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A New Explicit Linear Six-Step Methods with Vanished Phase-Lag and its First and Second Derivatives

T. E. Simos[1,2,*]

[1] Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia
[2] Laboratory of Computational Sciences, Department of Computer Science and Technology,Faculty of Sciences and Technology, University of Peloponnese, GR-22 100 Tripolis, Greece

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Abstract: The purpose of this paper is the development of an explicit linear sixth algebraic order six-step methods with vanished phase-lag and its first and second derivatives. The development of the new method is based on a theoretical and computational investigation. The theoretical investigation consists :

–The construction of the method
–The determination of the local truncation error
–The comparative local truncation error analysis
–The stability analysis

We note here that the stability analysis is is based on a scalar test equation with different frequency than the frequency of the scalar test equation used for the phase-lag analysis. The computational investigation of the new proposed method consists the application of the new obtained method to the resonance problem of the radial time independent Schrödinger equation. Based on the above mentioned studies we conclude that the new developed linear six-step method is more efficient (computationally and theoretically) than other well known methods for the approximate integration of the Schrödinger equation and related periodical/oscillatory initial or boundary value problems.

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

1. Introduction

In this paper we study the numerical solution of special second-order periodic and/or oscillatory initial or boundary value problems of the form

$$y''(x) = f(x, y), \;\; y(x_0) = y_0 \;\; and \;\; y'(x_0) = y'_0 \qquad (1)$$

The mathematical models which describe the above mentioned problems consist from systems of second order differential equations in which the first derivative y' does not appear explicitly (see for numerical methods for these problems [2] - [99] and references therein).

The numerical methods for the numerical integration of the one-dimensional time independent Schrödinger equation and related initial or boundary value problems with periodical or oscillating solution belong to one of the following categories:

–Methods with Coefficients Dependent on the Frequency of the periodic/oscillating problem
–Methods with Constant Coefficients

The numerical methods with coefficients dependent on the frequency of the periodic/oscillating problem belong into one of the following categories:

–Exponentially Fitted Methods
–Trigonometrically Fitted Methods
–Phase-Fitted and/or Amplification Fitted Methods (with or without Vanishing of the Derivatives of the Phase-Lag and/or the Amplification Error)

The numerical methods with constant coefficients belong into one of the following categories:

–Symplectic Integrators

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

–Other Finite Difference Methods

2. Phase-Lag For Symmetric Multistep Finite Difference Methods

For the numerical solution of the initial or boundary value problem 1) let us consider the multistep methods of the form:

$$\sum_{i=0}^{k} a_i\, y_{n+i} = h^2 \sum_{i=0}^{k} b_i\, f(x_{n+i}, y_{n+i}) \tag{2}$$

where:

–k are the number of steps over the equally spaced intervals $\{x_i\}_{i=0}^{k} \in [x_{begin}, x_{end}]$
–$h = |x_{i+1} - x_i|, \quad i = 0(1)k-1$, where h is called stepsize of integration

*Remark.*The finite difference method is called symmetric if $a_i = c_{k-i}$ and $b_i = b_{k-i}, \quad i = 0(1)\lfloor \frac{k}{2} \rfloor$.

The operator

$$L(x) = \sum_{i=0}^{k} c_i\, u(x + i\,h) - h^2 \sum_{i=0}^{k} b_i\, u''(x + i\,h) \tag{3}$$

where $u \in C^2$, is associated with the multistep finite difference method (2).

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

Application of the symmetric $2\,m$-step finite difference method, (i.e. for $i = -m(1)m$), to the scalar test equation

$$y'' = -\omega^2\, y \tag{4}$$

leads to the following difference equation:

$$A_m(v)\, y_{n+m} + \ldots + A_1(v)\, y_{n+1} + A_0(v)\, y_n + A_1(v)\, y_{n-1} + \ldots + A_m(v)\, y_{n-m} = 0 \tag{5}$$

where

–$v = \omega\, h$,
–h is the step length $A_j(v)\ j = 0(1)m$ are polynomials of v.

