J Math Chem (2011) 49:1330–1356
DOI 10.1007/s10910-011-9824-5

ORIGINAL PAPER

A hybrid method with phase-lag and derivatives equal to zero for the numerical integration of the Schrödinger equation

A. Konguetsof

Received: 3 November 2010 / Accepted: 18 April 2011 / Published online: 7 May 2011

Abstract A family of hybrid methods with algebraic order eight is proposed, with phase-lag and its first four derivatives eliminated. We investigate the behavior of the new algorithm and the property of the local truncation error and a comparison with other methods leads to conclusions and remarks about its accuracy and stability. The newly created method, as well as another Numerov-type methods, are applied to the resonance problem of the radial Schrödinger equation. The eigenenergies approximations, which are obtained prove the superiority of the new two-step method.

Keywords Multistep methods · Explicit methods · Hybrid methods · Phase-lag · Phase-fitted · Schrödinger equation

Abbreviation

LTE Local Truncation Error

1 Numerical methods for second order differential equations

Mathematical modelling with second order differential equations represents oscillatory problems and appears in many scientific fields, such as physics, chemistry, engineering, quantum mechanics, biology, economics etc.

A. Konguetsof
Department of Science, School of Technological Applications, Technological Education Institute of Kavala, 65404 Kavala, Greece

A. Konguetsof (✉)
1 Dimokritou Street, 67100 Xanthi, Greece
e-mail: aurka0@yahoo.com

The general second order initial value problem

$$\frac{d^2\psi(x)}{dx^2} = u(x, \psi(x)), \quad \psi(x_0) = \psi_0, \quad \psi'(x_0) = \psi_0' \tag{1}$$

has a periodic solution. According to our knowledge of the frequency of the above problem, the method chosen for its numerical solution will vary. In most cases the value of the frequency is not stable throughout the interval of the integration. The attempt made with this work, is to construct a method in order to deal with this kind of situation.

The last decades we encounter a lot of methods in numerical analysis for problems of the form (1) and the main categories of those methods are listed below.

- Runge–Kutta and Runge–Kutta–Nyström methods with constant coefficients (See [1–3]).
- Exponentially and trigonometrically fitted Runge–Kutta and Runge–Kutta–Nyström methods (See [4–11])
- Phase-fitted Runge–Kutta and Runge–Kutta–Nyström methods and Runge–Kutta and Runge–Kutta–Nyström methods with minimal phase-lag and dissipation (See [12–33]).
- Multistep methods with constant coefficients (See [34–40]).
- Multistep methods with vanished phase-lag and its derivatives (See [41–45])
- Exponentially and trigonometrically fitted multistep methods (See [46–80]).
- Hybrid(predictor-corrector) methods (See [81–88]).
- Exponentially and trigonometrically fitted hybrid methods (See [89–96]).
- Phase-fitted and minimal phase-lag hybrid methods (See [97–107]).
- Differential schemes as multilayer symplectic integrators (See [108–122])
- Symplectic methods (See [123–125]).
- Review papers (See [126–127]).
- The Bessel and Neumann fitted methods (See [128–129]).
- Non-linear schemes (See [132–133]).
- Conferences with related subject (See [134–139]).
- Other methods on the numerical solution of the Schrödinger equation (See [130, 131] and [140, 141]).
- Boundary value problems (See [142–147]).
- Stability of numerical methods for differential equations (See [148–150]).
- Special methods (See [151–160]).
- Mathematical software (See [161–167]).

The derivation of an eighth algebraic order set of explicit Numerov-type methods is explained and its main properties are studied. The free parameters of the methods have been calculated based on the frequency of the problem. The following paragraphs contain the relative theory, the development and the analysis of the family of methods and its numerical application.

- Necessary theoretical background is given in the second part.
- Description of each stage for the derivation of the new method appears in the third part.

- Comparison of the new method with other methods in accordance to their local truncation error and their stability is made and remarks and theorems are given in the fourth part.
- In the fifth part we have the presentation of the resonance problem of the radial Schrödinger equation and the application of the newly obtained methodology.
- In the sixth and final part we gather our observations and conclusions.

2 Theoretical background

A linear multistep method ([168]) with the general form

$$\sum_{i=0}^{j} \gamma_i^{\psi} \psi_{n+i} = h^2 \sum_{i=0}^{j} \gamma_i^{u} u_{n+i} \tag{2}$$

which has characteristic polynomials

$$p_1(\zeta) = \sum_{i=0}^{j} \gamma_i^{\psi} \psi_{n+i}, \quad p_2(\zeta) = \sum_{i=0}^{j} \gamma_i^{u} u_{n+i}, \quad \zeta \in \mathbb{C} \tag{3}$$

is said to have order method q and error constant c_{q+2}, if for a test equation

$$\sum_{i=0}^{j} \gamma_i^{\psi} z(x+ih) = h^2 \sum_{i=0}^{j} \gamma_i^{u} z''(x+ih) + c_{q+2} h^{q+2} z^{(q+2)}(x) + O(h^{q+3}) \tag{4}$$

The method (2) is called *symmetric*, when

$$\gamma_i^{\psi} = \gamma_{j-i}^{\psi}, \quad \gamma_i^{u} = \gamma_{j-i}^{u}, \quad i = 0, 1, \ldots, j \tag{5}$$

with $\gamma_0^{\psi} = \gamma_j^{\psi} \neq 0$ a necessary condition.

A numerical method of n steps will be considered over the intervals $[t_0, t_1], \ldots, [t_i, t_{i+1}], \ldots, [t_{n-1}, t_n]$, $i = 0, \ldots, (n-1)$ all of which have equal step length h for the initial value problem (1).

In order to study second order problems of this form, based on [34] we use the scalar test equation

$$\frac{d^2\psi(t)}{dt^2} = -\omega^2\, \psi(t) \tag{6}$$

Application of a symmetric $2m$-step method to the above equation, gives us the following difference equation

$$\begin{aligned} &U_m(H)\,\psi(t_0+mh) + \cdots + U_1(H)\,\psi(t_0+h) + U_0(H)\,\psi(t_0) \\ &\quad + U_1(H)\,\psi(t_0-h) + \cdots + U_m(H)\,\psi(t_0-mh) = 0, \end{aligned} \tag{7}$$

where U_j, $j = 0(1)m$ are polynomials of $H = \omega h$.

Thus the characteristic polynomial obtained is:

$$P(r, H) = U_m\, r^m + \cdots + U_1\, r + U_0 + U_1\, r^{-1} + \cdots + U_m\, r^{-m} \tag{8}$$

Theorem 1 [83] *The phase-lag order q_Φ and phase-lag constant c_Φ of a symmetric $2m$-step method with characteristic equation*

$$P(r, H) = 0 \tag{9}$$

are given by the formula

$$\frac{U_0(H) + 2\sum_{j=1}^{m} \cos(jH) U_j(H)}{2\sum_{j=1}^{m} j^2 U_j(H)} = -c_\Phi\, H^{q_\Phi+2} + O(H^{q_\Phi+4}) \tag{10}$$

3 Phase-fitted family of methods

We will study a four-layer method, which is given in the general form:

$$\begin{aligned} \overline{\psi}_{n+1} &= 2\psi_n - \psi_{n-1} + h^2\, \psi''_n \\ \overline{\psi}_n &= \psi_n - a_0\, h^2 \left(\overline{\psi}''_{n+1} - 2\psi''_n + \psi''_{n-1}\right) \\ \overline{\overline{\psi}}_n &= \psi_n - a_1\, h^2 \left(\overline{\psi}''_{n+1} - 2\overline{\psi}''_n + \psi''_{n-1}\right) \\ \psi_{n+1} + c_1\, \psi_n + \psi_{n-1} &= h^2 \left[b_0 \left(\overline{\psi}''_{n+1} + \psi''_{n-1}\right) + b_1\, \overline{\overline{\psi}}''_n\right] \end{aligned} \tag{11}$$

The new method is Numerov-type and has five free parameters a_0, a_1, c_0, b_0 and b_1. Our aim is to find these coefficients based on the requirement that the phase-lag and its first four derivatives are annihilated.

The stability polynomial is obtained, when we apply the above family of methods to the scalar test equation (6) and $H = \omega h$

$$S(\zeta) = \zeta^2 + C_p(H)\, \zeta + 1 \tag{12}$$

where h is the step length and $C_p(H) = \frac{B_p(H)}{A_p(H)}$ with

$$\begin{aligned} A_p(H) &= 1 \\ B_p(H) &= c_1 + (2\, b_0 + b_1)\; H^2 - b_0\, H^4 - b_1\, a_0\, H^6 + 2\, b_1\, a_0\, a_1\, H^8 \end{aligned}$$

As the phase-lag $\Phi(H)$ and its first derivatives should be equal to zero, we obtain the following system of equations:

$$\Phi(H) = \Phi'(H) = \Phi''(H) = \Phi^{(3)}(H) = \Phi^{(4)}(H) = 0 \tag{13}$$

The phase-lag formula is acquired from (10) with $m = 1$.

$$\Phi(H) = \cos(H) + \frac{1}{2}\,c_1 + \left(b_0 + \frac{1}{2}\,b_1\right)\,H^2 - \frac{1}{2}\,b_0\,H^4 - \frac{1}{2}\,b_1\,a_1\,H^6 + b_1\,a_1\,a_0\,H^8 \tag{14}$$

The expressions of the derivatives from first to fourth order of the phase-lag are

$$\Phi'(H) = -\sin(H) + (2\,b_0 + b_1)\,H - 2\,b_0\,H^3 - 3\,b_1\,a_1\,H^5 + 8\,b_1\,a_1\,a_0\,H^7 \tag{15}$$

$$\Phi''(H) = -\cos(H) + b_1 + 2\,b_0 - 6\,b_0\,H^2 - 15\,b_1\,a_1\,H^4 + 56\,b_1\,a_1\,a_0\,H^6 \tag{16}$$

$$\Phi^{(3)}(H) = -\sin(H) - 12\,b_0\,H - 60\,b_1\,a_1\,H^3 + 336\,b_1\,a_1\,a_0\,H^5 \tag{17}$$

$$\Phi^{(4)}(H) = -\cos(H) - 12\,b_0 - 180\,b_1\,a_1\,H^2 + 1680\,b_1\,a_1\,a_0\,H^4 \tag{18}$$

