A Family of Runge-Kutta Methods with Zero Phase-Lag and Derivatives for the Numerical Solution of the Schrödinger Equation and Related Problems

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Abstract. We construct a family of two new optimized explicit Runge-Kutta methods with zero phase-lag and derivatives for the numerical solution of the time-independent radial Schrödinger equation and related ordinary differential equations with oscillating solutions. The numerical results show the superiority of the new technique of nullifying both the phase-lag and its derivatives.

Keywords: Phase-Fitting, Derivative, Schrödinger Equation, Runge-Kutta, Explicit methods

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1. Introduction

Much research has been done on the numerical integration of the radial Schrödinger equation:

\[ y''(x) = \left( \frac{l(l+1)}{x^2} + V(x) - E \right) y(x) \]  

where \( \frac{l(l+1)}{x^2} \) is the centrifugal potential, \( V(x) \) is the potential, \( E \) is the energy and \( W(x) = \frac{l(l+1)}{x^2} + V(x) \) is the effective potential. It is valid that \( \lim_{x \to \infty} V(x) = 0 \) and therefore \( \lim_{x \to \infty} W(x) = 0 \).

Many problems in chemistry, physics, physical chemistry, chemical physics, electronics etc., are expressed by equation (1).

In this paper we will study the case of \( E > 0 \). We divide \([0, \infty]\) into subintervals \([a_i, b_i]\) so that \( W(x) \) is a constant with value \( W_i \). After this the problem (1) can be expressed by the approximation

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\[ y''_i = (\tilde{W} - E) y_i, \] whose solution is
\[ y_i(x) = A_i \exp \left( \sqrt{\tilde{W} - E} x \right) + B_i \exp \left( -\sqrt{\tilde{W} - E} x \right), \tag{2} \]
\[ A_i, B_i \in \mathbb{R}. \]

There has been an extended bibliography on the development and analysis of numerical methods for the efficient solution of the Schrödinger equation: see for example [1]-[129].

2. Basic theory

2.1. Explicit Runge-Kutta methods

An \( s \)-stage explicit Runge-Kutta method used for the computation of the approximation of \( y_{n+1}(x) \), when \( y_n(x) \) is known, can be expressed by the following relations:

\[
y_{n+1} = y_n + \sum_{i=1}^{s} b_i k_i
\]
\[
k_i = h f \left( x_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j \right), \quad i = 1, \ldots, s
\tag{3}
\]

where in this case \( f (x, y(x)) = (W(x) - E) y(x). \)

Actually to solve the second order ODE (1) using first order numerical method (3), (1) becomes:

\[
z'(x) = (W(x) - E) y(x)
\]
\[
y'(x) = z(x)
\tag{4}
\]

while we use two sets of equations (3): one for \( y_{n+1} \) and one for \( z_{n+1} \). The method shown above can also be presented using the Butcher table below:

\[
\begin{array}{c|ccc}
0 \\
c_2 & a_{21} \\
c_3 & a_{31} & a_{32} \\
\vdots & \vdots & \vdots \\
c_s & a_{s1} & a_{s2} & \ldots & a_{s,s-1} \\
\hline
b_1 & b_2 & \ldots & b_{s-1} & b_s
\end{array}
\tag{5}
\]

Coefficients \( c_2, \ldots, c_s \) must satisfy the equations:
\[ c_i = \sum_{j=1}^{i-1} a_{ij}, \quad i = 2, \ldots, s \]  
\hspace{20mm} (6)

**DEFINITION 1.** [3] A Runge-Kutta method has algebraic order \( p \) when the method’s series expansion agrees with the Taylor series expansion in the \( p \) first terms: \( y^{(n)}(x) = y^{(n)}_{\text{app}}(x), \quad n = 1, 2, \ldots, p. \)

A convenient way to obtain a certain algebraic order is to satisfy a number of equations derived from Tree Theory. These equations will be shown during the construction of the new methods.

### 2.2. Phase-Lag Analysis of Runge-Kutta Methods

The phase-lag analysis of Runge-Kutta methods is based on the test equation

\[ y' = I\omega y, \quad \omega \in \mathbb{R} \]  
\hspace{20mm} (7)

Application of the Runge-Kutta method described in (3) to the scalar test equation (7) produces the numerical solution:

\[ y_{n+1} = a^*_n y_n, \quad a_* = A_s(v^2) + ivB_s(v^2), \]  
\hspace{20mm} (8)

where \( v = \omega h \) and \( A_s, B_s \) are polynomials in \( v^2 \) completely defined by Runge-Kutta parameters \( a_{i,j}, b_i \) and \( c_i \), as shown in (5).

**DEFINITION 2.** [1] In the explicit \( s \)-stage Runge-Kutta method, presented in (5), the quantities

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

are respectively called the phase-lag or dispersion error and the dissipative error. If \( t(v) = O(v^{q+1}) \) and \( a(v) = O(v^{r+1}) \) then the method is said to be of dispersive order \( q \) and dissipative order \( r \).

