods are trigonometrically, exponentially-fitted, and phase-fitted, amplification-fitted for RK, Runge-Kutta–Nystrom (RKN), see [1-4]. For the numerical solution of the Schrödinger equation with an infinite phase-lag, Simos and Aguiar [5] suggested a modified RK procedure then an exponentially-fitted RK method was constructed, see [6]. Furthermore, Fawzi et al. [7] developed a four-stage phase-fitted and amplification-fitted RK device by combining the concept of infinite phase lag and zero amplification error. Then, Fang et al. [8] proposed a new embedded pair (RK) approach for numerical integration of the oscillatory problems with FSAL properties. Meanwhile, for solving oscillatory problems, Senu et al. [9] developed a new pair of embedded explicit RKN methods. In [10, 11], the authors established a new embedded 4(3) and 6(4) pairs of explicit RK methods, and they established a new phase suited to modified RK pair for the numerical solution of the Schrödinger equation, which was specially designed to the numerical solution of an oscillatory problem. After that, Fawzi et al. [12, 13] evolved a new efficient embedded 6(5) pair trigonometrically-fitted explicit RK method and created a new efficient embedded phase-fitted modified RK method. Recently, a new optimized RK method for solving oscillatory problems was developed, see [14, 15].

Finally, we construct a new form of phase-fitting RK embedded pair in this study by nullifying the phase-lag, the first derivative of the phase-lag of the fifth-order technique, and the phase-lag of the fourth-order technique.

The following is the structure of this paper: The phase-lag properties of the explicit RK method are presented in section 2. Section 3 explains how to derive the optimized RK process. Meanwhile, the description of the stability property is discussed in section 4. In section 5, numerical results are provided to demonstrate the efficiency and competency of the new method compared to the well-known RK method. Finally, the discussion and conclusion are dealt with in section 6.

2. Basic Concepts

2.1. Phase-Lag Analysis of Runge-Kutta Method

We look at the m-stage explicit RK technique, which is given as follows:

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

(2)

$$K_i = f \left( x_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} K_j \right). \quad i = 1, ..., m$$

(3)

When $a_{ij} = 0$ for $i, j$, the method is considered to be explicit; otherwise, it is said to be implicit. The methods in (2) and (3) can be condensed into a Butcher tableau, see Table 1.

**Table 1** m-stage explicit RK method

<table>
<thead>
<tr>
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<th>0</th>
<th>$c_2$</th>
<th>$a_{21}$</th>
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<tr>
<td>$c_m$</td>
<td>$a_{m1}$</td>
<td>...</td>
<td>$a_{m,m-1}$</td>
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<td>3890</td>
<td>$b_1$</td>
<td>...</td>
<td>$b_m$</td>
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To construct the new technique based on phase-lag analysis, we use the following test equation from [16].

\[ y' = ivy \]  

where \( v \) is real. Then we examine the theoretical and numerical solutions for this equation. By requiring that the solutions are to be in phase with maximal order in the step-size \( h \), the so-called dispersion relation [7] is constructed. When we apply the methods (2) and (3) above to the test equation (4), we get

\[ y_n = a^n y_0 \]

With

\[ a_* = A_m(H^2) + iHB_m(H^2), \quad H = vh \]  

\[ a_1 = a_*(H) \] is the amplification factor, and \( y_n \) is the approximation to \( y(x_n) \). The dispersion or phase error or phase-lag and the amplification error, are defined by comparing (5) with the solution to (4).

**Definition 2.1.** [7] The dispersion or phase error or phase lag and the amplification error are the quantities in an explicit \( m \)-stage RK, as it is shown in Table 1:

\[ t(H) = H - \arg[a_*(H)], \quad a(H) = 1 - |a_*(H)| \]  

Thus, the method is described as phase-lag order \( r \) with dissipative order \( s \). If \( t(H) = O(H^{r+1}) \), and \( a(H) = O(H^{s+1}) \)

, then from (6), it follows that

\[ a(H) = 1 - \sqrt{[A_m^2(H) + H^2B_m^2(H^2)]} \]  

Meanwhile, the direct computation of the phase-lag order \( r \) and the phase-lag constant \( q \) for the Runge-Kutta method indicated in Table 1 is done using the following formula.

\[ \tan(H) - H \frac{B_m(H^2)}{A_m(H^2)} = qH^{r+1} + O(H^{s+3}). \]  

The dispersion and dissipation variables that stated above are used to examine phase-fitted (order infinity dispersion) and amplification-fitted (order infinity dissipation). The RK system is phase-fitted and amplification-fitted if the following conditions are met.

\[ t(H) = 0 \quad \text{and} \quad a(H) = 0. \]  