The characteristic equation which is associated with (5) is given by:

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

The following definition have been introduced by Lambert and Watson [13] :

Definition 2.*A symmetric $2\,m$-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 $\lambda_i, i = 1(1)2\,m$ of Eq. (6) satisfy:*

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

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

Definition 3.*[11], [12] For any method corresponding to the characteristic equation (6) the phase-lag is defined as the leading term in the expansion of*

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

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

Definition 4.*[23] A method for which the phase-lag vanishes (which is the same with: phase-lag equal to zero), is called* **phase-fitted**

*Remark.*A method can also have derivatives of the phase-lag which are vanished (which is the same with: derivatives of the phase-lag equal to zero).

Theorem 1.[11] *The symmetric $2\,m$-step method with characteristic equation given by (6) has phase-lag order p and phase-lag constant c given by*

$$-cv^{p+2} + O(v^{p+4}) = \frac{2\,A_m(v)\,\cos(m\,v) + \ldots + 2\,A_j(v)\,\cos(j\,v) + \ldots + A_0(v)}{2\,m^2\,A_m(v) + \ldots + 2\,j^2\,A_j(v) + \ldots + 2\,A_1(v)} \tag{9}$$

*Remark.*For any symmetric $2\,m$-step finite difference method the above mentioned formula (9) gives us a direct method to compute its phase-lag.

Proposition 1.*A symmetric six-step method has phase-lag order p and phase-lag constant c given by:*

$$-cv^{p+2} + O(v^{p+4}) = \frac{T_0}{T_1} \tag{10}$$

$$T_0 = 2\,A_3(v)\,\cos(3\,v) + 2\,A_2(v)\,\cos(2\,v) + 2\,A_1(v)\,\cos(v) + A_0(v)$$

$$T_1 = 18\,A_3(v) +_8\ A_2(v) + 2\,A_1(v)$$

*Proof.*The above proposition can be proved easily putting $m = 3$ in the formula (9).

3. A Linear Symmetric Six-Step Method with Phase-Lag and Its First and Second Derivatives Equal to Zero

3.1. The General Algorithm

For the numerical solution of problems with mathematical models of the form 1) with periodical and/ir oscillating solution let us consider the symmetric linear six-step method :

$$y_{n+3}+a_2\,(y_{n+2}+y_{n-2})+a_1\,(y_{n+1}+y_{n-1})+ \\ +a_0\,y_n \;=\; h^2\Big[b_2\,(f_{n+2}+f_{n-2})+ \\ +b_1\,(f_{n+1}+f_{n-1})+b_0\,f_n\Big] \qquad (11)$$

where $f_i = y''(x_i, y_i)\,, i = n-2(1)n+2$ and $a_0 \;=\; -2$, $a_1 \;=\; 2$ and $a_2 \;=\; -2$.

3.2. Development of the Method with Vanished Phase-Lag and its First and Second Derivatives

The construction of the new method is based on the algorithm presented below:

–We apply the general method (11) to the scalar test equation (4).
–The above application leads to the difference equation (5) with $m = 3$ and:

$$A_3(v) \;=\; 1,\; A_2(v) \;=\; -2+b_2\,v^2, \\ A_1(v) \;=\; 2+b_1\,v^2, \\ A_0(v) \;=\; -2+b_0\,v^2 \qquad (12)$$

–The associated characteristic equation (6), with $m = 3$, is obtained based on the polynomials (12).
–The direct formula (10) for the calculation of the phase-lag of the symmetric six-step finite difference method (11) is obtained based on the polynomials $A_j(v),\; j = 0(1)3$ presented in (12).
–Requiring the symmetric linear six-step method method (11) to have the phase-lag equal to zero (i.e. to be phase-fitted), the following equation is obtained.

$$\frac{T_2}{2\,v^2\,b_1+8\,v^2\,b_2+6}=0 \qquad (13)$$

where:

$$T_2 \;=\; 2\,\cos(3\,v)+2\,\left(v^2\,b_2-2\right)\cos(2\,v) \\ +2\,\left(v^2\,b_1+2\right)\cos(v)+v^2\,b_0-2$$

–Requiring the symmetric linear six-step method method (11) to have the the first derivative of the phase-lag equal to zero , the following equation is obtained.

