

A Special High Order Runge-Kutta Type Method for the Solution of the Schrödinger Equation

Jing Ma^{1,*} and T. E. Simos^{2,3,*}

¹ School of Information Engineering, Changan University, Xian, 710064, China

² Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia

³ Laboratory of Computational Sciences, Department of Informatics and Telecommunications, Faculty of Economy, Management and Informatics, University of Peloponnese, GR-221 00 Tripolis, Greece

Received: 9 Feb. 2015, Revised: 11 May 2015, Accepted: 12 May 2015

Published online: 1 Sep. 2015

Abstract: A Runge-Kutta type eighth algebraic order two-step method with phase-lag and its first, second and third order derivatives equal to zero is produced in this paper. We will also investigate how the above described elimination of the phase-lag and its derivatives effects on the efficiency of the method. More specifically we will study the following: (1) the production of the method, (2) the local truncation error of the new obtained method and a comparative local truncation error analysis using other similar methods of the literature, (3) the interval of periodicity i.e the stability of the developed method using frequency for the scalar test equation for the stability analysis different than the frequency used in the scalar test equation for phase-lag analysis and (4) the effectiveness of the new obtained method applying it on the resonance problem of the radial Schrödinger equation. Based on the last study we will show the efficiency of new method.

Keywords: Phase-lag, derivative of the phase-lag, initial value problems, oscillating solution, symmetric, multistep, Schrödinger equation

1 Introduction

A new two-step eighth algebraic order Runge-Kutta type method is introduced in this paper. It is known from the literature (see [48]) than in order one to achieve high algebraic order needs many steps or stages. This increase the computational problems considerably since the approximate solution must be started using unstable methods (for problems with periodical and /or oscillating solutions) like Runge-Kutta or Runge-Kutta-Nystöm methods. Consequently, this has a great cost on the accuracy. We solved this problem with the new proposed method since it is two-step. The proposed method has also other very important properties like vanished phase-lag and its derivatives.

The proposed method will be used for the approximate solution of special second order initial value problems of the form:

$$q''(x) = f(x, q), \quad q(x_0) = q_0 \quad \text{and} \quad q'(x_0) = q'_0 \quad (1)$$

with solutions which have periodical and/or oscillatory behavior.

As it is shown from the mathematical model presented above, the main characteristic of the above problems is that their models consist of systems of ordinary differential equations of second order in which the first derivative q' does not appear explicitly.

2 Analysis of the Phase-lag Analysis for Symmetric $2m$ Finite Difference Methods

The following finite difference methods

$$\sum_{i=-m}^m c_i q_{n+i} = h^2 \sum_{i=-m}^m b_i f(x_{n+i}, q_{n+i}) \quad (2)$$

are used for the the approximate solution of the initial value problem (1). The above mentioned methods are used as following: the integration interval $[a, b]$ is divided into m equally spaced intervals i.e. $\{x_i\}_{i=-m}^m \in [a, b]$ and

* Corresponding author e-mail: icesmile1983@163.com; tsimos.conf@gmail.com

within each interval we apply the method (2). The quantity h , called stepsize of integration, is given by $h = |x_{i+1} - x_i|$, $i = 1 - m(1)m - 1$. For the specific finite difference method the number of steps, which are used for the integration, is equal to $2m$ (and for this reason is called multistep method).

Remark. The method (2) is called symmetric multistep method if and only if $c_{-i} = c_i$ and $b_{-i} = b_i$, $i = 0(1)m$.

Remark. The linear operator

$$L(x) = \sum_{i=-m}^m c_i q(x+ih) - h^2 \sum_{i=-k}^k b_i q''(x+ih) \tag{3}$$

is associated with the Multistep Method (2), where $q \in C^2$.

Definition 1.[1] The multistep method (2) is called algebraic of order k if the associated linear operator L given by (3) vanishes for any linear combination of the linearly independent functions $1, x, x^2, \dots, x^{k+1}$.

We apply the symmetric $2m$ -step method, ($i = -m(1)m$), to the scalar test equation

$$q'' = -\phi^2 q \tag{4}$$

The above application leads to the following difference equation:

$$A_m(v)q_{n+m} + \dots + A_1(v)q_{n+1} + A_0(v)q_n + A_1(v)q_{n-1} + \dots + A_m(v)q_{n-m} = 0 \tag{5}$$

where $v = \phi h$, h is the stepsize and $A_j(v) j = 0(1)m$ are polynomials of v .

An equation is associated with (5):

$$A_m(v)\lambda^m + \dots + A_1(v)\lambda + A_0(v) + A_1(v)\lambda^{-1} + \dots + A_m(v)\lambda^{-m} = 0. \tag{6}$$

This equation is called as characteristic equation.

Definition 2.[16] A symmetric $2m$ -step method with characteristic equation given by (6) is said to have an interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots $\lambda_i, i = 1(1)2m$ of Eq. (6) satisfy:

$$\lambda_1 = e^{i\theta(v)}, \lambda_2 = e^{-i\theta(v)}, \text{ and } |\lambda_i| \leq 1, i = 3(1)2m \tag{7}$$

where $\theta(v)$ is a real function of v .

Definition 3.[14], [15] For any finite difference method which is corresponded to the characteristic equation (6) the phase-lag is defined as the leading term in the expansion of

$$t = v - \theta(v) \tag{8}$$

The order of phase-lag is p , if the quantity $t = O(v^{p+1})$ as $v \rightarrow \infty$ is hold.

Definition 4.[2] A method is called **phase-fitted** if its phase-lag is equal to zero

Theorem 1.[14] The symmetric $2m$ -step method with characteristic equation given by (6) has phase-lag order p and phase-lag constant c given by

$$-cv^{p+2} + O(v^{p+4}) = \frac{P_0}{P_1} \tag{9}$$

where

$$P_0 = 2A_m(v) \cos(mv) + \dots + 2A_j(v) \cos(jv) + \dots + A_0(v) \\ P_1 = 2m^2 A_m(v) + \dots + 2j^2 A_j(v) + \dots + 2A_1(v).$$

Remark. The formula (9) is used for the direct computation of the phase-lag for any symmetric $2m$ -step finite difference method.

Remark. For the purpose of the present paper, a symmetric two-step method, with characteristic polynomials $A_j(v) j = 0, 1$, has phase-lag order p and phase-lag constant c given by:

$$-cv^{p+2} + O(v^{p+4}) = \frac{2A_1(v) \cos(v) + A_0(v)}{2A_1(v)} \tag{10}$$

3 The New High Algebraic Order Hybrid Two-Step Method with Vanished Phase-Lag and Its First and Second Derivatives

Consider the family of two-step methods

$$\begin{aligned} \hat{y}_{n+\frac{1}{2}} &= \frac{1}{52} (3y_{n+1} + 20y_n + 29y_{n-1}) \\ &+ \frac{h^2}{4992} (41f_{n+1} - 682f_n - 271f_{n-1}) \\ \hat{y}_{n-\frac{1}{2}} &= \frac{1}{104} (5y_{n+1} + 146y_n - 47y_{n-1}) \\ &+ \frac{h^2}{4992} (-59f_{n+1} + 1438f_n + 253f_{n-1}) \\ \tilde{y}_n &= y_n - a_0 h^2 (f_{n+1} - 4\hat{f}_{n+\frac{1}{2}} + 6f_n - 4\hat{f}_{n-\frac{1}{2}} + f_{n-1}) \\ y_{n+1} - 2y_n + y_{n-1} &= h^2 \left[b_1 (f_{n+1} + f_{n-1}) + b_0 \tilde{f}_n + b_2 (\hat{f}_{n+\frac{1}{2}} + \hat{f}_{n-\frac{1}{2}}) \right] \end{aligned} \tag{11}$$

where $f_i = y''(x_i, y_i), i = -1(\frac{1}{2})1$ and $a_0, b_j j = 0(1)2$ are free parameters.

We require the above method (11) to have vanished phase-lag and its first, second and third derivatives. Therefore, we have the following system of equations :

$$\text{Phase - Lag(PL)} = \frac{1}{2} \frac{T_0}{T_1} = 0 \tag{12}$$

$$\text{First Derivative of the Phase - Lag} = \frac{T_2}{T_3} = 0 \tag{13}$$

$$\text{Second Derivative of the Phase - Lag} = \frac{T_4}{T_5} = 0 \tag{14}$$

$$\text{Third Derivative of the Phase - Lag} = \frac{T_6}{T_7} = 0 \tag{15}$$

where $T_j, j = 0(1)7$ are given in the Appendix A.

If we solve the above system of equations (12)-(15), we will obtain the coefficients of the new proposed hybrid method :

$$a_0 = -\frac{T_8}{T_9}, b_0 = 2 \frac{T_{10}}{T_{11}}$$

$$b_1 = -\frac{1}{3} \frac{T_{12}}{T_{13}}, b_2 = -\frac{T_{14}}{T_{15}} \tag{16}$$

where $T_k, k = 8(1)15$ are given in the Appendix B.

If the above formulae given by (16) are subject to heavy cancellations for some values of $|v|$ then the following Taylor series expansions should be used :

$$a_0 = -\frac{2}{10647} + \frac{157v^2}{1384110}$$

$$+ \frac{423893v^4}{92630177640} + \frac{230868409v^6}{1770162694700400}$$

$$+ \frac{394343483v^8}{1025682841386403200}$$

$$- \frac{1448557506233543v^{10}}{3665349431493208883424000}$$

$$- \frac{6550465773056706437v^{12}}{329544236686691424290884992000}$$

$$- \frac{76563088235849088023v^{14}}{128522252307809655473445146880000}$$

$$+ \frac{5347067736337178560829413v^{16}}{1846395916486805859530239632769781760000} + \dots$$

$$b_0 = \frac{13}{30} - \frac{157v^4}{354900} - \frac{560641v^6}{76735058400}$$

$$+ \frac{41917747v^8}{79804460736000} + \frac{4490261v^{10}}{742725606168000}$$

$$+ \frac{28384666537v^{12}}{48148425295850880000}$$

$$+ \frac{4497551069057351v^{14}}{197798738551586183531520000}$$

$$- \frac{14561318668477807v^{16}}{14693620578117830776627200000} + \dots$$

$$b_1 = \frac{1}{60} - \frac{157v^4}{2129400} - \frac{97861v^6}{18416414016}$$

$$- \frac{42456803v^8}{478826764416000} + \frac{560383333v^{10}}{98039780014176000}$$

$$+ \frac{220927910953v^{12}}{433335827662657920000}$$

$$+ \frac{1387348047327731v^{14}}{69811319488795123599360000}$$

$$+ \frac{889893652697591v^{16}}{12100628711391154757222400000} + \dots$$

$$b_2 = \frac{4}{15} + \frac{157v^4}{532350} + \frac{64507v^6}{7193911725}$$

$$- \frac{16698133v^8}{29926672776000} - \frac{26474663v^{10}}{765935781360750}$$

$$- \frac{192615256241v^{12}}{216667913831328960000}$$

$$+ \frac{34742917493593v^{14}}{3708726347842240941216000}$$

$$+ \frac{2210605374155621v^{16}}{756289294461947172326400000} + \dots \tag{17}$$

In Figure 1 we present the behavior of the coefficients of the new method.