2.2. Derivation of Embedded Optimized RK Method

In (2), an explicit \( m \)-stage RK process formula is presented. The order \( q \) RK method \( (c, A, b) \) and another RK method \( (c, A, b') \) of the order \( p < q \) are used to create the embedded pair \( q(p) \). Butcher tableau is a feature of an embedded pair.

\[
\begin{array}{c|cc}
  c & A & b \\
  \hline
  b^r & b^s
\end{array}
\]

A variable step size algorithm uses an embedded pair of explicit Runge-Kutta methods since they provide a low-cost error estimate. We get an approximate error from the embedded method.

\[ EST_{n+1} = \|y_{n+1} - y_{n+1}^*\| \]  

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We used the step-size control method described in [17] to integrate the equation (1) numerically:

- if \( \frac{\text{EST}_{n+1}}{100} < \frac{\text{Tol}}{100} \), \( h_{n+1} = 2h_n \),
- if \( \frac{\text{Tol}}{100} \leq \frac{\text{EST}_{n+1}}{100} < \text{Tol} \), \( h_{n+1} = h_n \)
- if \( \text{EST}_{n+1} \geq \text{Tol} \), \( h_{n+1} = \frac{h_n}{2} \) and repeat the step.

\( TOL \) stands for the required local error. It is worth noting that the \((n + 1)\) th-step's initial value is the \(q\) th-order approximation \( y_n \), this implies that the embedded pair is employed in local extrapolation mode or higher-order mode.

3. Construction of the New Embedded Pair

In this section, we will develop an embedded pair optimized RK method based on [18] fifth-order RK method with seven stages, as it is illustrated in the tableau (see Table 2), where the method \((c, A, b)\) is of order five and \((c, A, b^\ast)\) is of order four. We set free coefficients \( b_1, b_2, b_3, b_1^\ast, b_2^\ast, b_3^\ast \), while keeping all other coefficients as the same as in Table 2. First, we compute the polynomials \( A^\ast_m \) and \( B^\ast_m \) in terms of RK coefficients in Table 2. The numbers \( t(H) \) and \( a(H) \) are then obtained by nullifying the phase-lag, amplification error, and phase-derivative lag from these polynomials.

As a result, when we solve the fifth-order as follows, we get a system of three equations:

**Table 2** - RK method of order five

\[
\begin{array}{cccccc}
0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\
\frac{2}{3} & \frac{1}{5} & 0 & 0 & 0 & 0 \\
\frac{4}{5} & \frac{1}{5} & \frac{9}{20} & \frac{1}{5} & 0 & 0 \\
\frac{8}{9} & \frac{13}{21} & \frac{64}{77} & \frac{212}{77} & 0 & 0 \\
1 & \frac{31}{38} & \frac{2}{5} & \frac{196}{115} & \frac{221}{115} & \frac{11}{15} \\
1 & \frac{31}{36} & 0 & \frac{100}{115} & \frac{125}{115} & \frac{11}{15} & 0 \\
1 & \frac{31}{36} & 0 & \frac{100}{115} & \frac{125}{115} & \frac{11}{15} & 0 \\
\end{array}
\]

\[a(H) = \left(1 - \frac{1}{24}H^4 + \frac{1}{24}H^4 + QH^2\right)^2 - 1 = 0\]  \( (11) \)

\[t(H) = \tan(H) - \frac{H\left(1 - \frac{1}{24}H^4 + \frac{1}{24}H^4 + QH^2\right)}{1 - \frac{1}{600}H^6 + \frac{1}{24}H^4 + QH^2} = 0\]  \( (12) \)
\[ t'(H) = 1 + (\tan(H))^2 - \left( \frac{1}{120} H^4 + PH^2 + b_1 + b_2 + b_3 + \frac{65479}{142464} \right) \left( 1 - \frac{1}{600} H^6 + \frac{1}{24} H^4 + QH^2 \right) \]
\[ + H \left( \frac{1}{120} H^4 + PH^2 + b_1 + b_2 + b_3 + \frac{65479}{142464} \right) \left( -\frac{1}{100} H^5 + \frac{1}{6} H^3 + 2QH \right) \]
\[ - \frac{H \left( \frac{1}{50} H^3 + 2PH \right)}{\left( 1 - \frac{1}{600} H^6 + \frac{1}{24} H^4 + QH^2 \right)^2} \]
(13)

Where
\[ p = -\frac{163}{1113} - \frac{9}{200} b_3 \quad \text{and} \quad Q = -\frac{3}{10} b_3 - \frac{1}{5} b_2 - \frac{271}{742} \]