Substituting the above formulae and solving system (13), we obtain the free parameters of the new Numerov-type method.

$$a_0 = \frac{1}{8}\,\frac{\sin(H)\,(15 - 6H^2) + \cos(H)\,(-15H + H^3)}{\sin(H)\,(21H^2 - 8H^4) + \cos(H)\,(-21H^3 + H^5)} \tag{19}$$

$$a_1 = \frac{\sin(H)\,(-21 + 8H^2) + \cos(H)\,(21H - H^3)}{\sin(H)\,(-105H^2 + 135H^4 - 12H^6) + \cos(H)\,(105H^3 - 60H^5 + H^7)} \tag{20}$$

$$c_1 = \cos(H)\left(-2 + \frac{29}{64}H^2 - \frac{1}{192}H^4\right) + \sin(H)\left(-\frac{93}{64}H + \frac{7}{96}H^3\right) \tag{21}$$

$$b_0 = \frac{\sin(H)\,(35 - 10H^2) + \cos(H)\,(-35H + H^3)}{32H^3} \tag{22}$$

$$b_1 = \frac{\sin(H)\,(-105 + 135H^2 - 12H^4) + \cos(H)\,(105H - 60H^3 + H^5)}{48\,H^3} \tag{23}$$

and their Taylor series expansions

$$\begin{aligned} a_0 = {} & \frac{1}{112} - \frac{1}{2016}\,H^2 + \frac{1}{34496}\,H^4 - \frac{11}{6604416}\,H^6 \\ & + \frac{113}{1173553920}\,H^8 - \frac{19013}{3423491495424}\,H^{10} \\ & + \frac{257611}{803513592161280}\,H^{12} - \frac{345841}{18692263565015040}\,H^{14} \\ & + \frac{4029945911}{3773855860195146485760}\,H^{16} + \cdots \end{aligned} \tag{24}$$

$$\begin{aligned} a_1 = {} & \frac{1}{112} - \frac{1}{2016}\,H^2 + \frac{1}{34496}\,H^4 - \frac{11}{6604416}\,H^6 \\ & + \frac{113}{1173553920}\,H^8 - \frac{19013}{3423491495424}\,H^{10} \end{aligned}$$

$$
\begin{aligned}
&+\frac{257611}{803513592161280} H^{12}-\frac{345841}{18692263565015040} H^{14} \\
&+\frac{4029945911}{3773855860195146485760} H^{16}+\cdots
\end{aligned}
\tag{25}
$$

$$
\begin{aligned}
c_1 = & -2+\frac{1}{1814400} H^{10}-\frac{1}{47900160} H^{12}+\frac{1}{2905943040} H^{14} \\
&-\frac{1}{298896998400} H^{16}+\frac{1}{45731240755200} H^{18}+\cdots
\end{aligned}
\tag{26}
$$

$$
\begin{aligned}
b_0 = & \frac{1}{12}-\frac{1}{181440} H^{6}+\frac{1}{5322240} H^{8}-\frac{1}{345945600} H^{10} \\
&+\frac{1}{37362124800} H^{12}-\frac{1}{5928123801600} H^{14} \\
&+\frac{1}{1287249739776000} H^{16}-\frac{1}{364935301226496000} H^{18}+\cdots
\end{aligned}
\tag{27}
$$

$$
\begin{aligned}
b_1 = & \frac{5}{6}+\frac{1}{90720} H^{6}-\frac{5}{1596672} H^{8}+\frac{1}{9434880} H^{10} \\
&-\frac{31}{18681062400} H^{12}+\frac{139}{8892185702400} H^{14} \\
&-\frac{193}{1930874609664000} H^{16}+\frac{1}{2146678242508800} H^{18}+\ldots
\end{aligned}
\tag{28}
$$

In order to find the local truncation error of the new method, we substitute the Taylor polynomials of ψ_{n+1}, ψ_{n-1}, ψ''_{n+1} and ψ''_{n-1}, as well as the Taylor polynomials of a_0, a_1, c_0, b_0 and b_1, into (11):

$$
\begin{aligned}
\mathrm{LTE} = & \frac{h^{10}}{1814400}\Big(\psi_n^{(10)}+5\omega^2\,\psi_n^{(8)}+10\omega^4\,\psi_n^{(6)} \\
&+10\omega^6\,\psi_n^{(4)}+5\omega^8\,\psi_n^{(2)}+10\omega^{10}\,\psi_n\Big)
\end{aligned}
\tag{29}
$$

Theorem 2 *The family of explicit two-step methods given by* (11) *with coefficients determined in* (19)–(23) *has algebraic order eight and phase-lag and its first four derivatives equal to zero (Fig. 1).*

4 Local truncation error—Stability

4.1 Error—Theory and analysis

In order to find the local truncation error we consider the general form

$$
\frac{d^2\psi(x)}{dx^2}=\varphi(x)\,\psi(x)
\tag{30}
$$

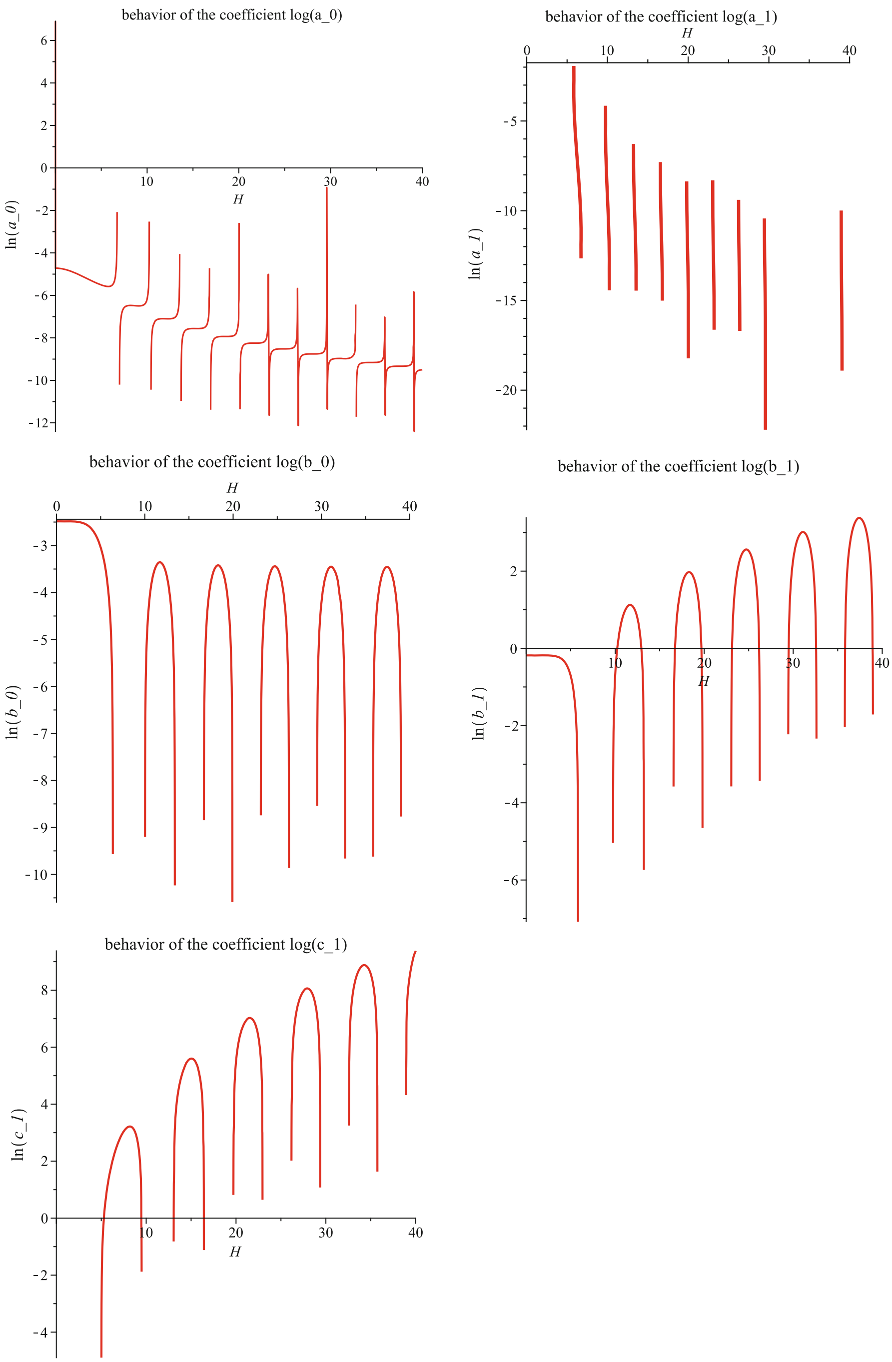

Fig. 1 Behavior of the coefficients of the new method given by (19)–(23) for several values of H

We will apply the newly obtained method (11) and another well known methods to the radial Schrödinger equation

$$\frac{d^2 y(x)}{dx^2} = \left[\frac{l^2}{x^2} + \frac{l}{x^2} + V(x) - k^2\right] y(x), \quad y(0) = 0 \tag{31}$$

and a second one boundary condition depending on physical considerations.

We substitute the function $\varphi(x)$ [47],

$$\varphi(x) = V(x) - V_c + G = g(x) + G \tag{32}$$

where $V(x)$ is the potential, V_c is the constant approximation of the potential and $G = v^2 = V_c - E$, with E denoting the energy.