3.1 The Local Truncation Error of the New Method

The local truncation error of the new obtained hybrid method (11) (mentioned as *ExpTwoStepHY8*) with the coefficients given by (16) - (17) is given by:

$$LTE_{ExpTwoStepHY8} = \frac{157}{204422400} h^{10} \left(q_n^{(10)} + 4\phi^2 q_n^{(8)} + 6\phi^4 q_n^{(6)} + 4\phi^6 q_n^{(4)} + \phi^8 q_n^{(2)} \right) + O(h^{12}) \tag{18}$$

4 Comparative Error Analysis

Considering the test problem

$$q''(x) = (V(x) - V_c + G) q(x) \tag{19}$$

where $V(x)$ is a potential function, V_c a constant value approximation of the potential for the specific x , $G = V_c - E$ and E is the energy, we will investigate the local truncation error of the following methods

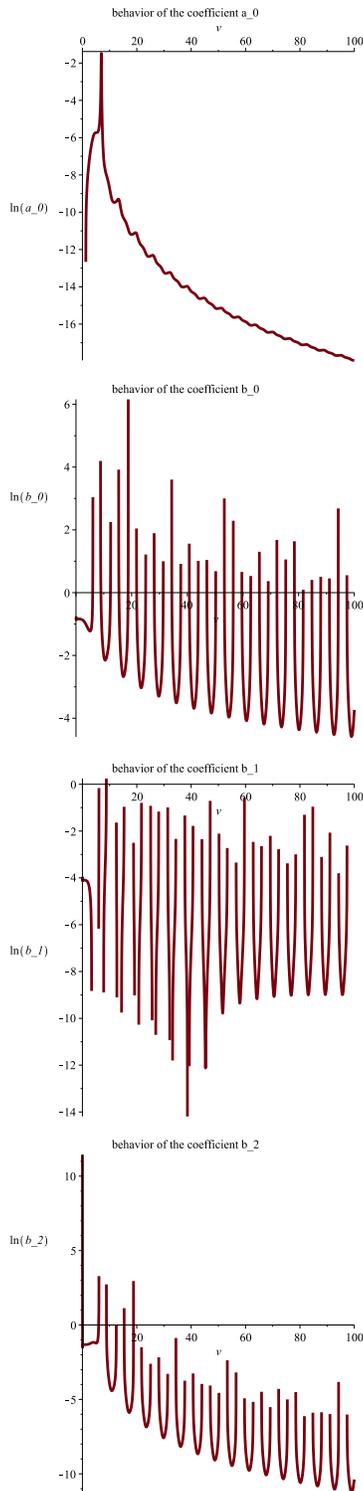


Fig. 1: Behavior of the coefficients of the new proposed method given by (16) for several values of $v = \phi h$.

4.1 Classical Method (i.e. the method (11) with constant coefficients)

$$LTE_{CL} = \frac{157}{204422400} h^{10} q_n^{(10)} + O(h^{12}) \quad (20)$$

4.2 The New Proposed Method with Vanished Phase-Lag and its First, Second and Third Derivatives Produced in Section 3

$$LTE_{ExpTwoStepHY8} = \frac{157}{204422400} h^{10} \left(q_n^{(10)} + 4\phi^2 q_n^{(8)} + 6\phi^4 q_n^{(6)} + 4\phi^6 q_n^{(4)} + \phi^8 q_n^{(2)} \right) + O(h^{12}) \quad (21)$$

The procedure contains the following stages

- Expressions of the derivatives which are included in the formulae of the Local Truncation Errors based on the test problem (19). The expressions of some derivatives are presented in the Appendix C.
- Based on the above step, production of the new form of the formulae of the Local Truncation Error for each method. These formulae are dependent from the energy E .
- Based on the above step, formulae of the Local Truncation Error which contain the parameter G (see (19)) are produced. Our investigation is based on two cases for the parameter G :

1. The Energy and the potential are closed each other. Therefore, $G = V_c - E \approx 0$ i.e. the value of the parameter G is approximately equal to zero. Consequently, all the terms in the expressions of the local truncation error with terms of several power of G are approximately equal to zero. Therefore, we consider only the terms of the expressions of the local truncation error for which the power to G is equal to zero i.e. the terms which are free from G . In this case (free from G terms) the local truncation error for the classical method (constant coefficients) and the methods with vanished the phase-lag and its first, second and third derivatives are the same since the expressions of the terms of the local truncation errors which are free from G in both cases are the same. Consequently, for these values of G , the methods are of comparable accuracy.

2. $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number. In these cases we wish to have expressions of the local truncation error with terms with minimum power of G .

–Finally the asymptotic expansions of the Local Truncation Errors are calculated.

The following asymptotic expansions of the Local Truncation Errors are obtained based on the analysis presented above :

4.3 Classical Method

$$LTE_{CL} = \frac{157}{204422400} h^{10} \left(q(x) G^5 + \dots \right) + O(h^{12}) \tag{22}$$

4.4 The New Proposed Method with Vanished Phase-Lag and its First and Second Derivatives Produced in Section 3

$$LTE_{ExpTwoStepHY8} = h^{10} \left[\left(\frac{157 \left(\frac{d}{dx} g(x) \right)^2 q(x)}{17035200} + \frac{157 g(x) q(x) \frac{d^2}{dx^2} g(x)}{12776400} + \frac{157 \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} q(x)}{25552800} + \frac{157 \left(\frac{d^4}{dx^4} g(x) \right) q(x)}{7300800} \right) G^2 + \dots \right] + O(h^{12}) \tag{23}$$

From the above equations we have the following theorem:

Theorem 2. –Classical Method (i.e. the method (11) with constant coefficients): For this method the error increases as the fifth power of G.

–Eighth Algebraic Order Two-Step Method with Vanished Phase-lag and its First, Second and Third Derivatives developed in Section 3: For this method the error increases as the Second power of G.

So, for the approximate integration of the time independent radial Schrödinger equation the New Obtained High Algebraic Order Method with Vanished Phase-Lag and its First, Second and Third Derivatives is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

5 Stability Analysis

The scalar test equation for the study of the stability of the new proposed method, given by :

$$q'' = -\omega^2 q. \tag{24}$$

has as characteristic $\omega \neq \phi$, i.e. the frequency of the scalar test equation for the phase-lag analysis (ϕ) - investigated above - is different with the frequency of the scalar test equation used for the stability analysis.

If we apply the new proposed methods to the scalar test equation (24), we have the following difference equation:

$$A_1(s, v) (q_{n+1} + q_{n-1}) + A_0(s, v) q_n = 0 \tag{25}$$

where

$$A_1(s, v) = \frac{S_0}{S_1}, A_0(s, v) = 2 \frac{S_2}{S_1} \tag{26}$$

where $S_i, i = 0(1)2$ are given in the Appendix D. We note that $s = \omega h$ and $v = \phi h$

Based on the analysis presented in Section 2, we have the following definitions:

Definition 5.(see [16]) We call P-stable a multistep method with interval of periodicity equal to $(0, \infty)$.

Definition 6.We call singularly almost P-stable a multistep method with interval of periodicity equal to $(0, \infty) - S$ ¹. The term singularly almost P-stable method is used only in the cases when the frequency of the scalar test equation for the phase-lag analysis is equal with the frequency of the scalar test equation for the stability analysis, i.e. $\omega = \phi$.

The $s - v$ plane for the method obtained in this paper is shown in Figure 2.

Remark. From the presented in Figure 2 $s - v$ region we can see the following:

1. The method is stable within the shadowed area,
2. The method is unstable within the white area.

Remark. There are mathematical models of real problems in Sciences, Engineering and Technology where the observation of **the surroundings of the first diagonal of the $s - v$ plane** is necessary. Such cases are the mathematical models which have only one frequency per differential equation in the model. In these cases the frequency of the scalar test equation used for the phase-lag analysis is equal with the frequency of the scalar test equation used for the stability analysis. An example is the time independent radial Schrödinger equation.

¹ where S is a set of distinct points

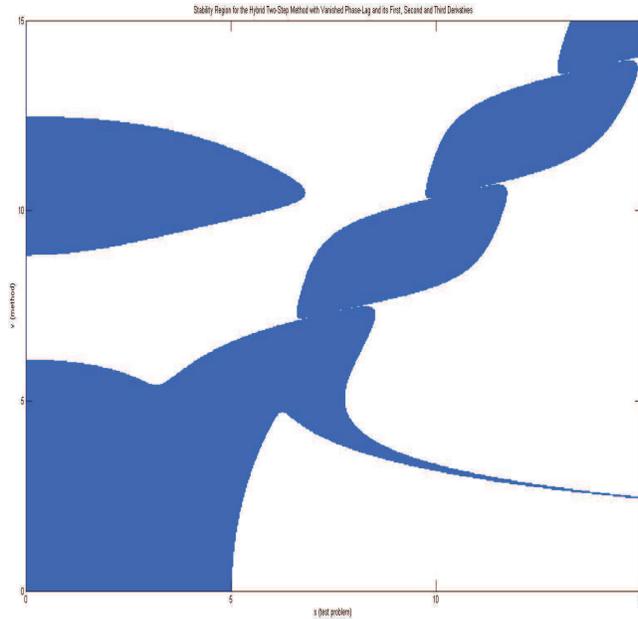


Fig. 2: $s - v$ plane of the new obtained two-step high order method with vanished phase-lag and its first and second derivatives

Based on the above remark, we investigate the case where the frequency of the scalar test equation used for the phase-lag analysis is equal with the frequency of the scalar test equation used for the stability analysis, i.e. we investigate the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s - v$ plane). Based on this investigation we extract the results that the new obtained methods has interval of periodicity equal to: $(0, \infty)$, i.e. is P-stable.

The above study leads to the following theorem:

Theorem 3. *The proposed method developed in section 3:*

- is of eighth algebraic order,
- has the phase-lag and its first, second and third derivatives equal to zero
- has an interval of periodicity equals to: $(0, \infty)$, i.e. is P-stable when the frequency of the scalar test equation used for the phase-lag analysis is equal with the frequency of the scalar test equation used for the stability analysis

6 Numerical Results

6.1 The Mathematical Model of the Radial Time-Independent Schrödinger Equation

The model of the radial time independent Schrödinger equation is given by :

$$q''(r) = [l(l + 1)/r^2 + V(r) - k^2]q(r). \quad (27)$$

where

- The function $W(r) = l(l + 1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(r) \rightarrow 0$ as $r \rightarrow \infty$,
- The quantity k^2 is a real number denoting *the energy*,
- The quantity l is a given integer representing *the angular momentum*,
- V is a given function which denotes *the potential*.

Since the problem (27) is belong to the category of the boundary value problems, then we need the boundary conditions. The initial condition is given by:

$$q(0) = 0 \quad (28)$$

while the final condition, for large values of r , determined by physical properties and characteristics of the specific problem.

The new proposed method is a frequency dependent method. Consequently we have to determine the parameter ϕ (frequency) of the coefficients of the method ($v = \phi h$). For the category of problems like the radial Schrödinger equation, the parameter ϕ (for $l = 0$) is given by :

$$\phi = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \quad (29)$$

where $V(r)$ is the potential and E is the energy.