The same case for the fourth-order method

\[ a(H) = \left( -\frac{1}{24000} H^6 + \frac{1097}{120000} H^4 + PH^2 + b_1' + b_2' + b_3' + \frac{3252437}{7123200} \right)^2 H^2 \]
\[ + \left( 1 - \frac{161}{120000} H^6 + \frac{1}{24} H^4 + QH^2 \right)^2 - 1 = 0 \]  
(14)

\[ t(H) = \tan(H) - \frac{H \left( -\frac{1}{24000} H^6 + \frac{1097}{120000} H^4 + PH^2 + b_1' + b_2' + b_3' + \frac{3252437}{7123200} \right)}{\left( 1 - \frac{161}{120000} H^6 + \frac{1}{24} H^4 + QH^2 \right)} \]
\[ = 0 \]  
(15)

\[ t'(H) = 1 + (\tan(H))^2 - \frac{\left( 1 \frac{407}{24000} H^6 + \frac{1097}{120000} H^4 + PH^2 + b_1' + b_2' + b_3' + \frac{3252437}{7123200} \right)}{\left( 1 - \frac{161}{120000} H^6 + \frac{1}{24} H^4 + QH^2 \right)^2} \]
\[ + H \left( -\frac{1}{24000} H^6 + \frac{1097}{120000} H^4 + PH^2 + b_1' + b_2' + b_3' + \frac{3252437}{7123200} \right) \left( -\frac{161}{2000} H^5 + \frac{1}{6} H^3 + 2QH \right) \]
\[ - \frac{H \left( -\frac{1}{4000} H^5 + \frac{1097}{30000} H^3 + 2PH \right)}{\left( 1 - \frac{161}{120000} H^6 + \frac{1}{24} H^4 + QH^2 \right)} \]
(16)

Where
\[ p = -\frac{9}{200} b'_3 - \frac{162787}{1113000} \quad \text{and} \quad Q = -\frac{10127}{27825} - \frac{3}{10} b'_3 - \frac{1}{5} b'_2 \]

When the system of equations (3) - (16) is solved simultaneously, the coefficients \( b_1, b_2, b_3, b'_1, b'_2 \) and \( b'_3 \) are obtained, which are completely contingent on \( H \) when \( H \) is the product of step-size \( h \) and frequency \( v \) because the expressions for \( b_1, b_2, b_3, b'_1, b'_2 \) and \( b'_3 \) are too complex, we replaced them with their Taylor series expansion, yielding the following expressions:

\[ b_1 = \frac{35}{384} + \frac{643}{45360} H^4 + \frac{62677}{16329600} H^6 + \frac{5933}{4435200} H^8 + \frac{50184187}{93405312000} H^{10} + \frac{11769096931200}{2560520257} H^{12} + \ldots \]
4. Stability of the New Method

The linear stability of the developed method is examined in this section. Consider the following test equation (4) where \( v > 0 \). The exact solution of this equation with the initial value \( y(x_0) = y_0 \) satisfies

\[
y(x_0 + h) = R(H)y_0 ,
\]

when applying (2), (3) to (4), we get

\[
y_{n+1} = R(H)y_0
\]

\[
R(H) = 1 + Hb^T (1 - HA)^{-1} e
\]

Where \( e = (1, \ldots, 1)^T \), \( A = [a_{ij}] \) and \( b^T = [b_1, b_2, b_3, \ldots, b_m] \). \( R(H) \) is referred to the stability function of the method (3).

**Definition 4.1.** If an RK method is absolutely stable, then for all \( H \in (-h, 0), |\hat{R}(H)| < 1 \).

The stability function of the high order of the new method is

\[
R(H) = 1 + H^{\frac{3}{2}}H^2 + H^3 + \frac{1}{3628800}H^6 + \frac{1}{479001600}H^{11} - \frac{1}{10378368000}H^{13}
\]
We repeat the procedure for the low order of the new method, and then the stability function is computed.

\[
R(H) = 1 + \frac{57671}{57600} H + \frac{13505}{27136} H^2 + \frac{1675}{10176} H^3 + \frac{311}{7632} H^4 + \frac{565457}{2268000} H^5 + \frac{97}{64800} H^6 \\
+ \frac{10176}{182673} H^7 - \frac{40320}{111961} H^8 + \frac{567705600}{165523} H^9 + \frac{3628800}{37065600000} H^{10} \\
+ \frac{49896000000}{479001600} H^{11} - \frac{1}{479001600} H^{12} + \frac{37065600000}{37065600000} H^{13}
\]

(23)

The stability region of the EORK5(4) method up to \( H^i \), where \( i = 10 \). The stability interval of the fifth-order and fourth-order methods with the coefficients \( H^{10} \) is \((-2,0)\). Our proposed technique is absolutely stable because \( |R(H)| < 1 \) as is shown in the stability areas that are displayed in Figures 1 and 2. We used the Maple program to collect this information.