Afterwards, we differentiate the function $\psi(x)$ and obtain the polynomials of G equal to $\psi_n^{(i)}$, $i = 2, 4, 6, \ldots$.

The expression of the local truncation error contains the following derivatives.

$$\begin{aligned}
\frac{d^2\psi_n}{dx^2} &= (V(x) - V_c + G)\,\psi(x) \\
\frac{d^4\psi_n}{dx^4} &= \left(\frac{d^2}{dx^2}\,V(x)\right)\psi(x) + 2\left(\frac{d}{dx}\,V(x)\right)\left(\frac{d}{dx}\,\psi(x)\right) \\
&\quad + (V(x) - V_c + G)\left(\frac{d^2}{dx^2}\,\psi(x)\right) \\
\frac{d^6\psi_n}{dx^6} &= \left(\frac{d^4}{dx^4}\,V(x)\right)\psi(x) + 4\left(\frac{d^3}{dx^3}\,V(x)\right)\left(\frac{d}{dx}\,\psi(x)\right) \\
&\quad + 3\left(\frac{d^2}{dx^2}\,V(x)\right)\left(\frac{d^2}{dx^2}\,\psi(x)\right) + 4\left(\frac{d}{dx}\,V(x)\right)^2 \psi(x) \\
&\quad + 6\,(V(x) - V_c + G)\left(\frac{d}{dx}\,\psi(x)\right)\left(\frac{d}{dx}\,V(x)\right) \\
&\quad + 4\,(U(x) - V_c + G)\,\psi(x)\left(\frac{d^2}{dx^2}\,V(x)\right) \\
&\quad + (V(x) - V_c + G)^2\left(\frac{d^2}{dx^2}\,\psi(x)\right)\ldots
\end{aligned}$$

We will compare the following methods:

- Numerov's Method (Φ_0)
- The Method developed by Konguetsof in [105] (Φ_1)
- The Method developed by Konguetsof in [106] (Φ_2)
- The Classical Method of the Family (Φ_3)
- The New Developed Method (Φ_4)

The expressions of the local truncation error are mentioned in Appendix.

Depending on the value of E, we distinguish two cases:

- **Case 1** When the energy E is found close to the potential, i.e. $V_c \approx E \Leftrightarrow G \approx 0$, we ignore the terms of the polynomial, which depend on the parameter G. In this case the accuracy of the methods does not differ very much. This is explained by the fact that the remaining terms are the same as those of the new family of methods.
- **Case 2** When $G \ll 0$ or $G \gg 0$, we obtain a large absolute value of G. So, we have the following asymptotic expansions of Eqs. (54–58).

Numerov's Method

$$\mathrm{LTE}_{\Phi_0} = h^6 \left(\frac{1}{240}\, \psi(x)\, G^3 + \cdots \right) \tag{33}$$

The Method developed by Konguets of [105]

$$\mathrm{LTE}_{\Phi_1} = h^6 \left(\frac{1}{90} \left(\frac{d^2}{dx^2}\, g(x) \right) \psi(x)\, G + \cdots \right) \tag{34}$$

The Method developed by Konguets of [106]

$$\begin{aligned} \mathrm{LTE}_{\Phi_2} = h^8 \Bigg[\Bigg(& \frac{1}{1680} \left(\frac{d^4}{dx^4}\, \mathrm{g}(x) \right) \psi(x) \\ & + \frac{1}{2520} \left(\frac{d^3}{dx^3}\, \mathrm{g}(x) \right) \left(\frac{d}{dx}\, \psi(x) \right) \\ & + \frac{1}{1260}\, \mathrm{g}(x)\, \psi(x) \left(\frac{d^2}{dx^2}\, \mathrm{g}(x) \right) \\ & + \frac{1}{1680} \left(\frac{d}{dx}\, \mathrm{g}(x) \right)^2 \psi(x) \Bigg) G + \cdots \Bigg] \end{aligned} \tag{35}$$

The Classical Method of the Family

$$\mathrm{LTE}_{\Phi_3} = h^{10} \left[\frac{1}{1814400}\, \psi(x)\, G^5 + \cdots \right] \tag{36}$$

The New Method

$$\mathrm{LTE}_{\Phi_4} = h^{10} \left[\left(\frac{1}{113400} \left(\frac{d^4}{dx^4}\, \mathrm{g}(x) \right) \psi(x) \right) G^2 + \cdots \right] \tag{37}$$

Comparing the expressions (33–37) we come to the following conclusion.

Theorem 3 – *Numerov's Method has algebraic order four and the error increases as the third power of G.*
- *The method developed by Konguetsof in* [105] *has algebraic order four and the error increases as the first power of G.*

- *The method developed by Konguetsof in* [106] *has algebraic order six and the error increases as the first power of G.*
- *The new method developed in this paper has algebraic order eight and the error increases as the second power of G.*

Thus, the newly obtained family of methods is the most accurate one for the numerical solution of the time independent radial Schrödinger equation, especially for large values of $\mid G \mid \gg 0$.

4.2 Stability—theory and Analysis

Application of the family of methods (11) to the scalar test equation

$$\psi'' = -\tau^2\, \psi(x), \quad \tau \neq \omega \tag{38}$$

leads to the difference equation

$$\psi_{n+1} + C_p(H, s)\, \psi_n + \psi_{n-1} = 0 \tag{39}$$

where $s = \tau h$, h the step length and

$$C_p(H) = c_1 + (2\, b_0 + b_1)\; s^2 - b_0\, s^4 - b_1\, a_0\, s^6 + 2\, b_1\, a_0\, a_1\, s^8 \tag{40}$$

The characteristic equation arising from (39) is

$$s^2 + C_p(H, s) s + 1 = 0 \tag{41}$$

Definition 1 *(see* [34]) A symmetric $2m$-step method with the characteristic equation given by (41) is considered to have an *interval of periodicity* $(0, \omega_0^2)$ if, for all $\omega \in (0, \omega_0^2)$, the roots $z_i,\ i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i\, \phi(\tau h)}, \quad |z_i| \le 1, \quad i = 3, 4 \ldots, 2m \tag{42}$$

where $\phi(\tau h)$ is a real function.

Definition 2 (see [34]) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Theorem 4 (see [97]) *A symmetric two-step method with the characteristic equation given by* (41) *is considered to have a nonzero interval of periodicity* $(0, s_0^2)$ *if, for all* $s \in (0, s_0^2)$ *the following relations hold*

$$Q_1(H, s)\, Q_2(H, s) < 0, \;\; H = \omega h, \quad s = \tau\, h \tag{43}$$

$$Q_1(H, s)\, Q_2(H, s) = C_p^2(H, s) - 4, \tag{44}$$

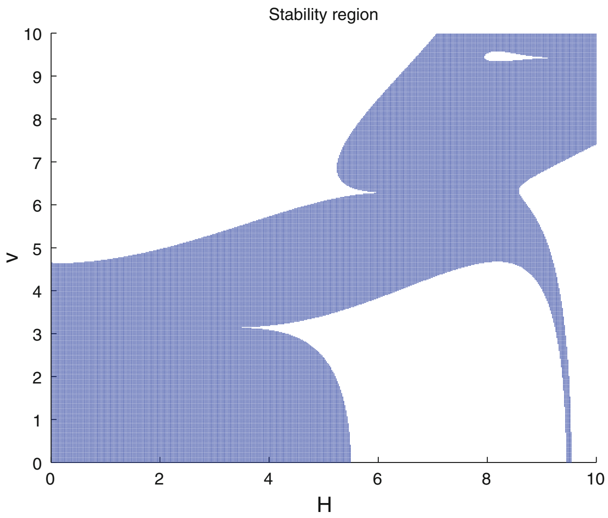

Fig. 2 $v - H$ plane of the new method of the family of method developed in this paper

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S$[1] only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $H = s$.

The obtained stability polynomials for the newly developed methods are given as follows:

$$
\begin{aligned}
Q_1(H, s) &= 2 + c_1 + (2\,b_0 + b_1)\; s^2 - b_0\, s^4 - b_1\, a_0\, s^6 + 2\, b_1\, a_0\, a_1\, s^8, \\
Q_2(H, s) &= -2 + c_1 + (2\,b_0 + b_1)\; s^2 - b_0\, s^4 - b_1\, a_0\, s^6 + 2\, b_1\, a_0\, a_1\, s^8
\end{aligned} \tag{45}
$$

In Fig. 2, the $\tau - H$ plane is shown for the the new family of methods constructed in this paper (Sect. 3).

A method is found to be P-stable, when the whole surface of the $\tau - H$ plane is covered. We note that the new method, which is explicit, does not have the property of P-stability, but from the diagram (Fig. 2) we observe that it is almost P-stable.

Remark 1 We use the results of the observation of the surroundings of the first diagonal of the $\tau - H$ plane, since it is known that, for the numerical solution of the Schrödinger equation, the frequencies of the exponential fitting and of the scalar test equation are equal.

[1] where S is a set of distinct points.

5 Application of the new method—comparison with other methods

In this section we will present the results of the application of some numerical methods to the radial Schrödinger equation. More specifically we will use Eq. (31). We present here some terminology:

– *Effective potential* is called the function $M(x) = l^2/x^2 + l/x^2 + V(x)$, with $\lim_{x\to\infty} M(x) = 0$.
– We call *energy* the real number k^2.
– *Angular momentum* is expressed by the integer l.
– *The potential* is the known function V.

The method developed in this paper belongs to the category of methods with frequency dependent coefficients. For this category of methods we should know the parameter ω in order to be able to apply the above methods. It is obvious from (31) that this parameter can be defined by the following equation

$$\omega = \sqrt{|g(x)|} = \sqrt{|V(x) - E|} \tag{46}$$

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

5.1 Woods–Saxon potential

For the numerical solution of (31) we need the potential function $V(x)$. For the purposes of this paper we use, as potential $V(x)$, the well known Woods-Saxon potential (see [169]) given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a\,(1+z)^2} \tag{47}$$

with $z = \exp[(x - X_0)/a]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

In Fig. 3, we present the behavior of the Woods-Saxon potential.