6.1.1 Woods-Saxon potential

For our numerical experiments we use the Woods-Saxon potential which is given by :

$$V(r) = \frac{u_0}{1 + q} - \frac{u_0 q}{a(1 + q)^2} \quad (30)$$

with $q = \exp\left[\frac{r-X_0}{a}\right]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

The Woods-Saxon potential is shown in Figure 5.

For the use of the potential we can follow two procedures:

- To approximate at every point r the potential and based on this to find the parameter ϕ . This procedure creates big computational cost
- To approximate the potential using some critical points of the potential. We use these critical points in order to determine the value of the parameter ϕ (see for details [43]).

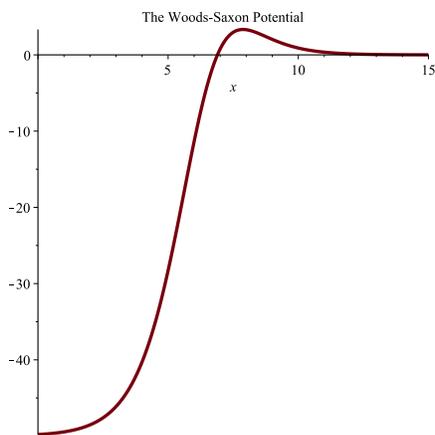


Fig. 3: The Woods-Saxon potential.

For our numerical experiments we use the second procedure.

For the purpose of our tests, we choose ϕ as follows (we use the methodology presented in [44] and [45]):

$$\phi = \begin{cases} \sqrt{-50 + E}, & \text{for } r \in [0, 6.5 - 2h], \\ \sqrt{-37.5 + E}, & \text{for } r = 6.5 - h \\ \sqrt{-25 + E}, & \text{for } r = 6.5 \\ \sqrt{-12.5 + E}, & \text{for } r = 6.5 + h \\ \sqrt{E}, & \text{for } r \in [6.5 + 2h, 15] \end{cases} \quad (31)$$

For example, in the point of the integration region $r = 6.5 - h$, the value of ϕ is equal to: $\sqrt{-37.5 + E}$. So, $w = \phi h = \sqrt{-37.5 + E}h$. In the point of the integration region $r = 6.5 - 3h$, the value of ϕ is equal to: $\sqrt{-50 + E}$, etc.

6.1.2 Radial Schrödinger Equation - The Resonance Problem

Our test for the efficiency of the obtained new high order hybrid method is the approximate solution of the radial time independent Schrödinger equation (27) with the Woods-Saxon potential (30).

Since, by theory, the integration interval for this problem is equal to $r \in (0, \infty)$, we have to approximate it by a finite one. For our numerical tests we use the integration interval $r \in [0, 15]$. The domain of energies in which we will solve the above problem is equal to: $E \in [1, 1000]$.

For the case of positive energies, $E = k^2$, the radial Schrödinger equation effectively reduces to:

$$y''(r) + \left(k^2 - \frac{l(l+1)}{r^2} \right) y(r) = 0 \quad (32)$$

for r greater than some value R . This is because the potential decays faster than the term $\frac{l(l+1)}{r^2}$.

Therefore, this differential equation has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Thus, the solution of equation (27) (when $r \rightarrow \infty$), has the asymptotic form

$$q(r) \approx Akrj_l(kr) - Bkrn_l(kr) \approx AC \left[\sin \left(kr - \frac{l\pi}{2} \right) + \tan d_l \cos \left(kr - \frac{l\pi}{2} \right) \right] \quad (33)$$

where δ_l is the phase shift that may be calculated from the formula

$$\tan \delta_l = \frac{y(r_2)S(r_1) - y(r_1)S(r_2)}{y(r_1)C(r_1) - y(r_2)C(r_2)} \quad (34)$$

for r_1 and r_2 distinct points in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. Since the problem is treated as an initial-value problem, we need $y_j, j = 0, 1$ before starting a two-step method. From the initial condition, we obtain y_0 . The value y_1 is obtained by using high order Runge-Kutta-Nyström methods(see [46] and [47]). With these starting values, we evaluate at r_2 of the asymptotic region the phase shift δ_l .

For the case of positive energies we have the known as resonance problem. We have two forms for this problem:

1. finding the phase-shift δ_l or
2. finding those E , for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$.

We actually solve the latter problem, known as **the resonance problem**.

The boundary conditions for this problem are:

$$q(0) = 0, q(r) = \cos(\sqrt{E}r) \text{ for large } r. \quad (35)$$

We compute the approximate positive eigenenergies of the Woods-Saxon resonance problem using:

- The eighth order multi-step method developed by Quinlan and Tremaine [48], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [48], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [48], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [50], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [49], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [51], which is indicated as **Method MCR6**

- The classical form of the eighth algebraic order two-step method developed in Section 3, which is indicated as **Method NMCL**².
- The Phase-Fitted Method (Case 1) developed in [1], which is indicated as **Method NMPF1**
- The Phase-Fitted Method (Case 2) developed in [1], which is indicated as **Method NMPF2**
- The Method developed in [42] (Case 2), which is indicated as **Method NMC2**
- The Method developed in [42] (Case 1), which is indicated as **Method NMC1**
- The New Obtained Two-Step Hybrid Method developed in Section 3, which is indicated as **Method NM2S8PL3DV**

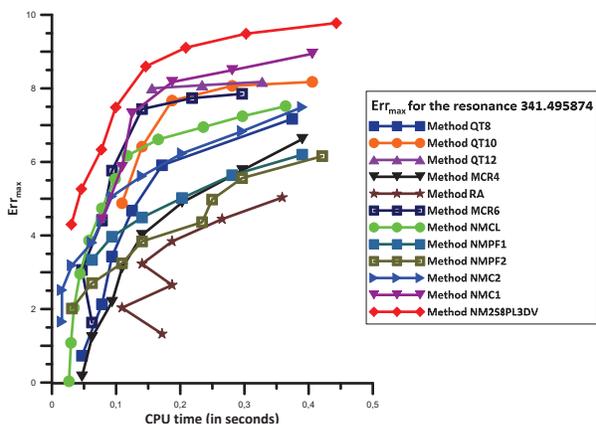


Fig. 4: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

We defined some reference values using the well known two-step method of Chawla and Rao [51] with small step size for the integration. We then compared the numerically calculated eigenenergies with these reference values. In Figures 4 and 5, we present the maximum absolute error $Err_{max} = |\log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{36}$$

of the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$ respectively, for several values of CPU time (in seconds). We note that the CPU time (in seconds) counts the computational cost for each method.

² with the term classical we mean the method of Section 3 with constant coefficients

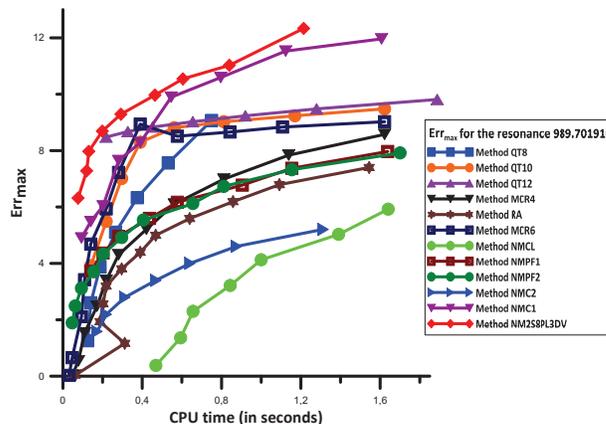


Fig. 5: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

7 Conclusions

In this paper, we studied a family of two-step hybrid methods. The main results of this investigation was:

- The proposed method is of eighth algebraic order
- The obtained method has vanished phase-lag and its first, second and third derivatives
- The obtained method is P-stable (for $\phi = \omega$).

From the numerical experiments mentioned above, we have the following conclusions:

1. The tenth algebraic order multistep method developed by Quinlan and Tremaine [48], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [50], which is indicated as **Method MCR4**. The **Method QT10** is also more efficient than the eighth order multi-step method developed by Quinlan and Tremaine [48], which is indicated as **Method QT8**. The **Method QT10** is also more efficient than the classical form of the eighth algebraic order two-step method developed in Section 3, which is indicated as **Method NMCL**³ Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [51], which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.
2. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [48], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan

³ with the term classical we mean the method of Section 3 with constant coefficients

and Tremaine [48], which is indicated as **Method QT10**

3.The Phase-Fitted Method (Case 1) developed in [1], which is indicated as **Method NMPF1** is more efficient than the classical form of the fourth algebraic order four-step method developed in Section 3, which is indicated as **Method NMCL**, the exponentially-fitted method of Raptis and Allison [49] and the Phase-Fitted Method (Case 2) developed in [1], which is indicated as **Method NMPF2**

4.The Method developed in [42] (Case 2), which is indicated as **Method NMC2** is more efficient than the classical form of the fourth algebraic order four-step method developed in Section 3, which is indicated as **Method NMCL**, the exponentially-fitted method of Raptis and Allison [49] and the Phase-Fitted Method (Case 2) developed in [1], which is indicated as **Method NMPF2** and the Phase-Fitted Method (Case 1) developed in [1], which is indicated as **Method NMPF1**

5.The Method developed in [42] (Case 1), which is indicated as **Method NMC1**, is the more efficient than all the other methods mentioned above.

6.The New Obtained Two-Step Hybrid Method developed in Section 3, which is indicated as **Method NM2S8PL3DV**, is the most efficient one.