$$-\frac{T_3}{\left(v^2\,b_1+4\,v^2\,b_2+3\right)^2}=0 \qquad (14)$$

where:

$$T_3 \;=\; 4\,\sin(v)\cos(v)\,v^4\,b_1\,b_2 \\ +16\,\sin(v)\cos(v)\,v^4\,{b_2}^2 \\ +\sin(v)\;v^4\,{b_1}^2+4\,\sin(v)\;v^4\,b_1\,b_2 \\ +12\,(\cos(v))^2\,\sin(v)\;v^2\,b_1 \\ +48\,(\cos(v))^2\,\sin(v)\;v^2\,b_2 \\ +8\,(\cos(v))^3\;v\,b_1 \\ +32\,(\cos(v))^3\;v\,b_2 \\ -8\,\sin(v)\cos(v)\;v^2\,b_1 \\ -20\,\sin(v)\cos(v)\;v^2\,b_2 \\ -8\,(\cos(v))^2\;v\,b_1 \\ -44\,(\cos(v))^2\;v\,b_2+2\,\sin(v)\;v^2\,b_1 \\ -4\,\sin(v)\;v^2\,b_2+36\,(\cos(v))^2\,\sin(v) \\ -8\,v\,b_1\,\cos(v)-8\,\cos(v)\;v\,b_2 \\ -24\,\sin(v)\cos(v) \\ -3\,v\,b_0+2\,v\,b_1+14\,v\,b_2-3\,\sin(v)$$

–Requiring the symmetric linear six-step method method (11) to have the the second derivative of the phase-lag equal to zero , the following equation is obtained.

$$\frac{T_4}{\left(v^2\,b_1+4\,v^2\,b_2+3\right)^3}=0 \qquad (15)$$

where:

$$T_4 \;=\; -72-120\,\cos(v)\;v^2\,b_1\,b_2-48\,\sin(v)\;v\,b_1 \\ -864\,(\cos(v))^3\;v^2\,b_2-48\,\sin(v)\;v\,b_2 \\ +192\,(\cos(v))^3\;v^2\,b_1\,b_2 \\ -32\,\sin(v)\cos(v)\;v^3\,{b_1}^2 \\ +768\,\sin(v)\,(\cos(v))^2\;v^3\,{b_2}^2 \\ +48\,\sin(v)\,(\cos(v))^2\;v^3\,{b_1}^2 \\ -288\,(\cos(v))^3\;v^4\,b_1\,b_2 \\ -16\,\cos(v)\;v^6\,b_1\,{b_2}^2-8\,\cos(v)\;v^6\,{b_1}^2\,b_2 \\ -8\,(\cos(v))^2\;v^6\,{b_1}^2\,b_2 \\ -64\,(\cos(v))^2\;v^6\,b_1\,{b_2}^2 \\ -304\,\sin(v)\cos(v)\;v^3\,b_1\,b_2+4\,v^6\,{b_1}^2\,b_2 \\ -528\,(\cos(v))^2\;v^2\,{b_2}^2 \\ -64\,\sin(v)\;v^3\,{b_2}^2-24\,\cos(v)\;v^2\,{b_1}^2 \\ -324\,(\cos(v))^3+32\,v^6\,b_1\,{b_2}^2 \\ -42\,b_2-24\,(\cos(v))^2\;v^2\,{b_1}^2 \\ +24\,(\cos(v))^3\;v^2\,{b_1}^2 \\ +16\,(\cos(v))^2\;v^4\,{b_1}^2 \\ -576\,(\cos(v))^3\;v^4\,{b_2}^2 \\ +384\,(\cos(v))^3\;v^2\,{b_2}^2$$