In some cases, the definition of the parameter ω is given based on some critical points, which are defined from the study of the function of the potential and is independent from the variant x) (see [35]).

For this paper we choose ω as follows (see [35] for details):

$$\omega = \begin{cases} \sqrt{-50+E}, & \text{for } 0 \le x \le 6.5 - 2h \\ \sqrt{-37.5+E}, & \text{for } x = 6.5 - h \\ \sqrt{-25+E}, & \text{for } x = 6.5 \\ \sqrt{-12.5+E}, & \text{for } x = 6.5 + h \\ \sqrt{E}, & \text{for } 6.5 + 2h \le x \le 15 \end{cases} \tag{48}$$

5.2 Resonance problem of the one-dimensional Schrödinger equation

In this section we will approximate the solution of the radial Schrödinger equation (31) using as potential the Woods–Saxon potential (47) presented above.

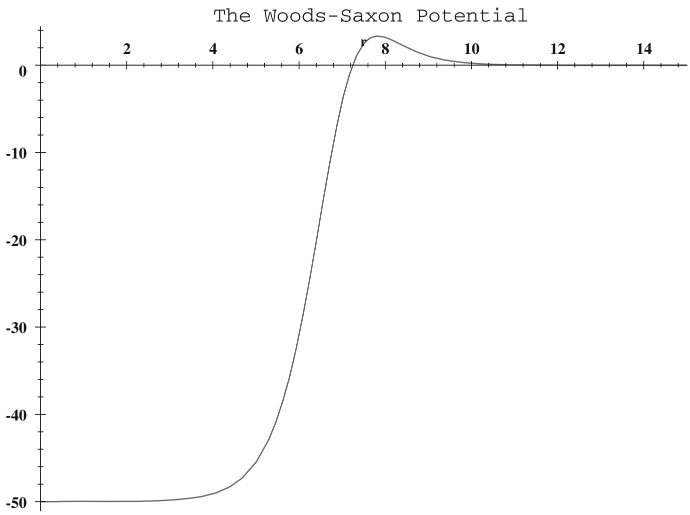

Fig. 3 The Woods–Saxon potential

The numerical solution is based on the approximation of the infinite true interval of integration by a finite one. For the specific example this finite interval is equal to [0, 15]. We will investigate a wide range of energies $E \in [1, 1000]$.

Since the potential vanishes faster than the quantity $l(l+1)/x^2$ for positive energies $E = k^2$, the radial Schrödinger equation can be simplified to the following form

$$y''(x) + y(x)\left(k^2 - \frac{l(l+1)}{x^2}\right) = 0, \quad x > X \tag{49}$$

The linearly independent solutions of Eq. (49) are $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions respectively.

Based on the above it is easy to see that the asymptotic form of Eq. (31) in the case of $x \to \infty$ can be written as

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan(\delta_l \cos\left(kx - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{50}$$

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

$$\tan(\delta_l) = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{51}$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$.

The problem we have to solve now is an initial value one. Since our method is a two-step method, we need the approximation of y_1 using a one-step method. The value of y_0 is determined using the initial condition. Based on formula (51) and using the above defined values y_0 and y_1 we can compute the phase shift δ_l at the point x_1 of the asymptotic region.

We will solve the resonance problem. This can be defined by determining the phase-shift δ_l or by finding those E, for $1 \leq E \leq 1000$, at which $\delta_l = \frac{\pi}{2}$. In the this case we will solve the second of the above problems, which is called *the resonance problem*, when the positive eigenenergies lie under the potential barrier.

For this problem, the boundary conditions are given by the following formulae

$$y(0) = 0,\ y(x) = \cos\left(\sqrt{E}x\right) \quad \text{for large } x. \tag{52}$$

The approximate positive eigenenergies of the Woods-Saxon resonance problem are calculated with the following numerical methods.

– Numerov's method (**Method I**)
– The two-step method developed by Raptis and Allison [46] (**Method II**)
– The two-step method developed by Ixaru and Rizea [35] (**Method III**)
– The Method developed by Konguetsof in [105] (**Method IV**)
– The two-step method developed by Raptis [49] (**Method V**)
– The two-step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero, which was developed by Konguetsof in [106] (**Method VI**)
– The new two-step Numerov-Type Method with phase-lag and its first, second, third and fourth derivatives equal to zero obtained in Sect. 3 (**Method VII**)

for several step sizes $h = 0.3 \times 2^{-n}$.

We compare the obtained approximations of the eigenenergies $\tilde{E}$ with the real values E. In Figs. 4, 5 and 6, the maximum absolute error $log_{10}(ER)$, is shown, where ER is given by

$$ER = |\tilde{E} - E| \tag{53}$$

of the eigenenergies E_1, E_2, E_3 for several values of n.

6 Final remarks and conclusions

In the present paper, a hybrid two-step method of eighth algebraic order is developed with phase-lag and its first, second, third and fourth derivatives equal to zero. The new method is applied to the resonance problem of the radial Schrödinger equation.

The following conclusions are extracted based on the results presented above:

– The two-step method developed by Raptis and Allison [46] (Method II) is more efficient than Numerov's Method (Method I) but less efficient than the other two methods.

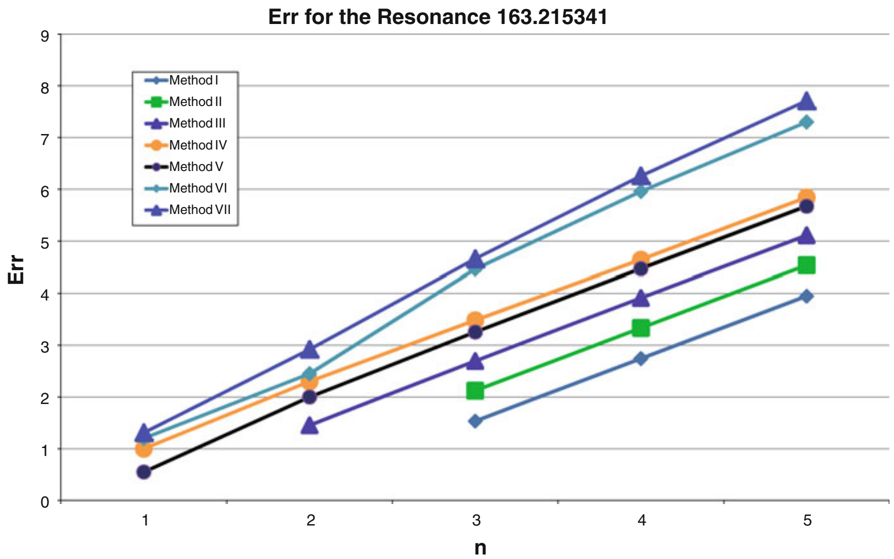

Fig. 4 Error Errmax for several values of n for the eigenvalue $E_1 = 163.215341$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

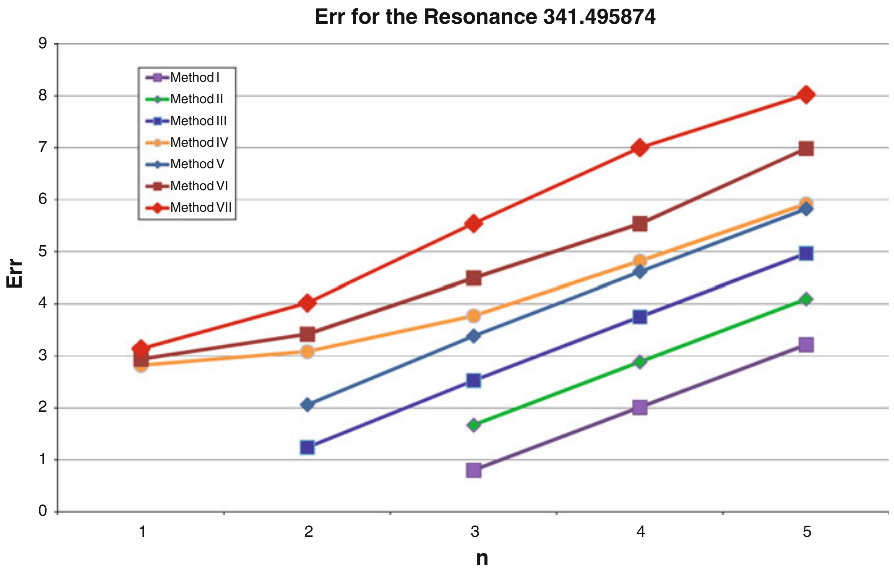

Fig. 5 Error Errmax for several values of n for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

– The two-step method developed by Ixaru and Rizea [35] (Method III) is more efficient than Numerov's Method (Method I) and the method developed by Raptis and Allison (Method II) but less efficient than the new obtained method.