All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

Appendix A: Formulae $T_j, j = 0(1)7$

$$\begin{aligned}
 T_0 &= 2 \left(1 + v^2 \left(b_1 + b_0 a_0 v^2 \left(\frac{15}{26} - \frac{3v^2}{208} \right) + b_2 \left(\frac{11}{104} + \frac{3v^2}{832} \right) \right) \right) \cos(v) \\
 &- 2 + v^2 \left(b_0 \left(1 + a_0 v^2 \left(-\frac{15}{13} + \frac{63v^2}{104} \right) \right) + b_2 \left(\frac{93}{52} - \frac{63v^2}{416} \right) \right) \\
 T_1 &= 1 + v^2 \left(b_1 + b_0 a_0 v^2 \left(\frac{15}{26} - \frac{3v^2}{208} \right) + b_2 \left(\frac{11}{104} + \frac{3v^2}{832} \right) \right) \\
 T_2 &= 1384448 b_2 v + 1384448 v b_1 - 199680 b_2 v^3 + 692224 v b_0 \\
 &- 15552 v^5 b_2^2 - 692224 \sin(v) + 72 \sin(v) v^{10} a_0 b_0 b_2 \\
 &+ 19968 \sin(v) v^8 a_0 b_0 b_1 - 768 \sin(v) v^8 a_0 b_0 b_2
 \end{aligned}$$

$$\begin{aligned}
 &- 798720 \sin(v) v^6 a_0 b_0 b_1 - 84480 \sin(v) v^6 a_0 b_0 b_2 \\
 &+ 1198080 v^5 a_0 b_0 + 230400 v^9 a_0^2 b_0^2 - 146432 \sin(v) b_2 v^2 \\
 &- 1384448 \sin(v) v^2 b_1 - 4992 \sin(v) v^4 b_2 - 7744 \sin(v) v^4 b_2^2 \\
 &- 9 \sin(v) v^8 b_2^2 - 692224 \sin(v) v^4 b_1^2 - 528 \sin(v) v^6 b_2^2 - 104832 v^5 b_1 b_2 \\
 &+ 19968 v^7 a_0 b_0^2 - 399360 v^5 a_0 b_0^2 - 2496 v^5 b_0 b_2 + 19968 \sin(v) v^6 a_0 b_0 + 838656 v^7 a_0 b_0 b_1 \\
 &+ 124416 v^7 a_0 b_0 b_2 - 798720 v^5 a_0 b_0 b_1 - 798720 v^5 a_0 b_0 b_2 - 144 \sin(v) v^{12} a_0^2 b_0^2 \\
 &+ 11520 \sin(v) v^{10} a_0^2 b_0^2 - 230400 \sin(v) v^8 a_0^2 b_0^2 - 4992 \sin(v) v^6 b_1 b_2 - 798720 \sin(v) b_0 a_0 v^4 \\
 &- 146432 \sin(v) v^4 b_1 b_2 \\
 T_3 &= \left(12 v^6 a_0 b_0 - 480 v^4 a_0 b_0 - 3 v^4 b_2 - 832 v^2 b_1 - 88 v^2 b_2 - 832 \right)^2
 \end{aligned}$$

$$\begin{aligned}
 T_4 &= 35143680 v^6 a_0 b_0^2 b_2 - 28753920 \cos(v) v^{10} a_0^2 b_0^2 - 1728 \cos(v) v^{18} a_0^3 b_0^3 + 1727791104 \cos(v) v^2 b_1 \\
 &+ 6230016 \cos(v) v^4 b_2 - 4984012800 b_0 a_0 v^4 + 19329024 \cos(v) v^4 b_2^2 + 1727791104 \cos(v) v^4 b_1^2 \\
 &+ 681472 \cos(v) v^6 b_2^3 + 1317888 \cos(v) v^6 b_2^2 - 575930368 b_0 + 575930368 \cos(v) v^6 b_1^3 \\
 &- 12460032 v^8 a_0 b_0^2 b_2 + 332267520 v^6 a_0 b_0^2 b_1 - 62429184 v^8 a_0 b_0 b_2^2 - 2093285376 v^8 a_0 b_0 b_1^2 \\
 &+ 359424 \cos(v) v^{14} a_0^2 b_0^2 b_1 + 19329024 \cos(v) v^6 b_1 b_2^2 - 49840128 \cos(v) v^8 a_0 b_0 b_1 \\
 &+ 11321856 v^{10} a_0 b_0 b_1 b_2 - 690094080 v^8 a_0 b_0 b_1 b_2 + 734822400 v^6 a_0 b_0 b_1 b_2
 \end{aligned}$$

$$\begin{aligned}
& +1296 \cos(v) v^{16} a_0^2 b_0^2 b_2 \\
& +22464 \cos(v) v^{10} b_1 b_2^2 \\
& -179712 \cos(v) v^{12} a_0 b_0 b_1 b_2 \\
& +1916928 \cos(v) v^{10} a_0 b_0 b_1 b_2 \\
& +210862080 \cos(v) v^8 a_0 b_0 b_1 b_2 \\
& -6063882240 v^6 a_0 b_0 b_1 + 2376 \cos(v) v^{10} b_2^3 \\
& +22464 \cos(v) v^8 b_2^2 \\
& +27 \cos(v) v^{12} b_2^3 + 69696 \cos(v) v^8 b_2^3 \\
& +1727791104 v^2 b_0 b_1 \\
& +22164480 v^6 b_1 b_2^2 + 87220224 v^6 b_1^2 b_2 \\
& +219648 v^6 b_0 b_2^2 \\
& -943488 v^8 b_1 b_2^2 - 575078400 v^8 a_0^2 b_0^3 \\
& -22464 v^8 b_0 b_2^2 \\
& +43130880 v^{10} a_0^2 b_0^3 - 110592000 v^{12} a_0^3 b_0^3 \\
& -1198080 v^{12} a_0^2 b_0^3 \\
& -8294400 v^{14} a_0^3 b_0^3 + 3821076480 v^2 b_1 b_2 \\
& +24920064 v^4 b_0 b_2 \\
& +3987210240 v^4 a_0 b_0^2 - 207667200 v^6 a_0 b_0^2 \\
& +182747136 v^2 b_0 b_2 \\
& +299040768 v^4 b_1 b_2 - 100638720 v^{10} a_0^2 b_0^2 \\
& +182747136 \cos(v) b_2 v^2 \\
& +2076672 v^6 b_0 b_1 b_2 + 70287360 v^6 a_0 b_0 b_2^2 \\
& +664535040 v^6 a_0 b_0 b_1^2 \\
& +575930368 \cos(v) + 359424 \cos(v) v^{12} a_0^2 b_0^2 \\
& -1150156800 v^8 a_0^2 b_0^2 b_1 \\
& -1150156800 v^8 a_0^2 b_0^2 b_2 \\
& -49840128 v^8 a_0 b_0^2 b_1 \\
& +1916928 \cos(v) v^8 a_0 b_0 b_2 \\
& +1368576 v^6 b_2^3 - 139968 v^8 b_2^3 \\
& -2995200 v^6 b_2^2 + 76197888 v^4 b_2^2 \\
& +365494272 v^2 b_2^2 + 3455582208 v^2 b_1^2 \\
& +498401280 b_2 v^2 - 1151860736 b_1 - 1151860736 b_2 \\
& +182747136 \cos(v) v^6 b_1^2 b_2 \\
& +32348160 v^8 a_0 b_0 b_2 \\
& +1317888 \cos(v) v^8 b_1 b_2^2 \\
& -8294400 \cos(v) v^{14} a_0^3 b_0^3 \\
& +110592000 \cos(v) v^{12} a_0^3 b_0^3 \\
& +12460032 \cos(v) v^6 b_1 b_2 \\
& +1679616 v^{10} a_0 b_0 b_2^2 \\
& +269568 v^{10} a_0 b_0^2 b_2 \\
& +25436160 v^{10} a_0^2 b_0^2 b_2 \\
& -488816640 v^{10} a_0^2 b_0^2 b_1 \\
& -8156160 v^{12} a_0^2 b_0^2 b_2 \\
& -50319360 v^{12} a_0^2 b_0^2 b_1 \\
& -24920064 \cos(v) v^6 a_0 b_0 \\
& +365494272 \cos(v) v^4 b_1 b_2 \\
& +575078400 \cos(v) v^8 a_0^2 b_0^2 \\
& +6230016 \cos(v) v^8 b_1^2 b_2 \\
& +996802560 \cos(v) b_0 a_0 v^4 \\
& +207360 \cos(v) v^{16} a_0^3 b_0^3 \\
& +1993605120 \cos(v) v^6 a_0 b_0 b_1 \\
& -65664 \cos(v) v^{14} a_0^2 b_0^2 b_2 \\
& -324 \cos(v) v^{14} a_0 b_0 b_2^2 \\
& -28753920 \cos(v) v^{12} a_0^2 b_0^2 b_1 \\
& -967680 \cos(v) v^{12} a_0^2 b_0^2 b_2 \\
& -6048 \cos(v) v^{12} a_0 b_0 b_2^2 \\
& +575078400 \cos(v) v^{10} a_0^2 b_0^2 b_1 \\
& +11151360 \cos(v) v^8 a_0 b_0 b_2^2 \\
& +60825600 \cos(v) v^{10} a_0^2 b_0^2 b_2 \\
& -24920064 \cos(v) v^{10} a_0 b_0 b_1^2 \\
& +481536 \cos(v) v^{10} a_0 b_0 b_2^2 \\
& -179712 \cos(v) v^{10} a_0 b_0 b_2 \\
& +996802560 \cos(v) v^8 a_0 b_0 b_1^2 \\
& +7974420480 v^4 a_0 b_0 b_2 \\
& +7974420480 v^4 a_0 b_0 b_1 \\
& -1492008960 v^6 a_0 b_0 b_2 \\
& +210862080 \cos(v) v^6 a_0 b_0 b_2 \\
& T_5 = \left(12 v^6 a_0 b_0 \right. \\
& \quad \left. -480 b_0 a_0 v^4 - 3 v^4 b_2 \right. \\
& \quad \left. -832 v^2 b_1 - 88 b_2 v^2 - 832 \right)^3 \\
& T_6 = -27644657664 \sin(v) v^6 a_0 b_0
\end{aligned}$$