### 3. Construction of the new trigonometrically fitted Runge-Kutta methods

We consider the explicit Runge-Kutta method with 3 stages and 3rd algebraic order given in table (9).
We will construct two new optimized methods.

3.1. First optimized method with zero phase-lag

In order to develop the new optimized method, we set free \( b_3 \), while all other coefficients are borrowed from the classical method. We want the phase-lag of the method to be null, so we satisfy the equation \( PL = 0 \), while solving for \( b_3 \), where

\[
PL = \frac{1}{6} \left(6 + (-2 - 6 b_3) v^2\right) \tan(v) + v^3 b_3 + \frac{1}{6} (-5 - 6 b_3) v
\]

So \( b_3 \) becomes

\[
b_3 = -\frac{6 \tan(v) + 2 \tan(v) v^2 + 5 v}{6v (v \tan(v) - v^2 + 1)}
\]

and its Taylor series expansion is

\[
b_3 = \frac{1}{6} - \frac{1}{30} v^4 - \frac{4}{315} v^6 + \frac{17}{2835} v^8 + \frac{206}{31185} v^{10} + \frac{7951}{12162150} v^{12} - \ldots
\]

where \( v = \omega h \), \( \omega \) is a real number and indicates the dominant frequency of the problem and \( h \) is the step-length of integration.

3.2. Second optimized method with zero phase-lag and derivative

As for the development of the second optimized method, we set free \( b_2 \) and \( b_3 \), while all other coefficients are borrowed from the classical method. We want the phase-lag and its first derivative of the method to be null, so we satisfy the equations \( \{PL = 0, PL' = 0\} \), while solving for \( b_2 \) and \( b_3 \), where

\[
PL = \frac{1}{6} \left(6 + (-3 b_2 - 6 b_3) v^2\right) \tan(v) + v (-1/6 - b_2 - b_3 + b_3 v^2)
\]

\[
PL' = -v \tan(v) b_2 - 2 v \tan(v) b_3 + 5/6 + (\tan(v))^2 - 1/2 v^2 b_2 -1/2 v^2 b_2 (\tan(v))^2 + 2 b_3 v^2 - b_3 v^2 (\tan(v))^2 - b_2 - b_3
\]

Then we have

\[
\begin{array}{c|c|c|c}
1 & 1/2 & 1/2 \\
1 & -1 & 2 \\
1/6 & 2/3 & 1/6
\end{array}
\]
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\[ b_2 = \frac{1}{6} \frac{12v + v^3 + \tan(v)e^2 - 12 \tan(v) + v^3(\tan(v))^2}{v^2(-3v + \tan(v) + v(\tan(v))^2 - \tan(v)e^2 + v(\tan(v))^2)} \]  
\[ b_3 = \frac{1}{3} \frac{5v^3(\tan(v))^2 + 7v^3 - 10 \tan(v)e^2 + 6v(\tan(v))^2 - 6v + 6 \tan(v)}{v^2(-3v + \tan(v) + v(\tan(v))^2 - \tan(v)e^2 + v(\tan(v))^2)} \]  
(11)

The Taylor series expansion of the coefficients are given below:

\[ b_2 = \frac{2}{3} - \frac{2}{15} v^2 - \frac{52}{315} v^4 - \frac{3726}{14175} v^6 - \frac{173788}{467775} v^8 - \frac{354768808}{638512875} v^{10} - \ldots \]  
\[ b_3 = \frac{1}{6} + \frac{2}{15} v^2 + \frac{25}{126} v^4 + \frac{4201}{14175} v^6 + \frac{207349}{467775} v^8 + \frac{423287713}{638512875} v^{10} + \ldots \]  
(12)

where \( v = \omega h \), \( \omega \) is a real number and indicates the dominant frequency of the problem and \( h \) is the step-length of integration.

4. Algebraic order of the new methods

The following 4 equations must be satisfied so that the new methods maintain the third algebraic order of the corresponding classical method (9). The number of stages is symbolized by \( s \), where \( s = 4 \). Then we are presenting the Taylor series expansions of the remainders of these equations, that is the difference of the right part minus the left part.