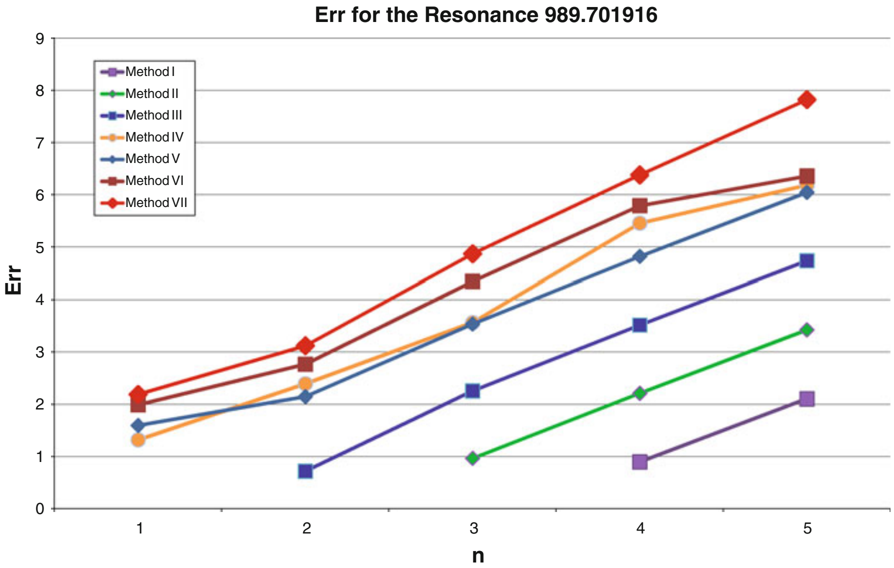

Fig. 6 Error Errmax for several values of n for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

- The method developed by Konguetsof in [105] (Method IV) is more efficient than Numerov's Method (Method I) and the method developed by Raptis and Allison (Method II), but less efficient than the newly obtained method and generally less efficient than the two-step method developed by Raptis [49] (Method V)
- The two-step Numerov-Type method developed by Konguetsof in [106] (Method VI) with phase-lag and its first, second and third derivatives equal to zero (Method VI) is the most efficient of all the previous methods.
- Finally the newly developed two-step Numerov-Type method with its first, second, third and fourth derivatives equal to zero (Method VII) is the most efficient of all the other methods.

From the above we conclude that the vanishing of the phase-lag and its derivatives produces very efficient methods. So, we must prefer to use the free parameters of a method in order to vanish the phase-lag and/or its derivatives in order to produce computationally very accurate methods.

Acknowledgments The author wishes to thank the anonymous referee and the Editor-in-Chief of the Journal for their careful reading of the manuscript and their fruitful comments and suggestions. All computations were carried out on an IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

Appendix

The Numerov's method

$$
\begin{aligned}
LTE_{\Phi_0} = h^6 \Bigg[& \frac{1}{240}\,\psi(x)\,G^3 + \frac{1}{80}\,g(x)\,\psi(x)\,G^2 \\
& + \left(\frac{1}{40}\left(\frac{d}{dx}\,g(x)\right)\left(\frac{d}{dx}\,\psi(x)\right) + \frac{7}{240}\left(\frac{d^2}{dx^2}\,g(x)\right)\psi(x) \right. \\
& \left. + \frac{1}{80}\,g(x)^2\,\psi(x) \right) G \\
& + \frac{1}{240}\left(\frac{d^4}{dx^4}\,g(x)\right)\psi(x) + \frac{1}{60}\left(\frac{d^3}{dx^3}\,g(x)\right)\left(\frac{d}{dx}\,\psi(x)\right) \\
& + \frac{7}{240}\,g(x)\,\psi(x)\left(\frac{d^2}{dx^2}\,g(x)\right) + \frac{1}{240}\,g(x)^3\,\psi(x) \\
& + \frac{1}{60}\left(\frac{d}{dx}\,g(x)\right)^2\psi(x) + \frac{1}{40}\,g(x)\left(\frac{d}{dx}\,\psi(x)\right)\left(\frac{d}{dx}\,g(x)\right) \Bigg]
\end{aligned} \tag{54}
$$

The method developed by Konguetsof in [105]

$$
\begin{aligned}
LTE_{\Phi_1} = h^6 \Bigg[& \frac{1}{90}\left(\frac{d^2}{dx^2}\,g(x)\right)\psi(x)\,G + \frac{7}{360}\,g(x)\,\psi(x)\left(\frac{d^2}{dx^2}\,g(x)\right) \\
& + \frac{1}{360}\,g(x)^3\,\psi(x) + \frac{1}{360}\left(\frac{d^4}{dx^4}\,g(x)\right)\psi(x) \\
& + \frac{1}{90}\left(\frac{d^3}{dx^3}\,g(x)\right)\left(\frac{d}{dx}\,\psi(x)\right) \\
& + \frac{1}{90}\left(\frac{d}{dx}\,g(x)\right)^2\psi(x) + \frac{1}{60}\,g(x)\left(\frac{d}{dx}\,\psi(x)\right)\left(\frac{d}{dx}\,g(x)\right) \Bigg]
\end{aligned} \tag{55}
$$

The method developed by Konguetsof in [106]

$$
\begin{aligned}
LTE_{\Phi_2} = h^8 \Bigg[& \left(\frac{1}{1680}\left(\frac{d^4}{dx^4}\,g(x)\right)\psi(x) + \frac{1}{2520}\left(\frac{d^3}{dx^3}\,g(x)\right)\left(\frac{d}{dx}\,\psi(x)\right) \right. \\
& \left. + \frac{1}{1260}\,g(x)\,\psi(x)\left(\frac{d^2}{dx^2}\,g(x)\right) + \frac{1}{1680}\left(\frac{d}{dx}\,g(x)\right)^2\psi(x) \right) G
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{1}{20160}\left(\frac{d^6}{dx^6}\,g(x)\right)\psi(x)+\frac{1}{3360}\left(\frac{d^5}{dx^5}\,g(x)\right)\left(\frac{d}{dx}\,\psi(x)\right)\\
&+\frac{1}{1260}\,g(x)\,\psi(x)\left(\frac{d^4}{dx^4}\,g(x)\right)+\frac{1}{1344}\left(\frac{d^2}{dx^2}\,g(x)\right)^2\psi(x)\\
&+\frac{13}{10080}\left(\frac{d}{dx}\,g(x)\right)\psi(x)\left(\frac{d^3}{dx^3}\,g(x)\right)+\frac{1}{840}\,g(x)\left(\frac{d}{dx}\,\psi(x)\right)\\
&\times\left(\frac{d^3}{dx^3}\,g(x)\right)+\frac{1}{1680}\,g(x)^2\left(\frac{d}{dx}\,\psi(x)\right)\left(\frac{d}{dx}\,g(x)\right)\\
&+\frac{1}{420}\left(\frac{d}{dx}\,g(x)\right)\left(\frac{d}{dx}\psi(x)\right)\\
&\times\left(\frac{d^2}{dx^2}\,g(x)\right)+\frac{11}{10080}\,g(x)^2\,\psi(x)\left(\frac{d^2}{dx^2}\,g(x)\right)\\
&+\frac{1}{720}\,g(x)\,\psi(x)\left(\frac{d}{dx}\,g(x)\right)^2+\frac{1}{20160}\,g(x)^4\,\psi(x)\Bigg]
\end{aligned}
\tag{56}
$$

The classical method (method with constant coefficients)

$$
\begin{aligned}
LTE_{\Phi_3}=h^{10}\Bigg[&\left(\frac{1}{1814400}\,\psi(x)\right)G^5+\left(\frac{1}{362880}\,g(x)\psi(x)\right)G^4\\
&+\left(\frac{1}{36288}\left(\frac{d^2}{dx^2}g(x)\right)\psi(x)+\frac{1}{90720}\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}\psi(x)\right.\\
&\left.+\frac{1}{181440}\,(g(x))^2\,\psi(x)\right)G^3\\
&+\left(\frac{43}{907200}\left(\frac{d^4}{dx^4}g(x)\right)\psi(x)+\frac{1}{12096}\,g(x)\psi(x)\frac{d^2}{dx^2}g(x)\right.\\
&+\frac{1}{30240}\,g(x)\left(\frac{d}{dx}\psi(x)\right)\frac{d}{dx}g(x)+\frac{1}{18144}\left(\frac{d}{dx}g(x)\right)^2\psi(x)\\
&\left.+\frac{1}{22680}\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}\psi(x)+\frac{1}{181440}\,(g(x))^3\,\psi(x)\right)G^2\\
&+\left(\frac{1}{5670}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}\psi(x)\right)\frac{d^2}{dx^2}g(x)+\frac{29}{1814400}\left(\frac{d^6}{dx^6}g(x)\right)\psi\,(x)\right.\\
&+\frac{43}{453600}\,g(x)\psi(x)\frac{d^4}{dx^4}g(x)+\frac{1}{12096}\,(g(x))^2\,\psi(x)\frac{d^2}{dx^2}g(x)\\
&+\frac{211}{1814400}\left(\frac{d^2}{dx^2}g(x)\right)^2\psi(x)+\frac{1}{30240}\,(g(x))^2\left(\frac{d}{dx}\psi(x)\right)\frac{d}{dx}g(x)
\end{aligned}
$$