$$
\begin{aligned}
&-128\,(\cos(v))^2\,v^6\,{b_2}^3\\
&-\cos(v)\,v^6\,{b_1}^3+600\cos(v)\,v^2\,b_2\\
&-6\,b_1+80\,(\cos(v))^2\,v^4\,b_1\,b_2\\
&-704\sin(v)\cos(v)\,v^3\,{b_2}^2\\
&-80\sin(v)\,v^3\,b_1\,b_2\\
&+144\,(\cos(v))^2\sin(v)\,v\,b_1\\
&+576\,(\cos(v))^2\sin(v)\,v\,b_2\\
&-96\sin(v)\cos(v)\,v\,b_1-528\sin(v)\cos(v)\,v\,b_2\\
&-36\,(\cos(v))^3\,v^4\,{b_1}^2-36\,v^2\,b_0\,b_2\\
&+66\,v^2\,b_1\,b_2+9\,b_0\\
&+400\cos(v)\,v^4\,{b_2}^2+312\,(\cos(v))^2\,v^2\,b_2\\
&+225\cos(v)+144\,(\cos(v))^2+6\,v^2\,{b_1}^2\\
&+168\,v^2\,{b_2}^2+176\cos(v)\,v^4\,b_1\,b_2\\
&-32\,v^4\,{b_2}^2-156\,v^2\,b_2-8\,v^4\,{b_1}^2\\
&-228\,(\cos(v))^2\,v^2\,b_1\,b_2-40\,v^4\,b_1\,b_2\\
&+132\,(\cos(v))^2\,b_2+24\,b_1\cos(v)\\
&+24\cos(v)\,b_2-48\,v^2\,b_1-216\,(\cos(v))^3\,v^2\,b_1\\
&+141\cos(v)\,v^2\,b_1+96\,(\cos(v))^2\,v^2\,b_1\\
&+64\,(\cos(v))^2\,v^4\,{b_2}^2-16\sin(v)\,v^3\,{b_1}^2\\
&-9\,v^2\,b_0\,b_1+19\cos(v)\,v^4\,{b_1}^2\\
&+384\sin(v)\,(\cos(v))^2\,v^3\,b_1\,b_2\\
&-96\cos(v)\,v^2\,{b_2}^2-24\,(\cos(v))^3\,b_1\\
&-96\,(\cos(v))^3\,b_2+24\,(\cos(v))^2\,b_1\\
&+64\,v^6\,{b_2}^3
\end{aligned}
$$

–The solution of the system of equations (13) - (15) leads to the determination of the coefficients $b_i\, i = 0(1)2$ of the symmetric linear six-step method method (11):

$$
\begin{aligned}
b_0 &= \frac{T_5}{3\,v^4\sin(v)-v^4\sin(3\,v)}\\
b_1 &= \frac{T_6}{3\,v^4\sin(v)-v^4\sin(3\,v)}\\
b_2 &= \frac{T_7}{3\,v^4\sin(v)-v^4\sin(3\,v)}
\end{aligned}
\tag{16}
$$

where

$$
\begin{aligned}
T_5 &= 6\,v^2\sin(v)-15\,v^2\sin(2\,v)+v^2\sin(6\,v)\\
&+6\,v^2\sin(4\,v)-2\,v^2\sin(3\,v)+50\cos(v)\,v\\
&-2\,v\cos(5\,v)+3\,v\cos(6\,v)+13\,v\cos(4\,v)\\
&-12\,v\cos(3\,v)-25\,v\cos(2\,v)+6\sin(v)\\
&-15\sin(2\,v)-3\sin(6\,v)-15\sin(4\,v)\\
&+6\sin(5\,v)+24\sin(3\,v)-27\,v\\
T_6 &= 9\,v^2\sin(v)-3\,v^2\sin(5\,v)+2\,v^2\sin(3\,v)\\
&+32\cos(v)\,v-8\,v\cos(5\,v)+8\,v\cos(4\,v)\\
&-8\,v\cos(2\,v)+6\sin(v)-12\sin(2\,v)\\
&-12\sin(4\,v)+6\sin(5\,v)+12\sin(3\,v)-24\,v\\
T_7 &= 6\,v^2\sin(v)-6\,v^2\sin(2\,v)+3\,v^2\sin(4\,v)\\
&-2\,v^2\sin(3\,v)+12\cos(v)\,v+5\,v\cos(4\,v)\\
&-6\,v\cos(3\,v)-5\,v\cos(2\,v)-3\sin(2\,v)\\
&-3\sin(4\,v)+6\sin(3\,v)-6\,v
\end{aligned}
$$