$$\begin{aligned}
 &+38277218304000 v^7 a_0^2 b_0^2 b_1 \\
 &+1602551808 \sin(v) v^{12} a_0 b_0 b_1 b_2^2 \\
 &\quad +5750088794112 v^3 b_0 b_1^2 \\
 &\quad +38277218304000 v^7 a_0^2 b_0^2 b_2 \\
 &-598081536 \sin(v) v^{12} a_0 b_0 b_1 b_2 \\
 &\quad +81 \sin(v) v^{16} b_2^4 \\
 &+32163495936 \sin(v) v^8 b_1^2 b_2^2 \\
 &\quad +16586794598400 b_0 a_0 v^3 \\
 &+20733493248 \sin(v) v^8 b_1^2 b_2 \\
 &\quad +2267938816 \sin(v) v^8 b_1 b_2^3 \\
 &\quad +19138609152000 v^7 a_0^2 b_0^3 \\
 &\quad +829339729920 v^7 a_0 b_0 b_2^2 \\
 &\quad +26538871357440 v^5 a_0 b_0 b_1^2 \\
 &\quad +479174066176 \sin(v) \\
 &\quad -33173589196800 v^3 a_0 b_0 b_1 \\
 &+690094080 \sin(v) v^{16} a_0^3 b_0^3 \\
 &\quad -4140564480 v^{15} a_0^3 b_0^4 \\
 &+9661317120 v^{15} a_0^3 b_0^3 + 7907328 v^9 b_0 b_2^3 \\
 &\quad -5750784 \sin(v) v^{18} a_0^3 b_0^3 \\
 &+202427596800 \sin(v) v^{12} a_0^2 b_0^2 b_1 b_2 \\
 &\quad +1403498004480 v^5 a_0 b_0^2 b_2 \\
 &\quad -33173589196800 v^3 a_0 b_0 b_2 \\
 &\quad +202727489536 \sin(v) v^8 b_1^3 b_2 \\
 &+3189768192 \sin(v) v^{12} a_0 b_0 b_1^2 b_2 \\
 &\quad +1216364937216 v^3 b_0 b_1 b_2 \\
 &\quad +747601920 v^7 b_0 b_2^2 \\
 &\quad -430618705920 v^7 a_0 b_0 b_2 \\
 &\quad +22226304761856 v^5 a_0 b_0 b_1 \\
 &\quad +9212050538496 v^5 a_0 b_0 b_2 \\
 &\quad +598081536 \sin(v) v^{12} a_0^2 b_0^2 \\
 &-47846522880 \sin(v) v^{10} a_0^2 b_0^2 \\
 &+956930457600 \sin(v) v^8 a_0^2 b_0^2 \\
 &\quad -19138609152000 v^7 a_0^2 b_0^2 \\
 &\quad -16586794598400 v^3 a_0 b_0^2 \\
 &+1161075621888 v^5 a_0 b_0^2 + 1674628300800 v^9 a_0^2 b_0^2 \\
 &\quad +183411671040 v^5 b_1 b_2^2 \\
 &\quad +622004797440 v^3 b_1 b_2 \\
 &\quad +37380096 \sin(v) v^8 b_2^2 \\
 &\quad +2192965632 \sin(v) v^6 b_2^2 \\
 &+6911164416 \sin(v) v^4 b_2 + 797921280 v^9 b_1 b_2^3 \\
 &\quad +5199322152960 v^7 a_0 b_0 b_1 b_2 \\
 &\quad +8771862528 v^5 b_0 b_2^2 + 13456834560 v^7 b_1 b_2^2 \\
 &\quad +2806996008960 v^5 a_0 b_0 b_2^2 \\
 &\quad +231948288 \sin(v) v^{10} b_1 b_2^3 \\
 &\quad +74760192 \sin(v) v^{10} b_1 b_2^2 \\
 &\quad +1104150528000 v^{11} a_0^3 b_0^3 \\
 &\quad -1104150528000 v^{11} a_0^3 b_0^4 \\
 &\quad +165867945984 v^5 b_1^2 b_2 \\
 &\quad -1626781777920 v^9 a_0^2 b_0^3 \\
 &+2875044397056 \sin(v) v^4 b_1^2 \\
 &\quad +32163495936 \sin(v) v^4 b_2^2 \\
 &+1916696264704 \sin(v) v^2 b_1 \\
 &\quad +202727489536 \sin(v) b_2 v^2 \\
 &\quad +4385931264 \sin(v) v^8 b_1 b_2^2 \\
 &+608182468608 \sin(v) v^6 b_1^2 b_2 \\
 &\quad +64326991872 \sin(v) v^6 b_1 b_2^2 \\
 &\quad +26873856 v^{13} a_0 b_0 b_2^3 \\
 &\quad -2208301056000 v^{11} a_0^3 b_0^3 b_1 \\
 &\quad -2208301056000 v^{11} a_0^3 b_0^3 b_2 \\
 &\quad -287079137280 v^{11} a_0^2 b_0^3 b_1 \\
 &-20127744 \sin(v) v^{14} a_0 b_0 b_1 b_2^2 \\
 &\quad +13932907462656 v^3 b_1^2 b_2 \\
 &+2561383858176 v^3 b_1 b_2^2 - 5750088794112 v b_0 b_1 \\
 &\quad +64326991872 v^3 b_0 b_2^2 \\
 &-608182468608 v b_0 b_2 - 12716542525440 v b_1 b_2 \\
 &\quad +2267938816 \sin(v) v^6 b_2^3 \\
 &\quad +1916696264704 \sin(v) v^6 b_1^3 \\
 &\quad +398131200 v^{19} a_0^4 b_0^4
 \end{aligned}$$

$$\begin{aligned}
& +15925248000v^{17}a_0^4b_0^4 & +3189768192\sin(v)v^8a_0b_0b_2 \\
+86261760v^{17}a_0^3b_0^4 + 110415052800v^{13}a_0^3b_0^4 & -299040768\sin(v)v^{10}a_0b_0b_2 \\
& -269568v^{11}b_0b_2^3 & +13563002880v^{13}a_0^2b_0^2b_2^2 \\
+41865707520v^{11}a_0^2b_0^3 + 3139928064v^9b_1^2b_2^2 & -20736\sin(v)v^{22}a_0^3b_0^3b_2 \\
-11321856v^{11}b_1b_2^3 - 307413909504v^9a_0b_0b_1b_2 & -5750784\sin(v)v^{20}a_0^3b_0^3b_1 \\
& +302399225856v^9a_0b_0b_1b_2^2 & +1880064\sin(v)v^{20}a_0^3b_0^3b_2 \\
& +1779890651136v^9a_0b_0b_1^2b_2 & +7776\sin(v)v^{20}a_0^2b_0^2b_2^2 \\
& +41466986496v^9a_0b_0^2b_1b_2 & +690094080\sin(v)v^{18}a_0^3b_0^3b_1 \\
+4232577024000v^9a_0^2b_0^2b_1b_2 & -26542080\sin(v)v^{18}a_0^3b_0^3b_2 \\
& -51066961920v^{11}a_0^2b_0^3b_2 & -165888\sin(v)v^{18}a_0^2b_0^2b_2^2 \\
-2488019189760v^{11}a_0^2b_0^2b_1^2 & -1296\sin(v)v^{18}a_0b_0b_2^3 \\
-152740823040v^{11}a_0^2b_0^2b_2^2 & -27603763200\sin(v)v^{16}a_0^3b_0^3b_1 \\
+393813688320v^{11}a_0^2b_0^2b_2 & -1592524800\sin(v)v^{16}a_0^3b_0^3b_2 \\
-319168512v^{11}a_0b_0^2b_2^2 & +598081536\sin(v)v^{16}a_0^2b_0^2b_1^2 \\
-1806188544v^{11}a_0b_0b_2^3 & -17362944\sin(v)v^{16}a_0^2b_0^2b_2^2 \\
+819486720v^{11}a_0b_0b_2^2 & +4313088\sin(v)v^{16}a_0^2b_0^2b_2 \\
-27603763200\sin(v)v^{14}a_0^3b_0^3 & -62208\sin(v)v^{16}a_0b_0b_2^3 \\
& +231948288\sin(v)v^8b_2^3 & +368050176000\sin(v)v^{14}a_0^3b_0^3b_1 \\
& +20733493248\sin(v)v^6b_1b_2 & +38928384000\sin(v)v^{14}a_0^3b_0^3b_2 \\
+1105786306560\sin(v)b_0a_0v^4 & -47846522880\sin(v)v^{14}a_0^2b_0^2b_1^2 \\
& +608182468608\sin(v)v^4b_1b_2 & +194641920\sin(v)v^{14}a_0^2b_0^2b_2^2 \\
& +59969536\sin(v)v^8b_2^4 & +1196163072\sin(v)v^{14}a_0^2b_0^2b_1 \\
& +479174066176\sin(v)v^8b_1^4 & -218529792\sin(v)v^{14}a_0^2b_0^2b_2 \\
& +8177664\sin(v)v^{10}b_2^4 & +1216512\sin(v)v^{14}a_0b_0b_2^3 \\
& +7907328\sin(v)v^{10}b_2^3 & -1078272\sin(v)v^{14}a_0b_0b_2^2 \\
& +89856\sin(v)v^{12}b_2^3 & +956930457600\sin(v)v^{12}a_0^2b_0^2b_1^2 \\
& +418176\sin(v)v^{12}b_2^4 & +10705305600\sin(v)v^{12}a_0^2b_0^2b_2^2 \\
& +9504\sin(v)v^{14}b_2^4 & -95693045760\sin(v)v^{12}a_0^2b_0^2b_1 \\
-103667466240v^3b_0b_2 & -3220439040\sin(v)v^{12}a_0^2b_0^2b_2 \\
-1078272\sin(v)v^{16}a_0b_0b_1b_2^2 & -27644657664\sin(v)v^{12}a_0b_0b_1^3 \\
-3220439040\sin(v)v^{14}a_0^2b_0^2b_1b_2 & \\
-299040768\sin(v)v^{14}a_0b_0b_1^2b_2 & \\
+29345867366400v^5a_0b_0b_1b_2 & \\
+3317358919680\sin(v)v^6a_0b_0b_1 & \\
+350874501120\sin(v)v^6a_0b_0b_2 & \\
-82933972992\sin(v)v^8a_0b_0b_1 &
\end{aligned}$$