$$+\frac{1}{9072}\,g(x)\psi(x)\left(\frac{d}{dx}g(x)\right)^2+\frac{169}{907200}\left(\frac{d}{dx}g(x)\right)\psi(x)\frac{d^3}{dx^3}g(x)$$
$$+\frac{31}{907200}\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}\psi(x)+\frac{1}{11340}\,g(x)\left(\frac{d}{dx}\psi(x)\right)\frac{d^3}{dx^3}g(x)$$
$$+\frac{1}{362880}\,(g(x))^4\,\psi(x)\Bigg)\,G+\frac{43}{907200}\,(g(x))^2\,\psi(x)\frac{d^4}{dx^4}g(x)$$
$$+\frac{1}{5670}\,g(x)\left(\frac{d}{dx}\psi(x)\right)\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}g(x)$$
$$+\frac{31}{907200}\,g(x)\left(\frac{d}{dx}\psi(x)\right)\frac{d^5}{dx^5}g(x)+\frac{1}{36288}\,(g(x))^3\,\psi(x)\frac{d^2}{dx^2}g(x)$$
$$+\frac{211}{1814400}\,g(x)\psi(x)\left(\frac{d^2}{dx^2}g(x)\right)^2+\frac{29}{226800}\left(\frac{d}{dx}g(x)\right)^2\psi(x)\frac{d^2}{dx^2}g(x)$$
$$+\frac{1}{22680}\left(\frac{d}{dx}g(x)\right)^3\frac{d}{dx}\psi(x)+\frac{1}{18144}\,(g(x))^2\,\psi(x)\left(\frac{d}{dx}g(x)\right)^2$$
$$+\frac{29}{1814400}\,g(x)\psi(x)\frac{d^6}{dx^6}g(x)+\frac{1}{32400}\left(\frac{d^3}{dx^3}g(x)\right)^2\psi(x)$$
$$+\frac{1}{90720}\,(g(x))^3\left(\frac{d}{dx}\psi(x)\right)\frac{d}{dx}g(x)+\frac{1}{1814400}\left(\frac{d^8}{dx^8}g(x)\right)\psi(x)$$
$$+\frac{1}{226800}\left(\frac{d^7}{dx^7}g(x)\right)\frac{d}{dx}\psi(x)+\frac{1}{6480}\left(\frac{d^2}{dx^2}g(x)\right)\left(\frac{d}{dx}\psi(x)\right)$$
$$\times\frac{d^3}{dx^3}g(x)+\frac{1}{10080}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}\psi(x)\right)\frac{d^4}{dx^4}g(x)$$
$$+\frac{169}{907200}\,g(x)\psi(x)\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}g(x)$$
$$+\frac{1}{28350}\left(\frac{d}{dx}g(x)\right)\psi(x)\frac{d^5}{dx^5}g(x)$$
$$+\frac{1}{22680}\,(g(x))^2\left(\frac{d}{dx}\psi(x)\right)\frac{d^3}{dx^3}g(x)$$
$$+\frac{7}{129600}\left(\frac{d^2}{dx^2}g(x)\right)\psi(x)\frac{d^4}{dx^4}g(x)+\frac{1}{1814400}\,(g(x))^5\,\psi(x)\Bigg] \quad (57)$$

The new method

$$LTE_{\Phi_4}=h^{10}\Bigg[\left(\frac{1}{113400}\left(\frac{d^4}{dx^4}g(x)\right)\psi(x)\right)G^2+\Bigg(\frac{1}{30240}\,g(x)\,\psi(x)\left(\frac{d}{dx}g(x)\right)^2$$
$$+\frac{1}{75600}\left(\frac{d^6}{dx^6}g(x)\right)\psi(x)+\frac{1}{56700}\left(\frac{d^5}{dx^5}g(x)\right)\left(\frac{d}{dx}\psi(x)\right)$$

$$+\frac{23}{453600}\,g(x)\,\psi(x)\,\left(\frac{d^4}{dx^4}g(x)\right)+\frac{17}{226800}\,\left(\frac{d^2}{dx^2}g(x)\right)^2\,\psi(x)$$
$$+\frac{13}{113400}\,\psi(x)\,\left(\frac{d}{dx}g(x)\right)\left(\frac{d^3}{dx^3}g(x)\right)$$
$$+\frac{1}{45360}\,g(x)\,\left(\frac{d}{dx}\psi(x)\right)\left(\frac{d^3}{dx^3}g(x)\right)$$
$$+\frac{1}{22680}\,\left(\frac{d}{dx}\psi(x)\right)\left(\frac{d}{dx}g(x)\right)\left(\frac{d^2}{dx^2}g(x)\right)$$
$$+\frac{1}{45360}\,g(x)^2\,\psi(x)\,\left(\frac{d^2}{dx^2}\,g(x)\right)\Bigg)\,G$$
$$+\frac{1}{22680}\,(g(x))^2\left(\frac{d}{dx}\psi(x)\right)\frac{d^3}{dx^3}g(x)+\frac{1}{1814400}\,(g(x))^5\,\psi(x)$$
$$+\frac{211}{1814400}\,g(x)\psi(x)\left(\frac{d^2}{dx^2}g(x)\right)^2+\frac{1}{18144}\,(g(x))^2\,\psi(x)\left(\frac{d}{dx}g(x)\right)^2$$
$$+\frac{31}{907200}\,g(x)\left(\frac{d}{dx}\psi(x)\right)\frac{d^5}{dx^5}g(x)$$
$$+\frac{169}{907200}\,g(x)\psi(x)\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}g(x)$$
$$+\frac{1}{6480}\,\left(\frac{d^2}{dx^2}g(x)\right)\left(\frac{d}{dx}\psi(x)\right)\frac{d^3}{dx^3}g(x)$$
$$+\frac{1}{36288}\,(g(x))^3\,\psi(x)\frac{d^2}{dx^2}g(x)$$
$$+\frac{1}{226800}\,\left(\frac{d^7}{dx^7}g(x)\right)\frac{d}{dx}\psi(x)+\frac{43}{907200}\,(g(x))^2\,\psi(x)\frac{d^4}{dx^4}g(x)$$
$$+\frac{1}{28350}\,\left(\frac{d}{dx}g(x)\right)\psi(x)\frac{d^5}{dx^5}g(x)+\frac{1}{90720}\,(g(x))^3\left(\frac{d}{dx}\psi(x)\right)\frac{d}{dx}g(x)$$
$$+\frac{29}{226800}\,\left(\frac{d}{dx}g(x)\right)^2\psi(x)\frac{d^2}{dx^2}g(x)+\frac{1}{5670}\,g(x)\left(\frac{d}{dx}\psi(x)\right)$$
$$\times\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}g(x)+\frac{1}{32400}\,\left(\frac{d^3}{dx^3}g\,(x)\right)^2\psi(x)+\frac{1}{10080}$$
$$\times\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}\psi(x)\right)\frac{d^4}{dx^4}g(x)+\frac{7}{129600}\,\left(\frac{d^2}{dx^2}g(x)\right)\psi(x)\frac{d^4}{dx^4}g(x)$$
$$+\frac{29}{1814400}\,g(x)\psi(x)\frac{d^6}{dx^6}g(x)$$
$$+\frac{1}{22680}\,\left(\frac{d}{dx}g(x)\right)^3\frac{d}{dx}\psi(x)+\frac{1}{1814400}\,\left(\frac{d^8}{dx^8}g(x)\right)\psi(x)\Bigg] \tag{58}$$

References

1. S.D. Capper, D.R. Moore, On high order MIRK schemes and Hermite-Birkhoff interpolants. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 27–47 (2006)
2. J.R. Cash, S. Girdlestone, Variable step Runge–Kutta–Nyström methods for the numerical solution of reversible systems. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 59–80 (2006)
3. M. Calvo, J.I. Montijano, M.P. Laburta, L. Rández, On the long time error of first integrals for some RK numerical integrators. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 77–86 (2009)
4. T.E. Simos, A fourth algebraic order exponentially-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation. IMA J. Numer. Anal. **21**(4), 919–931 (2001)
5. T.E. Simos, Exponentially-fitted Runge–Kutta–Nyström method for the numerical solution of initial-value problems with oscillating solutions. Appl. Math. Lett. **15**(2), 217–225 (2002)
6. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge–Kutta–Nyström methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. J. Math. Chem. **31**(2), 211–232 (2002)
7. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge–Kutta methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 281–293 (2005)
8. Z. Kalogiratou, T. Monovasilis, T.E. Simos, New modified Runge–Kutta–Nyström methods for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **60**(6), 1639–1647 (2010)
9. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Computation of the eigenvalues of the Schrödinger equation by exponentially-fitted Runge–Kutta–Nyström methods. Comput. Phys. Commun. **180**(2), 167–176 (2009)
10. T. Monovasilis, Z. Kalogiratou, T.E. Simos, A family of trigonometrically fitted partitioned Runge–Kutta symplectic methods. Appl. Math. Comput. **209**(1), 91–96 (2009)
11. Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge–Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation. J. Math. Chem. **41**(1), 79–100 (2007)
12. T.E. Simos, E. Dimas, A.B. Sideridis, A Runge–Kutta–Nyström method for the numerical-integration of special 2nd-order periodic initial-value problems. J. Comput. Appl. Math. **51**(3), 317–326 (1994)
13. K. Tselios, T.E. Simos, Runge–Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. J. Comput. Appl. Math. **175**(1), 173–181 (2005)
14. Z.A. Anastassi, T.E. Simos, An optimized Runge–Kutta method for the solution of orbital problems. J. Comput. Appl. Math. **175**(1), 1–9 (2005)
15. A.B. Sideridis, T.E. Simos, A low-order embedded Runge–Kutta Method for periodic initial-value problems. J. Comput. Appl. Math. **44**(2), 235–244 (1992)
16. T.E. Simos, A Runge–Kutta Fehlberg method with phase-lag of order infinity for initial value problems with oscillating solution. Comput. Math. Appl. **25**, 95–101 (1993)
17. T.E. Simos, Runge–Kutta interpolants with minimal phase-lag. Comput. Math. Appl. **26**, 43–49 (1993)
18. T.E. Simos, Runge–Kutta–Nyström interpolants for the numerical integration of special second-order periodic initial-value problems. Comput. Math. Appl. **26**, 7–15 (1993)
19. T.E. Simos, A high-order predictor-corrector method for periodic IVPs. Appl. Math. Lett. **6**(5), 9–12 (1993)
20. T.E. Simos, An explicit high-order predictor-corrector method for periodic initial-value problems. Math. Models Methods Appl. Sci. **5**(2), 159–166 (1995)
21. G. Avdelas, T.E. Simos, Block Runge–Kutta methods for periodic initial-value problems. Comput. Math. Appl. **31**, 69–83 (1996)
22. G. Avdelas, T.E. Simos, Embedded methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **31**, 85–102 (1996)
23. T.E. Simos, A modified Runge–Kutta method for the numerical solution of ODE's with oscillation solutions. Appl. Math. Lett. **9**(6), 61–66 (1996)
24. T.E. Simos, Some embedded modified Runge–Kutta methods for the numerical solution of some specific Schrödinger equations. J. Math. Chem. **24**(1–3), 23–37 (1998)
25. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation. J. Math. Chem. **30**(1), 121–131 (2001)
26. T.E. Simos, P.S. Williams, A new Runge–Kutta–Nyström method with phase-Lag of order infinity for the numerical solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **45**, 123–137 (2002)