The above mentioned formulae (given by (16)) may subject to heavy cancelations for some values of $|v|$. In this case the following Taylor series expansions should be used :

$$
\begin{aligned}
b_0 &= \frac{97}{40}-\frac{275}{224}\,v^2+\frac{9559}{22400}\,v^4\\
&-\frac{679541}{6652800}\,v^6+\frac{300755969}{24216192000}\,v^8\\
&-\frac{1936967}{1845043200}\,v^{10}+\frac{30681216749}{592812380160000}\,v^{12}\\
&-\frac{11352810559}{3942202328064000}\,v^{14}\\
&-\frac{1786305431}{14867734494412800000}\,v^{16}\\
&-\frac{184467544202363}{17234677825923317760000}\,v^{18}+\ldots\\
b_1 &= -\frac{31}{30}+\frac{275}{336}\,v^2-\frac{10901}{50400}\,v^4\\
&+\frac{50009}{2851200}\,v^6-\frac{21107707}{18162144000}\,v^8\\
&+\frac{1389683}{174356582400}\,v^{10}-\frac{134286989}{34200714240000}\,v^{12}\\
&-\frac{18277572601}{47306427936768000}\,v^{14}\\
&-\frac{1667121262381}{33452402612428800000}\,v^{16}\\
&-\frac{156882478987937}{25852016738884976640000}\,v^{18}+\ldots\\
b_2 &= \frac{317}{240}-\frac{275}{1344}\,v^2+\frac{1177}{403200}\,v^4\\
&-\frac{22753}{39916800}\,v^6-\frac{8001571}{145297152000}\,v^8\\
&-\frac{452299}{63402393600}\,v^{10}-\frac{5876029}{6599024640000}\,v^{12}\\
&-\frac{260344639}{2365321396838400}\,v^{14}\\
&-\frac{3596712394753}{2676192208994304000000}\,v^{16}\\
&-\frac{8825566741177}{5442529839765258240000}\,v^{18}+\ldots
\end{aligned}
\tag{17}
$$

The behavior of the coefficients is given in the following Figure 1.

In the below mentioned formula we give the local truncation error of the new developed method (11) (men-

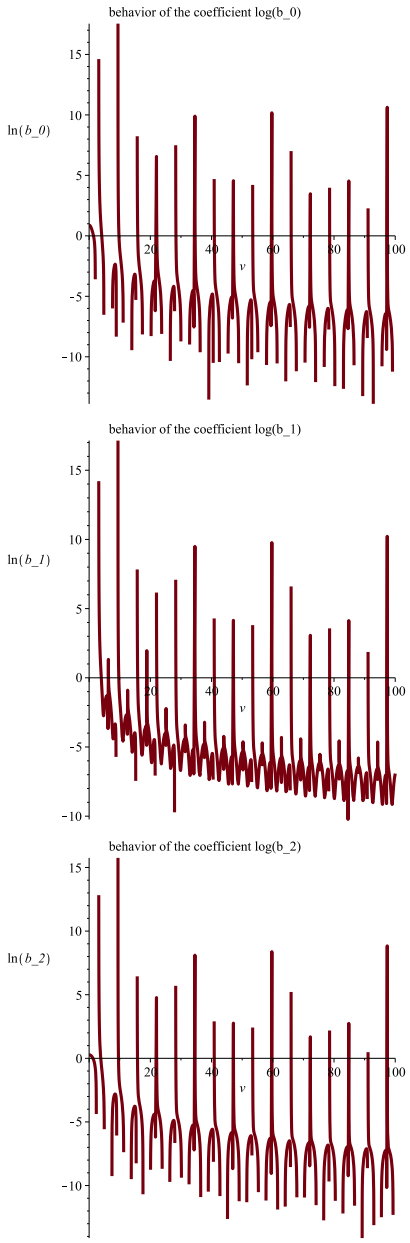

Figure 1 Behavior of the coefficients of the new proposed method given by (16) for several values of $v = \omega\, h$.

tioned as $SixStepMethod$) with the coefficients given by (16)-(17):

$$LTE_{Linear\ Six\ Step} = \frac{275\, h^8}{4032}\left(y_n^{(8)} + \right.$$
$$+3\,\omega^2\, y_n^{(6)} + 3\,\omega^4\, y_n^{(4)} +$$
$$\left. +\omega^6\, y_n^{(2)}\right) + O\left(h^{10}\right) \tag{18}$$