$$\begin{aligned}
 &+101105664 \sin(v) v^{12} a_0 b_0 b_2^3 \\
 &\quad -20127744 \sin(v) v^{12} a_0 b_0 b_2^2 \\
 &+1913860915200 \sin(v) v^{10} a_0^2 b_0^2 b_1 \\
 &\quad +2760376320 v^7 b_2^3 \\
 &+202427596800 \sin(v) v^{10} a_0^2 b_0^2 b_2 \\
 &+1105786306560 \sin(v) v^{10} a_0 b_0 b_1^3 \\
 &\quad +1308426240 \sin(v) v^{10} a_0 b_0 b_2^3 \\
 &\quad -82933972992 \sin(v) v^{10} a_0 b_0 b_1^2 \\
 &\quad +1602551808 \sin(v) v^{10} a_0 b_0 b_2^2 \\
 &+3317358919680 \sin(v) v^8 a_0 b_0 b_1^2 \\
 &\quad +37111726080 \sin(v) v^8 a_0 b_0 b_2^2 \\
 &+49268736 v^9 b_2^4 - 53913600 v^9 b_2^3 \\
 &\quad -11500177588224 v b_1^2 \\
 &-1216364937216 v b_2^2 - 1679616 v^{11} b_2^4 \\
 &\quad +17543725056 v^5 b_2^3 \\
 &\quad +11500177588224 v^3 b_1^3 \\
 &\quad +128653983744 v^3 b_2^3 \\
 &\quad -829339729920 b_2 v \\
 &\quad +29904076800 v^5 b_2^2 \\
 &\quad -119616307200 v^3 b_2^2 \\
 &\quad -1086898176 v^{15} a_0^2 b_0^2 b_1 b_2 \\
 &\quad +158031544320 v^{13} a_0^2 b_0^2 b_1 b_2 \\
 &\quad +181149696 v^{13} a_0 b_0 b_1 b_2^2 \\
 &-1357185024000 v^{11} a_0^2 b_0^2 b_1 b_2 \\
 &\quad -1794244608 v^{11} a_0 b_0^2 b_1 b_2 \\
 &\quad -75358273536 v^{11} a_0 b_0 b_1^2 b_2 \\
 &\quad -22859366400 v^{11} a_0 b_0 b_1 b_2^2 \\
 &\quad +4313088 v^{13} a_0 b_0^2 b_2^2 \\
 &\quad -4485611520 v^{13} a_0^2 b_0^2 b_2 \\
 &+701749002240 \sin(v) v^8 a_0 b_0 b_1 b_2 \\
 &\quad +6379536384 \sin(v) v^{10} a_0 b_0 b_1 b_2 \\
 &+37111726080 \sin(v) v^{10} a_0 b_0 b_1 b_2^2 \\
 &+350874501120 \sin(v) v^{10} a_0 b_0 b_1^2 b_2 \\
 &\quad +2192965632 \sin(v) v^{10} b_1^2 b_2^2 \\
 &\quad +6911164416 \sin(v) v^{10} b_1^3 b_2 \\
 &\quad -14736729047040 v^9 a_0^2 b_0^2 b_1 \\
 &\quad +1710513192960 v^{11} a_0^2 b_0^2 b_1 \\
 &\quad -218529792 \sin(v) v^{16} a_0^2 b_0^2 b_1 b_2 \\
 &\quad +4313088 \sin(v) v^{18} a_0^2 b_0^2 b_1 b_2 \\
 &\quad +502388490240 v^{13} a_0^2 b_0^2 b_1^2 \\
 &\quad +2645360640 v^{13} a_0^2 b_0^3 b_2 \\
 &\quad +11961630720 v^{13} a_0^2 b_0^3 b_1 \\
 &\quad +220830105600 v^{13} a_0^3 b_0^3 b_2 \\
 &\quad +220830105600 v^{13} a_0^3 b_0^3 b_1 \\
 &\quad -161243136 v^{15} a_0^2 b_0^2 b_2^2 \\
 &\quad -25878528 v^{15} a_0^2 b_0^3 b_2 \\
 &\quad +3397386240 v^{15} a_0^3 b_0^3 b_2 \\
 &\quad +102133923840 v^{15} a_0^3 b_0^3 b_1 \\
 &\quad +637009920 v^{17} a_0^3 b_0^3 b_2 \\
 &\quad +3622993920 v^{17} a_0^3 b_0^3 b_1 \\
 &\quad +7907328 \sin(v) v^{12} b_1 b_2^3 \\
 &\quad +37380096 \sin(v) v^{12} b_1^2 b_2^2 \\
 &+368050176000 \sin(v) v^{12} a_0^3 b_0^3 \\
 &\quad +89856 \sin(v) v^{14} b_1 b_2^3 \\
 &+53084160000 \sin(v) v^{16} a_0^4 b_0^4 \\
 &\quad -5308416000 \sin(v) v^{18} a_0^4 b_0^4 \\
 &\quad +199065600 \sin(v) v^{20} a_0^4 b_0^4 \\
 &\quad -3317760 \sin(v) v^{22} a_0^4 b_0^4 \\
 &\quad +20736 \sin(v) v^{24} a_0^4 b_0^4 \\
 &\quad +82933972992 v^5 b_0 b_1 b_2 \\
 &\quad +13269435678720 v^5 a_0 b_0^2 b_1 \\
 &\quad +13269435678720 v^7 a_0 b_0 b_1^2 \\
 &\quad +239232614400 v^7 a_0 b_0^2 b_2 + 74760192 v^9 b_0 b_1 b_2^2 \\
 &\quad -67951263744 v^9 a_0 b_0 b_2^2 - 10167386112 v^9 a_0 b_0^2 b_2 \\
 &\quad +16194207744 v^9 a_0 b_0 b_2^3 + 3483226865664 v^9 a_0 b_0 b_1^3 \\
 &\quad +3458138112 v^9 a_0 b_0^2 b_2^2 + 82933972992 v^9 a_0 b_0^2 b_1^2 \\
 &\quad -5848317296640 v^9 a_0^2 b_0^2 b_2 + 404855193600 v^9 a_0^2 b_0^2 b_2^2 \\
 &\quad +3827721830400 v^9 a_0^2 b_0^2 b_1^2 + 202427596800 v^9 a_0^2 b_0^3 b_2 \\
 &\quad +1913860915200 v^9 a_0^2 b_0^3 b_1 \\
 T_7 = &\left(12 v^6 a_0 b_0 - 480 b_0 a_0 v^4 - 3 v^4 b_2 \right. \\
 &\quad \left. - 832 v^2 b_1 - 88 b_2 v^2 - 832 \right)^4
 \end{aligned}$$

Appendix B: Formulae T_k , $k = 8(1)15$

$$\begin{aligned}
 T_8 &= 104 (\cos(v))^2 \sin(v) v^2 \\
 &\quad - 520 (\cos(v))^2 v^3 \\
 &\quad + 312 (\cos(v))^3 v \\
 &\quad + 4576 \cos(v) v^2 \sin(v) \\
 &\quad + 312 (\cos(v))^2 \sin(v) \\
 &\quad + 10920 (\cos(v))^2 v + 1560 v^2 \sin(v) \\
 &\quad - 1040 v^3 - 6864 \cos(v) \sin(v) \\
 &\quad - 7176 v \cos(v) + 6552 \sin(v) - 4056 v \\
 T_9 &= -178560 v - 45672 (\cos(v))^2 \sin(v) v^2 \\
 &\quad + 173694 \cos(v) v^4 \sin(v) \\
 &\quad - 524976 \cos(v) v^2 \sin(v) \\
 &\quad + 1329 (\cos(v))^2 \sin(v) v^4 \\
 &\quad - 5796 v^6 \sin(v) \cos(v) \\
 &\quad - 129 (\cos(v))^2 \sin(v) v^6 \\
 &\quad + 9633 v^5 + 630 v^7 + 407952 (\cos(v))^2 v^3 \\
 &\quad - 89280 (\cos(v))^3 v + 570648 v^2 \sin(v) \\
 &\quad + 178560 \cos(v) \sin(v) + 267840 v \cos(v) \\
 &\quad - 158040 \cos(v) v^3 - 3195 v^6 \sin(v) - 3267 \cos(v) v^5 \\
 &\quad - 8703 v^4 \sin(v) + 315 (\cos(v))^2 v^7 \\
 &\quad + 17640 (\cos(v))^3 v^3 \\
 &\quad + 144 (\cos(v))^4 v^3 \\
 &\quad - 35535 (\cos(v))^2 v^5 \\
 &\quad - 351 (\cos(v))^3 v^5 \\
 &\quad - 89280 (\cos(v))^2 \sin(v) \\
 &\quad - 89280 \sin(v) - 267696 v^3 \\
 T_{10} &= -59520 v - 15224 (\cos(v))^2 \sin(v) v^2 \\
 &\quad + 57898 \cos(v) v^4 \sin(v) \\
 &\quad - 174992 \cos(v) v^2 \sin(v) \\
 &\quad + 443 (\cos(v))^2 \sin(v) v^4 \\
 &\quad - 1932 v^6 \sin(v) \cos(v) \\
 &\quad - 43 (\cos(v))^2 \sin(v) v^6 \\
 &\quad + 3211 v^5 + 210 v^7 + 135984 (\cos(v))^2 v^3 \\
 &\quad - 29760 (\cos(v))^3 v \\
 &\quad + 190216 v^2 \sin(v) + 59520 \cos(v) \sin(v) \\
 &\quad + 89280 v \cos(v) \\
 &\quad - 52680 \cos(v) v^3 - 1065 v^6 \sin(v) \\
 &\quad - 1089 \cos(v) v^5 \\
 &\quad - 2901 v^4 \sin(v) + 105 (\cos(v))^2 v^7 \\
 &\quad + 5880 (\cos(v))^3 v^3
 \end{aligned}$$

$$\begin{aligned}
 &+ 48 (\cos(v))^4 v^3 - 11845 (\cos(v))^2 v^5 \\
 &\quad - 117 (\cos(v))^3 v^5 \\
 &\quad - 29760 (\cos(v))^2 \sin(v) \\
 &\quad - 29760 \sin(v) - 89232 v^3 \\
 T_{11} &= v^5 \left(- (\cos(v))^2 \sin(v) v^3 \right. \\
 &\quad + 3 (\cos(v))^3 v^2 \\
 &\quad - 84 \cos(v) v^3 \sin(v) \\
 &\quad + 3 (\cos(v))^2 \sin(v) v \\
 &\quad \left. + 200 (\cos(v))^2 v^2 \right. \\
 &\quad - 435 v^3 \sin(v) - 126 v \cos(v) \sin(v) \\
 &\quad - 1329 \cos(v) v^2 + 600 (\cos(v))^2 \\
 &\quad \left. + 1323 v \sin(v) + 526 v^2 - 600 \right) \\
 T_{12} &= 21120 v + 1144 (\cos(v))^2 \sin(v) v^2 \\
 &\quad - 17010 \cos(v) v^4 \sin(v) \\
 &\quad + 30352 \cos(v) v^2 \sin(v) \\
 &\quad - 327 (\cos(v))^2 \sin(v) v^4 \\
 &\quad - 516 v^6 \sin(v) \cos(v) \\
 &\quad - 9 (\cos(v))^2 \sin(v) v^6 \\
 &\quad + 6293 v^5 + 30 v^7 - 42192 (\cos(v))^2 v^3 \\
 &\quad + 10560 (\cos(v))^3 v \\
 &\quad - 31496 v^2 \sin(v) \\
 &\quad - 21120 \cos(v) \sin(v) \\
 &\quad - 31680 v \cos(v) + 97224 \cos(v) v^3 \\
 &\quad - 1395 v^6 \sin(v) - 11547 \cos(v) v^5 \\
 &\quad + 33897 v^4 \sin(v) \\
 &\quad + 15 (\cos(v))^2 v^7 \\
 &\quad - 120 (\cos(v))^3 v^3 \\
 &\quad + 685 (\cos(v))^2 v^5 \\
 &\quad + 9 (\cos(v))^3 v^5 \\
 &\quad + 10560 (\cos(v))^2 \sin(v) \\
 &\quad + 10560 \sin(v) - 54912 v^3 \\
 T_{13} &= v^5 \left(- (\cos(v))^2 \sin(v) v^3 \right. \\
 &\quad + 3 (\cos(v))^3 v^2 \\
 &\quad - 84 \cos(v) v^3 \sin(v) \\
 &\quad + 3 (\cos(v))^2 \sin(v) v \\
 &\quad + 200 (\cos(v))^2 v^2 - 435 v^3 \sin(v) \\
 &\quad - 126 v \cos(v) \sin(v) - 1329 \cos(v) v^2 \\
 &\quad \left. + 600 (\cos(v))^2 + 1323 v \sin(v) + 526 v^2 - 600 \right)
 \end{aligned}$$

$$\begin{aligned}
 T_{14} &= 2496 (\cos(v))^2 \sin(v) v^4 \\
 &\quad - 8320 (\cos(v))^2 v^5 \\
 &+ 2496 (\cos(v))^3 v^3 + 109824 \cos(v) v^4 \sin(v) \\
 &\quad - 10816 (\cos(v))^2 \sin(v) v^2 \\
 &\quad + 374400 (\cos(v))^2 v^3 \\
 &+ 37440 v^4 \sin(v) - 16640 v^5 - 99840 (\cos(v))^3 v \\
 &\quad - 627328 \cos(v) v^2 \sin(v) - 57408 \cos(v) v^3 \\
 &\quad - 99840 (\cos(v))^2 \sin(v) + 638144 v^2 \sin(v) \\
 &\quad - 319488 v^3 + 199680 \cos(v) \sin(v) \\
 &\quad + 299520 v \cos(v) - 99840 \sin(v) - 199680 v \\
 T_{15} &= 3 v^5 \left(-(\cos(v))^2 \sin(v) v^3 \right. \\
 &\quad \left. + 3 (\cos(v))^3 v^2 \right. \\
 &\quad \left. - 84 \cos(v) v^3 \sin(v) \right. \\
 &\quad \left. + 3 (\cos(v))^2 \sin(v) v \right. \\
 &+ 200 (\cos(v))^2 v^2 - 435 v^3 \sin(v) \\
 &\quad \left. - 126 v \cos(v) \sin(v) \right. \\
 &\left. - 1329 \cos(v) v^2 + 600 (\cos(v))^2 \right. \\
 &\quad \left. + 1323 v \sin(v) + 526 v^2 - 600 \right)
 \end{aligned}$$