5. Tested Problems and Numerical Results

The output of the proposed method EORK5(4) is compared to that of existing RK methods in this section, which takes into account the following issues. All of the problems below are evaluated using the \( C++ \) program for solving differential equations with periodic solutions.

- **TOL**: Tolerance.
- **FCN**: Number of function evaluations.
- **FSTEP**: Failure steps.
- **MAXE**: Maximum error of the computed solution.
- **EORK5(4)**: the new embedded RK5(4) pair given in this paper.
• MODRK54: Modified RK method derived in [19].
• MODPHARK5(4): A phase-fitted modified RK pair is given in [10].
• MODDPHARK5(4): The higher order Optimized Runge-Kutta Pair proposed in [20].

**Problem 1: (Inhomogeneous Equation) [12]**

\[ y'' = -100y + 99 \sin(x), \quad y(x_0) = 1, \quad y'(x_0) = 11 \]

Estimated frequency: \( v = 10 \)

Theoretical solution:

\[ y_1(x) = \cos(vx) + \sin(vx) + \sin(x) \]

**Problem 2: (Inhomogeneous linear system) [21]**

\[
\begin{align*}
    y''(x) + \left( \frac{101}{2} y - \frac{99}{2} \right) y &= \left( \frac{93}{2} \cos(2x) - \frac{99}{2} \sin(2x) \right) y(x) = \left( \frac{93}{2} \right) \sin(2x) - \frac{99}{2} \cos(2x) \\
    y(0) &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} -10 \\ 12 \end{pmatrix}
\end{align*}
\]

The frequency is \( w = 10 \), and the exact solution is

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

**Problem 3: (Inhomogeneous system) [13]**

\[
\begin{align*}
    y''_1 &= \frac{-y_1}{\left(\sqrt{y_1^2 + y_2^2}\right)^3}, \quad y_1(0) = 1, \quad y_1'(0) = 0 \\
    y''_2 &= \frac{-y_2}{\left(\sqrt{y_1^2 + y_2^2}\right)^3}, \quad y_2(0) = 0, \quad y_2'(0) = 1
\end{align*}
\]

Exact solutions:

\[
    y_1(t) = \cos(t), \quad y_2(t) = \sin(t)
\]

**Problem 4: (The oscillatory system) [21]**

\[
\begin{align*}
    y''(t) + \left( \frac{13}{12} \right) y(t) &= \begin{pmatrix} 9 \cos(2x) & -12 \sin(2x) \\ -12 \cos(2x) & +9 \sin(2x) \end{pmatrix}, \\
    y(0) &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} -4 \\ 8 \end{pmatrix}
\end{align*}
\]

The frequency is \( w = 5 \), and the exact solution is

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

**Table 3—Comparison of Numerical Results When Solving Problem 1**

<table>
<thead>
<tr>
<th>TOL</th>
<th>Method</th>
<th>STEP</th>
<th>FCN</th>
<th>FSTEP</th>
<th>MAXE</th>
</tr>
</thead>
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<td>10^{-2}</td>
<td>EORK5(4)</td>
<td>132</td>
<td>1038</td>
<td>19</td>
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Figure 3-Curves of efficiency for Problem 1 with $X_{\text{end}} = 10$

Table 4-Comparison of Numerical Results When Solving Problem 2

<table>
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<th>TOL</th>
<th>Method</th>
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<th>FCN</th>
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Figure 4-Curves of efficiency for Problem 2 with $X_{end} = 5$

Table 5- Comparison of Numerical Results When Solving Problem 3

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Figure 5- Curves of efficiency for Problem 3 with $X_{end} = 3$

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Figure 6-Curves of efficiency for Problem 4 with $X_{end} = 10$

6. Discussion and Conclusion

We have developed a new embedded RK method for solving first-order (ODEs) called EORK5(4) by converting second-order ODEs to equivalent first-order ODEs with phase-lag and amplification error, as well as the first derivative of phase-lag of order infinity. The comparison is made with other well-known existing explicit RK methods with the same algebraic order found in [10] and [19, 20]. We apply criteria based on determining the largest error in the solution $(max\ error = max(|y(t_n - y_n)|))$ in numerical comparisons, which is equivalent to the maximum difference between absolute errors of true and computed solutions. The numerical obtained as it is shown in Table 3 to 6 and graphically as it is shown in Figures 3-6 which displays the efficiency curves of $Log10$ (max error) against the computational effort calculated by $Log10$ (function evaluations) required by each method, and we observed that the new EORK5(4) method is more effective than other existing RK methods for integration first-order ODEs with an oscillatory solution.

References
[8] Y. Fang, Y. Song, X. Wu, New embedded pairs of explicit runge–kutta methods with fsal