**1st Alg. Order (1 equation)**  
\[ \sum_{i=1}^{s} b_i = 1 \]

**3rd Alg. Order (4 equations)**  
\[ \sum_{i=1}^{s} b_ic_i^2 = \frac{1}{3} \]

**2nd Alg. Order (2 equations)**  
\[ \sum_{i,j=1}^{s} b_ia_{ij}c_j = \frac{1}{6} \]

\[ \sum_{i=1}^{s} b_ic_i = \frac{1}{2} \]  
(13)

4.1. Equations remainders for the first method

We are presenting \( Rem \) which is the remainder for all four equations for the first method:

\[ Rem = -\frac{1}{30} v^4 - \frac{4}{315} v^6 + \frac{17}{2835} v^8 + \frac{206}{31185} v^{10} + \ldots \]  
(14)

4.2. Equations remainders for the second method

The four remainders of the equations for the second method are:
\[ Rem_1 = \frac{1}{30} v^4 + \frac{1}{21} v^6 + \frac{113}{1575} v^8 + \frac{7171}{66825} v^{10} + \ldots \]
\[ Rem_2 = \frac{1}{15} v^2 + \frac{73}{630} v^4 + \frac{2438}{14175} v^6 + \frac{24091}{93555} v^8 + \frac{2459033}{638512875} v^{10} + \ldots \]
\[ Rem_3 = \frac{1}{10} v^2 + \frac{11}{70} v^4 + \frac{2213}{9450} v^6 + \frac{54634}{155925} v^8 + \frac{371772}{638512875} v^{10} + \ldots \]
\[ Rem_4 = \frac{2}{15} v^2 + \frac{25}{126} v^4 + \frac{4201}{14175} v^6 + \frac{207349}{65832875} v^8 + \frac{423287713}{638512875} v^{10} + \ldots \]

(15)

We see that the two optimized methods retain the third algebraic order, since the constant term of all the remainders is zero.

5. Numerical results

5.1. The inverse resonance problem

The efficiency of the two new constructed methods will be measured through the integration of problem (1) with \( l = 0 \) at the interval \([0, 15]\) using the well known Woods-Saxon potential

\[ V(x) = \frac{u_0}{1 + q} + \frac{u_1 q}{(1 + q)^2}, \quad q = \exp \left( \frac{x - x_0}{a} \right), \quad \text{where} \]
\[ u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a} \]

and with boundary condition \( y(0) = 0 \).

The potential \( V(x) \) decays more quickly than \( \frac{l(l+1)}{x^2} \), so for large \( x \) (asymptotic region) the Schrödinger equation (1) becomes

\[ y''(x) = \left( \frac{l(l+1)}{x^2} - E \right) y(x) \]

(17)

The last equation has two linearly independent solutions \( k x j_l(k x) \) and \( k x n_l(k x) \), where \( j_l \) and \( n_l \) are the spherical Bessel and Neumann functions. When \( x \to \infty \) the solution takes the asymptotic form

\[ y(x) \approx A k x j_l(k x) - B k x n_l(k x) \]
\[ \approx D [\sin(k x - \pi l/2) + \tan(\delta_l) \cos(k x - \pi l/2)], \]

(18)

where \( \delta_l \) is called scattering phase shift and it is given by the following expression:

\[ \tan(\delta_l) = \frac{y(x_i) S(x_{i+1}) - y(x_{i+1}) S(x_i)}{y(x_{i+1}) C(x_i) - y(x_i) C(x_{i+1})}, \]

(19)
where $S(x) = k x j_l(k x)$, $C(x) = k x n_l(k x)$ and $x_i < x_{i+1}$ and both belong to the asymptotic region. Given the energy we approximate the phase shift, the accurate value of which is $\pi/2$ for the above problem.

We will use three different values for the energy: i) 989.701916, ii) 341.495874 and iii) 163.215341. As for the frequency $\omega$ we will use the suggestion of Ixaru and Rizea [2]:

$$\omega = \begin{cases} \sqrt{E - 50} & x \in [0, 6.5] \\ \sqrt{E} & x \in [6.5, 15] \end{cases} \quad (20)$$

5.2. **Nonlinear Problem**

\[ y'' = -100y + \sin(y), \quad \text{with} \quad y(0) = 0, \quad y'(0) = 1, \quad t \in [0, 20 \pi], \quad y(20\pi) = 3.92823991 \cdot 10^{-4} \quad \text{and} \quad \omega = 10 \quad \text{as frequency of this problem.} \]

5.3. **Comparison**

We present the accuracy of the tested methods expressed by the $-\log_{10}(\text{error at the end point})$ when comparing the phase shift to the actual value $\pi/2$ versus the $\log_{10}(\text{total function evaluations})$. The function evaluations per step are equal to the number of stages of the method multiplied by two that is the dimension of the vector of the functions integrated for the Schrödinger ($y(x)$ and $z(x)$). In Figure 1 we use $E = 989.701916$, in Figure 2 $E = 341.495874$ and in Figure 3 $E = 163.215341$.

6. **Conclusions**

We compare the two optimized methods and the corresponding classical explicit Runge-Kutta method for the integration of the Schrödinger equation and the Nonlinear problem. We see that the second method with the phase-lag and its first derivative nullified is the most efficient in all cases, followed in terms of efficiency by the optimized method with zero phase-lag and then by the corresponding classical method.

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Figure 2. Efficiency for the Schrödinger equation using $E = 341.495874$

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