Formulae of the derivatives which presented in the formulae of the Local Truncation Errors:

$$\begin{aligned}
 q_n^{(2)} &= (V(x) - V_c + G) q(x) \\
 q_n^{(3)} &= \left(\frac{d}{dx} g(x) \right) q(x) \\
 &\quad + (g(x) + G) \frac{d}{dx} q(x) \\
 q_n^{(4)} &= \left(\frac{d^2}{dx^2} g(x) \right) q(x) \\
 &\quad + 2 \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + (g(x) + G)^2 q(x) \\
 q_n^{(5)} &= \left(\frac{d^3}{dx^3} g(x) \right) q(x) \\
 &\quad + 3 \left(\frac{d^2}{dx^2} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + 4 (g(x) + G) q(x) \frac{d}{dx} g(x) \\
 &\quad + (g(x) + G)^2 \frac{d}{dx} q(x) \\
 q_n^{(6)} &= \left(\frac{d^4}{dx^4} g(x) \right) q(x) \\
 &\quad + 4 \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + 7 (g(x) + G) q(x) \frac{d^2}{dx^2} g(x) \\
 &\quad + 4 \left(\frac{d}{dx} g(x) \right)^2 q(x) \\
 &\quad + 6 (g(x) + G) \left(\frac{d}{dx} q(x) \right) \frac{d}{dx} g(x) \\
 &\quad + (g(x) + G)^3 q(x) \\
 q_n^{(7)} &= \left(\frac{d^5}{dx^5} g(x) \right) q(x) \\
 &\quad + 5 \left(\frac{d^4}{dx^4} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + 11 (g(x) + G) q(x) \frac{d^3}{dx^3} g(x) \\
 &\quad + 15 \left(\frac{d}{dx} g(x) \right) q(x)
 \end{aligned}$$

Appendix C: Formulae of the derivatives of q_n

Expressions of the derivatives are necessary since they are included in the formulae of the Local Truncation Errors based on the test problem (19).

$$\begin{aligned}
& \frac{d^2}{dx^2}g(x) + 13(g(x) + G) \\
& \quad \left(\frac{d}{dx}q(x)\right) \frac{d^2}{dx^2}g(x) \\
& + 10 \left(\frac{d}{dx}g(x)\right)^2 \frac{d}{dx}q(x) \\
& \quad + 9(g(x) + G)^2 q(x) \\
& \frac{d}{dx}g(x) + (g(x) + G)^3 \frac{d}{dx}q(x) \\
& q_n^{(8)} = \left(\frac{d^6}{dx^6}g(x)\right) q(x) \\
& \quad + 6 \left(\frac{d^5}{dx^5}g(x)\right) \frac{d}{dx}q(x) \\
& + 16(g(x) + G)q(x) \frac{d^4}{dx^4}g(x) \\
& \quad + 26 \left(\frac{d}{dx}g(x)\right) q(x) \\
& \frac{d^3}{dx^3}g(x) + 24(g(x) + G) \\
& \quad \left(\frac{d}{dx}q(x)\right) \frac{d^3}{dx^3}g(x) \\
& + 15 \left(\frac{d^2}{dx^2}g(x)\right)^2 q(x) \\
& \quad + 48 \left(\frac{d}{dx}g(x)\right) \\
& \quad \left(\frac{d}{dx}q(x)\right) \frac{d^2}{dx^2}g(x) \\
& \quad + 22(g(x) + G)^2 q(x) \\
& \frac{d^2}{dx^2}g(x) + 28(g(x) + G) \\
& \quad q(x) \left(\frac{d}{dx}g(x)\right)^2 \\
& \quad + 12(g(x) + G)^2 \\
& \quad \left(\frac{d}{dx}q(x)\right) \frac{d}{dx}g(x) \\
& \quad + (g(x) + G)^4 q(x) \\
& \quad \dots
\end{aligned}$$

Appendix D: Formulae S_i , $i = 0(1)2$

$$\begin{aligned}
S_0 = & -126v^6 \sin(v) \cos(v) \\
& + 3(\cos(v))^2 \sin(v) v^6 - 600v^5 \\
& + 526v^7 + 1323v^6 \sin(v) \\
& + 200(\cos(v))^2 v^7 \\
& + 600(\cos(v))^2 v^5 \\
& + 69 \cos(v) s^4 v^3 + 3849 \cos(v) s^2 v^5 \\
& - 4200(\cos(v))^2 s^4 v \\
& + 864(\cos(v))^2 s^2 v^3 \\
& - 1367 \sin(v) s^4 v^2 - 12619 \sin(v) s^2 v^4 \\
& + 2400 \cos(v) \sin(v) s^4 \\
& + 2400 \cos(v) s^4 v - 30384 \cos(v) s^2 v^3 \\
& - 12000 \sin(v) s^2 v^2 \\
& - (\cos(v))^2 \sin(v) v^8 \\
& - 5(\cos(v))^2 s^6 v^3 \\
& + 10(\cos(v))^2 s^4 v^5 \\
& - 5(\cos(v))^2 s^2 v^7 \\
& + 3(\cos(v))^3 s^6 v \\
& - 3(\cos(v))^3 s^4 v^3 \\
& - 3(\cos(v))^3 s^2 v^5 \\
& - 84 \cos(v) \sin(v) v^8 \\
& + 3(\cos(v))^2 \sin(v) s^6 \\
& + 105(\cos(v))^2 s^6 v \\
& - 250(\cos(v))^2 s^4 v^3 \\
& + 65(\cos(v))^2 s^2 v^5 \\
& + 15 \sin(v) s^6 v^2 - 45 \sin(v) s^4 v^4 \\
& + 465 \sin(v) s^2 v^6 \\
& - 48(\cos(v))^3 s^2 v^3 \\
& - 66 \cos(v) \sin(v) s^6 \\
& - 69 \cos(v) s^6 v + (\cos(v))^2 \sin(v) s^6 v^2 \\
& - 3(\cos(v))^2 \sin(v) s^4 v^4 \\
& + 3(\cos(v))^2 \sin(v) s^2 v^6 \\
& + 44 \cos(v) \sin(v) s^6 v^2 \\
& - 132 \cos(v) \sin(v) s^4 v^4 \\
& + 172 \cos(v) \sin(v) s^2 v^6 \\
& - 27(\cos(v))^2 \sin(v) s^4 v^2 \\
& + 21(\cos(v))^2 \sin(v) s^2 v^4 \\
& - 1006 \cos(v) \sin(v) s^4 v^2 \\
& + 1798 \cos(v) \sin(v) s^2 v^4 \\
& + 12000 \cos(v) \sin(v) s^2 v^2
\end{aligned}$$

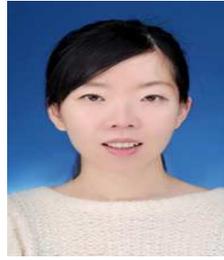
$$\begin{aligned}
 &+784s^4v^3 + 1800s^4v + 29568s^2v^3 - 1065 \sin(v)s^2v^6 \\
 &\quad -1511s^2v^5 - 10s^6v^3 + 20s^4v^5 + 5136 (\cos(v))^3 s^2v^3 \\
 &-10s^2v^7 - 39s^6v + 3 (\cos(v))^3 v^7 + 1386 \cos(v) \sin(v)s^6 + 1449 \cos(v)s^6v \\
 &-435 \sin(v)v^8 - 1329 \cos(v)v^7 - 21 (\cos(v))^2 \sin(v)s^6v^2 \\
 &\quad +63 \sin(v)s^6 - 2400 \sin(v)s^4 + 63 (\cos(v))^2 \sin(v)s^4v^4 \\
 S_1 = v^5 &\left(-(\cos(v))^2 \sin(v)v^3 - 43 (\cos(v))^2 \sin(v)s^2v^6 \right. \\
 &\quad +3 (\cos(v))^3 v^2 - 924 \cos(v) \sin(v)s^6v^2 \\
 &\quad -84 \cos(v)v^3 \sin(v) + 2772 \cos(v) \sin(v)s^4v^4 \\
 &\quad +3 (\cos(v))^2 \sin(v)v - 1932 \cos(v) \sin(v)s^2v^6 \\
 &\quad \left. +200 (\cos(v))^2 v^2 - 233 (\cos(v))^2 \sin(v)s^4v^2 \right. \\
 &-435 v^3 \sin(v) - 126 v \cos(v) \sin(v) - 301 (\cos(v))^2 \sin(v)s^2v^4 \\
 &\quad -1329 \cos(v)v^2 + 600 (\cos(v))^2 - 14074 \cos(v) \sin(v)s^4v^2 \\
 &\quad \left. +1323 v \sin(v) + 526 v^2 - 600 \right) + 25162 \cos(v) \sin(v)s^2v^4 \\
 S_2 = 126v^6 &\sin(v) \cos(v) + 12000 \cos(v) \sin(v)s^2v^2 \\
 &\quad -3 (\cos(v))^2 \sin(v)v^6 - 8464s^4v^3 - 6600s^4v + 6000s^2v^3 + 8171s^2v^5 \\
 &\quad +600v^5 - 526v^7 - 1323v^6 \sin(v) + 210s^6v^3 - 420s^4v^5 + 210s^2v^7 + 819s^6v \\
 &\quad -200 (\cos(v))^2 v^7 - 3 (\cos(v))^3 v^7 + 435 \sin(v)v^8 + 1329 \cos(v)v^7 \\
 &\quad -600 (\cos(v))^2 v^5 - 1323 \sin(v)s^6 \\
 &\quad +48 (\cos(v))^4 s^2v^3 \\
 &\quad -2400 (\cos(v))^3 s^4v \\
 &\quad -2400 (\cos(v))^2 \sin(v)s^4 \\
 &\quad -12000 (\cos(v))^2 \sin(v)s^2v^2 \\
 &-1449 \cos(v)s^4v^3 - 1089 \cos(v)s^2v^5 \\
 &\quad +4200 (\cos(v))^2 s^4v \\
 &\quad +24384 (\cos(v))^2 s^2v^3 \\
 +16707 \sin(v)s^4v^2 &- 14061 \sin(v)s^2v^4 \\
 &\quad +2400 \cos(v) \sin(v)s^4 \\
 +4800 \cos(v)s^4v &- 35568 \cos(v)s^2v^3 \\
 &\quad + (\cos(v))^2 \sin(v)v^8 \\
 &\quad +105 (\cos(v))^2 s^6v^3 \\
 &\quad -210 (\cos(v))^2 s^4v^5 \\
 &\quad +105 (\cos(v))^2 s^2v^7 \\
 &\quad -63 (\cos(v))^3 s^6v \\
 &\quad +63 (\cos(v))^3 s^4v^3 \\
 &\quad -117 (\cos(v))^3 s^2v^5 \\
 &\quad +84 \cos(v) \sin(v)v^8 \\
 -63 (\cos(v))^2 &\sin(v)s^6 \\
 &\quad -2205 (\cos(v))^2 s^6v \\
 &\quad +9250 (\cos(v))^2 s^4v^3 \\
 &\quad -9365 (\cos(v))^2 s^2v^5 \\
 -315 \sin(v)s^6v^2 &+ 945 \sin(v)s^4v^4
 \end{aligned}$$