27. Ch. Tsitouras, T.E. Simos, Optimized Runge–Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
28. K. Tselios, T.E. Simos, Optimized Runge–Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. Phys. Lett. A **363**(1–2), 38–47 (2007)
29. A.A. Kosti, Z.A. Anastassi, T.E. Simos, An optimized explicit Runge–Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems. J. Math. Chem. **47**(1), 315–330 (2010)
30. D.F. Papadopoulos, Z.A. Anastassi, T.E. Simos, A modified phase-fitted and amplification-fitted Runge–Kutta–Nyström method for the numerical solution of the radial Schrödinger equation. J. Mol. Model. **16**(8), 1339–1346 (2010)
31. T.V. Triantafyllidis, Z.A. Anastassi, T.E. Simos, Two optimized Runge–Kutta methods for the solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**(3), 753–771 (2008)
32. D.F. Papadopoulos, Z.A. Anastassi, T.E. Simos, An optimized Runge–Kutta–Nyström method for the numerical solution of the Schrödinger equation and related problems. MATCH Commun. Math. Comput. Chem. **64**(2), 551–566 (2010)
33. D.F. Papadopoulos, Z.A. Anastassi, T.E. Simos, A phase-fitted Runge–Kutta–Nyström method for the numerical solution of initial value problems with oscillating solutions. Comput. Phys. Commun. **180**(10), 1839–1846 (2009)
34. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
35. L.Gr. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum ofenergies. Comput. Phys. Commun. **19**, 23–27 (1980)
36. M.M. Chawla, Uncoditionally stable Noumerov-type methods for second order differential equations. BIT **23**, 541–542 (1983)
37. F. Mazzia, A. Sestini, D. Trigiante, BS linear multistep methods on non-uniform meshes. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 131–144 (2006)
38. G. Psihoyios, A block implicit advanced step-point (BIAS) algorithm for stiff differential systems. Comput. Lett. **2**(1–2), 51–58 (2006)
39. L. Aceto, R. Pandolfi, D. Trigiante, Stability analysis of linear multistep methods via polynomial type variation. JNAIAM J. Numer. Anal. Ind. Appl. Math. **2**(1–2), 1–9 (2007)
40. A.T. Hill, Linear multistep approximation of nonsymmetric rotating systems. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 103–112 (2009)
41. I. Alolyan, T.E. Simos, High algebraic order methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation. J. Math. Chem. **48**(4), 925–958 (2010)
42. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions. J. Math. Chem. **46**(2), 604–620 (2009)
43. I. Alolyan, T.E. Simos, Multistep methods with vanished phase-lag and its first and second derivatives for the numerical integration of the Schrödinger equation. J. Math. Chem. **48**(4), 1092–1143 (2010)
44. G.A. Panopoulos, Z.A. Anastassi, 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)
45. I. Alolyan, T.E. Simos, A family of eight-step methods with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation. J. Math. Chem. (to appear).
46. A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
47. L.Gr. Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **38**(3), 329–337 (1985)
48. A.D. Raptis, On the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **24**, 1–4 (1981)
49. A.D. Raptis, Two-step methods for the numerical solution of the Schrödinger equation. Computing **28**, 373–378 (1982)
50. A.D. Raptis, Exponentially-fitted solutions of the eigenvalue Shrödinger equation with automatic error control. Comput. Phys. Commun. **28**, 427–431 (1983)
51. T.E. Simos, A 4-step method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **30**(3), 251–255 (1990)
52. T.E. Simos, Some new 4-step exponential-fitting methods for the numerical solution of the radial Schrödinger equation. IMA J. Numer. Anal. **11**(3), 347–356 (1991)

53. T.E. Simos, G.V. Mitsou, A family of four-step exponential fitted methods for the numerical integration of the radial Schrödinger equation. Comput. Math. Appl. **28**, 41–50 (1994)
54. T.E. Simos, A family of P-stable exponentially-fitted methods forthe numerical solution of the Schrödinger equation. J. Math. Chem. **25**(1), 65–84 (1999)
55. T.E. Simos, An exponentially fitted eighth-order method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **108**(1–2), 177–194 (1999)
56. Z. Kalogiratou, T.E. Simos, A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation. Appl. Math. Comput. **112**, 99–112 (2000)
57. A. Konguetsof, T.E. Simos, On the Construction of exponentially-fitted methods for the numerical solution of the Schrödinger equation. J. Comput. Methods Sci. Eng. **1**, 143–165 (2001)
58. J. Vigo-Aguiar, T.E. Simos, A family of P-stable eighth algebraic order methods with exponential fitting facilities. J. Math. Chem. **29**(3), 177–189 (2001)
59. J. Vigo-Aguiar, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **32**(3), 257–270 (2002)
60. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **31**(4), 371–404 (2002)
61. T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems. J. Math. Chem. **34**(1–2), 39–58 (2003)
62. A. Konguetsof, T.E. Simos, An exponentially-fitted and trigonometrically-fitted method for the numerical solution of periodic initial-value problems. Comput. Math. Appl. **45**, 547–554 (2003)
63. T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution. Appl. Math. Lett. **17**(5), 601–607 (2004)
64. T.E. Simos, Exponentially—fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
65. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **37**(3), 263–270 (2005)
66. T.E. Simos, P-stable four-step exponentially-fitted method for the numerical integration of the Schrödinger equation. Comput. Lett. **1**(1), 37–45 (2005)
67. D.P. Sakas, T.E. Simos, Trigonometrically-fitted multiderivative methods for the numerical solution of the radial Schrödinger equation. MATCH Commun. Math. Comput. Chem. **53**(2), 299–320 (2005)
68. Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**, 162–174 (2005)
69. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **40**(3), 257–267 (2006)
70. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. J. Math. Chem. **40**(3), 305–318 (2006)
71. G. Vanden Berghe, M. Van Daele, Exponentially-fitted Stormer/Verlet methods. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(3), 241–255 (2006)
72. T.E. Simos, Stabilization of a four-step exponentially-fitted method and its application to the Schrödinger equation. Int. J. Modern Phys. C **18**(3), 315–328 (2007)
73. T. Monovasilis, T.E. Simos, New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation. J. Math. Chem. **42**(3), 535–545 (2007)
74. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation. J. Math. Chem. **44**(2), 483–499 (2008)
75. T.E. Simos, A family of four-step trigonometrically-fitted methods and its application to the Schrödinger equation. J. Math. Chem. **44**(2), 447–466 (2009)
76. T.E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation. Acta Appl. Math. **110**(3), 1331–1352 (2010)
77. T.E. Simos, P-stability, trigonometric-fitting and the numerical solution of the radial Schrödinger equation. Comput. Phys. Commun. **180**(7), 1072–1085 (2009)
78. Z.A. Anastassi, T.E. Simos, New trigonometrically fitted six-step symmetric methods for the efficient solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**(3), 733–752 (2008)

79. Z.A. Anastassi, T.E. Simos, A six-step P-stable trigonometrically-fitted method for the numerical integration of the radial Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**(3), 803–830 (2008)
80. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. J. Math. Chem. **45**(4), 1102–1129 (2009)
81. T.E. Simos, Explicit 2-step methods with minimal phase-lag for the numerical integration of special 2nd-order initial value problems and their application to the one-dimensional Schrödinger equation. J. Comput. Appl. Math. **39**(1), 89–94 (1992)
82. G. Avdelas, T.E. Simos, A generator of high-order embedded P-stable methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **72**(2), 345–358 (1996)
83. T.E. Simos, P.S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **79**(2), 189–205 (1997)
84. T.E. Simos, An accurate finite difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **91**(1), 47–61 (1998)
85. T.E. Simos, A new hybrid imbedded variable-step procedure for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **36**, 51–63 (1998)
86. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. J. Math. Chem. **29**(4), 281–291 (2001)
87. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. J. Math. Chem. **29**(4), 293–305 (2001)
88. J.R. Cash, F. Mazzia, Hybrid mesh selection algorithms based on conditioning for two-point boundary value problems. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 81–90 (2006)
89. T.E. Simos, A family of 4-step exponentially fitted Predictor-Corrector methods for the numerical integration of the Schrödinger equation. J. Comput. Appl. Math. **58**(3), 337–344 (1995)
90. R.M. Thomas, T.E. Simos, G.V. Mitsou, A family of Numerov-type exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **67**(2), 255–270 (1996)
91. R.M. Thomas, T.E. Simos, A family of hybrid exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **87**(2), 215–226 (1997)
92. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
93. G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation. J. Math. Chem. **37**(3), 295–316 (2005)
94. G. Psihoyios, T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions. J. Comput. Appl. Math. **175**(1), 137–147 (2005)
95. G. Psihoyios, T.E. Simos, A family of fifth algebraic order trigonometrically fitted P-C schemes for the numerical solution of the radial Schrödinger equation. MATCH Commun. Math. Comput. Chem. **53**(2), 321–344 (2005)
96. G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order Predictor-Corrector methods. J. Math. Chem. **40**(3), 269–293 (2006)
97. A.D. Raptis, T.E. Simos, A 4-step phase-fitted method for the numerical integration of 2nd-order initialvalue problems. BIT **31**(1), 160–168 (1991)
98. T.E. Simos, A Numerov-type method for the numerical solution of the radial Schröding er-equation. Appl. Numer. Math. **7**(2), 201–206 (1991)
99. T.E. Simos, Two-step almost P-stable complete in phase methods for the numerical integration of second order periodic initial-value problems. Inter. J. Comput. Math. **46**, 77–85 (1992)
100. T.E. Simos, A new variable step method for the numerical integration of special 2nd order initial value problems and their application to the one dimensional Schrödinger equation. Appl. Math. Lett. **6**(3), 67–73 (1993)
101. T.E. Simos, Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. J. Math. Chem. **21**(4), 359–372 (1997)