References

- [1] Z. A. Anastassi and T.E. Simos, A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 236 3880-3889(2012)
- [2] A.D. Raptis and T.E. Simos: A four-step phase-fitted method for the numerical integration of second order initial-value problem, *BIT*, 31, 160-168(1991)
- [3] D.G. Quinlan and S. Tremaine, Symmetric Multistep Methods for the Numerical Integration of Planetary Orbits, *The Astronomical Journal*, 100, 5, 1694-1700 (1990)
- [4] J.M. Franco, M. Palacios, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS*, 30, 1 (1990)
- [5] J.D.Lambert, Numerical Methods for Ordinary Differential Systems, The Initial Value Problem, Pages 104-107, John Wiley and Sons. (1991)
- [6] E. Stiefel, D.G. Bettis, Stabilization of Cowell's method, *Numer. Math.* 13, 154-175 (1969)
- [7] G.A. Panopoulos, Z.A. Anastassi and T.E. Simos: Two New Optimized Eight-Step Symmetric Methods for the Efficient Solution of the Schrödinger Equation and Related Problems, *MATCH Commun. Math. Comput. Chem.*, 60, 3, 773-785 (2008)
- [8] G.A. Panopoulos, Z.A. Anastassi and T.E. Simos, Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions, *Journal of Mathematical Chemistry*, 46(2), 604-620(2009)
- [9] <http://www.burtleburgle.net/bob/math/multistep.html>

- [10] T.E. Simos and P.S. Williams, Bessel and Neumann fitted methods for the numerical solution of the radial Schrödinger equation, *Computers and Chemistry*, 21, 175-179 (1977)
- [11] T.E. Simos and Jesus Vigo-Aguiar, A dissipative exponentially-fitted method for the numerical solution of the Schrödinger equation and related problems, *Computer Physics Communications*, 152, 274-294 (2003)
- [12] T.E. Simos and G. Psihoyios, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 175 (1): IX-IX MAR 1 2005
- [13] T. Lyche, Chebyshevian multistep methods for Ordinary Differential Eqations, *Num. Math.* 19, 65-75 (1972)
- [14] T.E. Simos and P.S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation, *Journal of Computational and Applied Mathematics* 79, 189205 (1997).
- [15] R.M. Thomas, Phase properties of high order almost P-stable formulae, *BIT* 24, 225238(1984).
- [16] J.D. Lambert and I.A. Watson, Symmetric multistep methods for periodic initial values problems, *J. Inst. Math. Appl.* 18 189202 (1976)
- [17] A. Konguetsof and T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 158(1) 93-106(2003)
- [18] Z. Kalogiratou, T. Monovasilis and T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 158(1) 83-92(2003)
- [19] Z. Kalogiratou and T.E. Simos, Newton-Cotes formulae for long-time integration, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 158(1) 75-82(2003)
- [20] G. Psihoyios and T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 158(1) 135-144(2003)
- [21] T.E. Simos, I.T. Famelis and C. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions, *NUMERICAL ALGORITHMS* 34(1) 27-40(2003)
- [22] T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution, *APPLIED MATHEMATICS LETTERS* 17(5) 601-607(2004)
- [23] K. Tselios and T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* Volume: 175(1) 173-181(2005)
- [24] D.P. Sakas and T.E. Simos, Multiderivative methods of eighth algebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 175(1) 161-172(2005)
- [25] G. Psihoyios and T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 175(1) 137-147(2005)
- [26] Z. A. Anastassi and T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* 175(1) 1-9(2005)
- [27] T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems, *APPLIED MATHEMATICS LETTERS* Volume: 22 (10) 1616-1621(2009)
- [28] S. Stavroyiannis and T.E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs, *APPLIED NUMERICAL MATHEMATICS* 59(10) 2467-2474(2009)
- [29] T.E. Simos, Exponentially and Trigonometrically Fitted Methods for the Solution of the Schrödinger Equation, *ACTA APPLICANDAE MATHEMATICAE* 110(3) 1331-1352(2010)
- [30] T. E. Simos, New Stable Closed Newton-Cotes Trigonometrically Fitted Formulae for Long-Time Integration, *Abstract and Applied Analysis*, Volume 2012, Article ID 182536, 15 pages, 2012 doi:10.1155/2012/182536
- [31] T.E. Simos, Optimizing a Hybrid Two-Step Method for the Numerical Solution of the Schrödinger Equation and Related Problems with Respect to Phase-Lag, *Journal of Applied Mathematics*, Volume 2012, Article ID 420387, 17 pages, doi:10.1155/2012/420387, 2012
- [32] G.A. Panopoulos and T.E. Simos, An eight-step semi-embedded predictor-corrector method for orbital problems and related IVPs with oscillatory solutions for which the frequency is unknown, *Journal of Computational and Applied Mathematics* **290** 115(2015)
- [33] D. F. Papadopoulos, T. E Simos, The Use of Phase Lag and Amplification Error Derivatives for the Construction of a Modified Runge-Kutta-Nyström Method, *Abstract and Applied Analysis* Article Number: 910624 Published: 2013
- [34] I. Alolyan, Z.A. Anastassi, Z. A. and T.E. Simos, A new family of symmetric linear four-step methods for the efficient integration of the Schrödinger equation and related oscillatory problems, *Applied Mathematics and Computation*, 218(9), 5370-5382(2012)
- [35] Ibraheem Alolyan and T.E. Simos, A family of high-order multistep methods with vanished phase-lag and its derivatives for the numerical solution of the Schrödinger equation, *Computers & Mathematics with Applications*, 62(10), 3756-3774(2011)
- [36] Ch Tsitouras, I. Th. Famelis, and T.E. Simos, On modified Runge-Kutta trees and methods, *Computers & Mathematics with Applications*, 62(4), 2101-2111(2011)
- [37] A. A. Kosti, Z. A. Anastassi and T.E. Simos, Construction of an optimized explicit Runge-Kutta-Nyström method for the numerical solution of oscillatory initial value problems, *Computers & Mathematics with Applications*, 61(11), 3381-3390(2011)
- [38] Z. Kalogiratou, Th. Monovasilis, and T.E. Simos, New modified Runge-Kutta-Nyström methods for the numerical integration of the Schrödinger equation, *Computers & Mathematics with Applications*, 60(6), 1639-1647(2010)
- [39] Th. Monovasilis, Z. Kalogiratou and T.E. Simos, A family of trigonometrically fitted partitioned Runge-Kutta symplectic methods, *Applied Mathematics and Computation*, 209(1), 91-96(2009)
- [40] T.E. Simos, High order closed Newton-Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation, *Applied Mathematics and Computation*, 209(1) 137-151(2009)

- [41] A. Konguetsof and T.E. Simos, An exponentially-fitted and trigonometrically-fitted method for the numerical solution of periodic initial-value problems, *Computers & Mathematics with Applications*, 45(1-3), 547-554 Article Number: PII S0898-1221(02)00354-1 (2003)
- [42] T.E. Simos, On the Explicit Four-Step Methods with Vanished Phase-Lag and its First Derivative, *Applied Mathematics & Information Sciences*, 8(2), 447-458 (2014)
- [43] L. Gr. Ixaru and M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation, *Comput. Phys. Commun.*, 38(3) 329-337(1985)
- [44] L.Gr. Ixaru and M. Micu, *Topics in Theoretical Physics*, Central Institute of Physics, Bucharest, 1978.
- [45] L.Gr. Ixaru and M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies, *Computer Physics Communications* 19, 23-27(1980).
- [46] J.R. Dormand, M.E.A. El-Mikkawy and P.J. Prince, Families of Runge-Kutta-Nyström formulae, *IMA J. Numer. Anal.* 7 235-250 (1987).
- [47] J.R. Dormand and P.J. Prince, A family of embedded RungeKutta formulae, *J. Comput. Appl. Math.* 6 19-26 (1980).
- [48] G.D. Quinlan and S. Tremaine, Symmetric Multistep Methods for the Numerical Integration of Planetary Orbits, *The Astronomical Journal*, 100 1694-1700(1990)
- [49] A. D. Raptis and A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation, *Computer Physics Communications*, 14, 1-5(1978)
- [50] M.M. Chawla and P.S. Rao, An Noumerov-typ method with minimal phase-lag for the integration of second order periodic initial-value problems II Explicit Method, *Journal of Computational and Applied Mathematics*, 15, 329-337(1986)
- [51] M.M. Chawla and P.S. Rao, An explicit sixth - order method with phase-lag of order eight for $y'' = f(t,y)$, *Journal of Computational and Applied Mathematics*, 17, 363-368(1987)
- [52] T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation, *Journal of Mathematical Chemistry*, 46, 981-1007(2009)
- [53] A.D. Raptis and J.R. Cash, A variable step method for the numerical integration of the one-dimensional Schrödinger equation, *Comput. Phys. Commun.* 36 113-119(1985).
- [54] A.C. Allison, The numerical solution of coupled differential equations arising from the Schrödinger equation, *J. Comput. Phys.* 6 378-391(1970).
- [55] R.B. Bernstein, A. Dalgarno, H. Massey and I.C. Percival, Thermal scattering of atoms by homonuclear diatomic molecules, *Proc. Roy. Soc. Ser. A* 274 427-442(1963).
- [56] R.B. Bernstein, Quantum mechanical (phase shift) analysis of differential elastic scattering of molecular beams, *J. Chem. Phys.* 33 795-804(1960).
- [57] T.E. Simos, Exponentially fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation and related problems, *Comput. Mater. Sci.* 18 315-332(2000).
- [58] J.R. Dormand and P.J. Prince, A family of embedded Runge-Kutta formula, *J. Comput. Appl. Math.* 6 19-26(1980).



Jing Ma received the PhD degree in Transportation Planning and Management at Chang'an University, China. In the same University, she entered the post-doc position at present. Her research activity is mainly focused on topics of traffic information engineering and control, such as, traffic modeling, simulation and optimization. She has published research articles in international refereed journals of applied traffic information control.



Theodore E. Simos (b. 1962 in Athens, Greece) is a Visiting Professor within the Distinguished Scientists Fellowship Program at the Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia and Professor at the Laboratory of Computational Sciences of the Department of Computer Science and Technology, Faculty of Sciences and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece. He holds a Ph.D. on Numerical Analysis (1990) from the Department of Mathematics of the National Technical University of Athens, Greece. He is Highly Cited Researcher in Mathematics (<http://isihighlycited.com/> and <http://highlycited.com/>), Active Member of the European Academy of Sciences and Arts, Active Member of the European Academy of Sciences and Corresponding Member of European Academy of Sciences, Arts and Letters. He is Editor-in-Chief of three scientific journals and editor of more than 25 scientific journals. He is reviewer in several other scientific journals and conferences. His research interests are in numerical analysis and specifically in numerical solution of differential equations, scientific computing and optimization. He is the author of over 400 peer-reviewed publications and he has more than 2000 citations (excluding self-citations).