102. T.E. Simos, G. Mousadis, A two-step method for the numerical solution of the radial Schrödinger equation. Comput. Math. Appl. **29**, 31–37 (1995)
103. T.E. Simos, An extended Numerov-type method for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **33**, 67–78 (1997)
104. T.E. Simos, I.T. Famelis, Ch. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions. Numer. Algorithms **34**(1), 27–40 (2003)
105. A. Konguetsof, A new two-step hybrid method for the numerical solution of the Schrödinger equation. J. Math. Chem. **47**(2), 871–890 (2010)
106. A. Konguetsof, Two-step high order hybrid explicit method for the numerical solution of the Schrödinger equation. J. Math. Chem. **48**, 224–252 (2010)
107. T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation. J. Math. Chem. **46**(3), 981–1007 (2009)
108. Z. Kalogiratou, T.E. Simos, Newton-Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
109. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for long-time integration. Int. J. Modern Phys. C **14**(8), 1061–1074 (2003)
110. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 83–92 (2003)
111. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation. J. Math. Chem. **34**(1–2), 83–94 (2003)
112. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrödinger equation. J. Math. Chem **35**(1), 55–63 (2004)
113. T.E. Simos, Multiderivative methods for the numerical solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **45**, 7–26 (2004)
114. Z. Kalogiratou, T.E. Simos, Newton-Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
115. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems. Appl. Math. Lett. **22**(10), 1616–1621 (2009)
116. T.E. Simos, High order closed Newton-Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation. Appl. Math. Comput. **209**(1), 137–151 (2009)
117. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for the solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**(3), 787–801 (2008)
118. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation. J. Math. Chem. **44**(2), 483–499 (2008)
119. T.E. Simos, High-order closed Newton-Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. Comput. Phys. Commun. **178**(3), 199–207 (2008)
120. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for numerical integration of the Schrödinger equation. Comput. Lett. **3**(1), 45–57 (2007)
121. T.E. Simos, New closed Newton-Cotes type formulae as multilayer symplectic integrators. J. Chem. Phys. **133**(10): Art. No. 104108 (2010)
122. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. Revista Mexicana de Astronomia y Astrofysica **42**(2), 167–177 (2006)
123. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Families of third and fourth algebraic order trigonometrically fitted symplectic methods for the numerical integration of Hamiltonian systems. Comput. Phys. Commun. **177**(10), 757–763 (2007)
124. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Computation of the eigenvalues of the Schrödinger equation by symplectic and trigonometrically fitted symplectic partitioned Runge–Kutta methods. Phys. Lett. A **372**(5), 569–573 (2008)
125. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Symplectic partitioned Runge–Kutta methods with minimal phase-lag. Comput. Phys. Commun. **181**(7), 1251–1254 (2010)
126. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. Comput. Chem. **23**, 513–554 (1999)
127. Z.A. Anastassi, T.E. Simos, Numerical multistep methods for the efficient solution of quantum mechanics and related problems. Phys. Rep. Rev. Sect. Phys. Lett. **482**, 1–240 (2009)
128. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. J. Math. Chem. **27**(4), 343–356 (2000)

129. T.E. Simos, Bessel and Neumann fitted methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **42**, 833–847 (2001)
130. T.E. Simos, A.D. Raptis, A 4th-order Bessel fitting method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **43**(3), 313–322 (1992)
131. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Numerical solution of the two-dimensional time independent Schrödinger equation with Numerov-type methods. J. Math. Chem. **37**(3), 271–279 (2005)
132. S. Stavroyiannis, T.E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs. Appl. Numer. Math. **59**(10), 2467–2474 (2009)
133. S. Stavroyiannis, T.E. Simos, A nonlinear explicit two-step fourth algebraic order method of order infinity for linear periodic initial value problems. Comput. Phys. Commun. **181**(8), 1362–1368 (2010)
134. T.E. Simos, A.D. Zdetsis, G. Psihoyios, Z.A. Anastassi, Special issue on mathematical chemistry based on papers presented within ICCMSE 2005 preface. J. Math. Chem. **46**(3), 727–728 (2009)
135. T.E. Simos, G. Psihoyios, Special issue: the International Conference on Computational Methods in Sciences and Engineering 2004—Preface. J. Comput. Appl. **191**(2), 165–165 (2006)
136. T.E. Simos, G. Psihoyios, Special issue—selected papers of the International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003) Kastoria, Greece, 12–16 September 2003—Preface. J. Comput. Appl. Math. **175**(1), IX–IX (2005)
137. T.E. Simos, G. Psihoyios, Z. Anastassi, Preface, Proceedings of the International Conference of Computational Methods in Sciences and Engineering 2005. Math. Comput. Model. **51**(3–4), 137 (2010)
138. K. Gurlebeck, T. Simos, Special issue: approximation, stability and error analysis—Preface. Math. Methods Appl. Sci. **30**(14), 1609–1610 (2007)
139. T.E. Simos, J. Vigo-Aguiar, Special issue—selected papers from the Conference on Computational and Mathematical Methods for Science and Engineering (CMMSE-2002)—Alicante University, Spain, 20–25 September 2002—Preface. J. Comput. Appl. Math. **158**(1), IX–IX (2003)
140. C.D. Papageorgiou, A.D. Raptis, T.E. Simos, A method for computing phase-shifts for scattering. J. Comput. Appl. Math. **29**(1), 61–67 (1990)
141. T.E. Simos, P.S. Williams, Bessel and Neumann fitted methods for the numerical solution of the radial Schrödinger equation. Comput. Chem. **21**, 175–179 (1997)
142. P. Amodio, I. Gladwell, G. Romanazzi, Numerical solution of general bordered ABD linear systems by cyclic reduction. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 5–12 (2006)
143. J.R. Cash, N. Sumarti, T.J. Abdulla, I. Vieira, The derivation of interpolants for nonlinear two-point boundary value problems. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 49–58 (2006)
144. L.F. Shampine, P.H. Muir, H. Xu, A user-friendly Fortran BVP solver. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(2), 201–217 (2006)
145. J. Kierzenka, L.F. Shampine, A BVP solver that controls residual and error. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 27–41 (2008)
146. L. Aceto, P. Ghelardoni, C. Magherini, BVMs for Sturm-Liouville eigenvalue estimates with general boundary conditions. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 113–127 (2009)
147. J. Cash, G. Kitzhofer, O. Koch, G. Moore, E. Weinmller, Numerical solution of singular two point BVPs. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 129–149 (2009)
148. F. Iavernaro, F. Mazzia, D. Trigiante, Stability and conditioning in numerical analysis. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 91–112 (2006)
149. J.C. Butcher, Forty-five years of A-stability. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 1–9 (2009)
150. L. Brugnano, C. Magherini, Blended general linear methods based on boundary value methods in the generalized BDF family. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 23–40 (2009)
151. F. Iavernaro, D. Trigiante, Discrete conservative vector fields induced by the trapezoidal method. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 113–130 (2006)
152. S.D. Capper, J.R. Cash, D.R. Moore, Lobatto-Obrechkoff formulae for 2nd order two-point boundary value problems. JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**(1), 13–25 (2006)
153. F. Iavernaro, D. Trigiante, High-order symmetric schemes for the energy conservation of polynomial Hamiltonian problems. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 87–101 (2009)
154. R.M. Corless, A. Shakoori, D.A. Aruliah, L. Gonzalez-Vega, Barycentric Hermite interpolants for event location in initial-value problems. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 1–16 (2008)
155. N.S. Nedialkov, J.D. Pryce, Solving differential algebraic equations by Taylor series (III): the DAETS Code. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 61–80 (2008)
156. S.P. Corwin, S. Thompson, S.M. White, Solving ODEs and DDEs with impulses. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 139–149 (2008)

157. A. Fichtner, H. Igel, H.-P. Bunge, B.L.N. Kennett, Simulation and inversion of seismic wave propagation on continental scales based on a spectral-element method. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 11–22 (2009)
158. K. Burrage, Z. Jackiewicz, B.D. Welfert, Spectral approximation of time windows in the solution of dissipative linear differential equations. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 41–64 (2009)
159. P. Amodio, G. Settanni, Variable step/order generalized upwind methods for the numerical solution of second order singular perturbation problems. JNAIAM J. Numer. Anal. Ind. Appl. Math. **4**, 65–76 (2009)
160. W.H. Enright, On the use of 'arc length' and 'defect' for mesh selection for differential equations. Comput. Lett. **1**(2), 47–52 (2005)
161. W. Weckesser, VFGEN: a code generation tool. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 151–165 (2008)
162. M. Dewar, Embedding a general-purpose numerical library in an interactive environment. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 17–26 (2008)
163. R. Knapp, A method of lines framework in Mathematica. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 43–59 (2008)
164. R.L. Lipsman, J.E. Osborn, J.M. Rosenberg, The SCHOL Project at the University of Maryland: using mathematical software in the teaching of sophomore differential equations. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 81–103 (2008)
165. M. Sofroniou, G. Spaletta, Extrapolation methods in Mathematica. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 105–121 (2008)
166. R.J. Spiteri, T.-P. Ter, pythNon: a PSE for the numerical solution of nonlinear algebraic equations. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 123–137 (2008)
167. A. Wittkopf, Automatic code generation and optimization in Maple. JNAIAM J. Numer. Anal. Ind. Appl. Math. **3**, 167–180 (2008)
168. P. Henrici, *Discrete Variable Methods in Ordinary Diferential Equations* (Wiley, NewYork, USA, 1962)
169. L.Gr. Ixaru, *Numerical Methods for Differential Equations and Applications* (Reidel, Dordrecht, Boston, Lancaster, 1984)