4. Comparative Local Truncation Error Analysis

We will investigate the following methods :

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

$$LTE_{CL} = \frac{275\, h^8}{4032}\, y_n^{(8)} + O\left(h^{10}\right) \tag{19}$$

4.2. The Phase-Fitted Method Produced in [39]

$$LTE_{Linear\ Six\ Step\ PF} = \frac{275\, h^8}{4032}\left(y_n^{(8)} + \right.$$
$$\left. \omega^6\, y_n^{(2)}\right) + O\left(h^{10}\right) \tag{20}$$

4.3. The Method with Vanished Phase-Lag and its First Derivative Produced Obtained in [39]

$$LTE_{Linear\ Six\ Step} = \frac{275\, h^8}{4032}\left(y_n^{(8)} - 3\,\omega^4\, y_n^{(4)}\right.$$
$$\left. -2\,\omega^6\, y_n^{(2)}\right) + O\left(h^{10}\right) \tag{21}$$

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

$$LTE_{Linear\ Six\ Step} = \frac{275\, h^8}{4032}\left(y_n^{(8)} + \right.$$
$$+3\,\omega^2\, y_n^{(6)} + 3\,\omega^4\, y_n^{(4)} +$$
$$\left. +\omega^6\, y_n^{(2)}\right) + O\left(h^{10}\right) \tag{22}$$

The following steps are followed in order to obtain the asymptotic expansions of the Local Truncation Error for the algorithms mentioned above :

–In this step we compute the derivatives of the function y_n (approximation of the function $y(x)$ at x_n). These derivatives are based on the main derivative : $y_n^{(2)} = (V(x) - V_c + G)\ y(x)$ which is followed from the mathematical model of the problem. The above mentioned derivatives are occurred in the formulae of the Local Truncation Errors. Therefore we have:

$$y_n^{(2)} = (V(x) - V_c + G)\ y(x)$$

$$y_n^{(3)} = \left(\frac{d}{dx}g(x)\right) y(x) + (g(x) + G)\ \frac{d}{dx}y(x)$$

$$y_n^{(4)} = \left(\frac{d^2}{dx^2}g(x)\right) y(x) + 2\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}y(x) + (g(x) + G)^2\, y(x)$$

$$y_n^{(5)} = \left(\frac{d^3}{dx^3}g(x)\right) y(x) + 3\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}y(x) + 4\ (g(x) + G)\, y(x)\ \frac{d}{dx}g(x) + (g(x) + G)^2\ \frac{d}{dx}y(x)$$

$$y_n^{(6)} = \left(\frac{d^4}{dx^4}g(x)\right) y(x) + 4\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}y(x) + 7\ (g(x) + G)\, y(x)\ \frac{d^2}{dx^2}g(x) + 4\left(\frac{d}{dx}g(x)\right)^2 y(x) + 6\ (g(x) + G)\left(\frac{d}{dx}y(x)\right)\frac{d}{dx}g(x) + (g(x) + G)^3\, y(x)$$

$$y_n^{(7)} = \left(\frac{d^5}{dx^5}g(x)\right) y(x) + 5\left(\frac{d^4}{dx^4}g(x)\right)\frac{d}{dx}y(x) + 11\ (g(x) + G)\, y(x)\ \frac{d^3}{dx^3}g(x) + 15\left(\frac{d}{dx}g(x)\right) y(x)\ \frac{d^2}{dx^2}g(x) + 13\ (g(x) + G)\left(\frac{d}{dx}y(x)\right)\frac{d^2}{dx^2}g(x) + 10\left(\frac{d}{dx}g(x)\right)^2\frac{d}{dx}y(x) + 9\ (g(x) + G)^2\, y(x)\ \frac{d}{dx}g(x) + (g(x) + G)^3\ \frac{d}{dx}y(x)$$

$$y_n^{(8)} = \left(\frac{d^6}{dx^6}g(x)\right) y(x) + 6\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}y(x) + 16\ (g(x) + G)\, y(x)\ \frac{d^4}{dx^4}g(x) + 26\left(\frac{d}{dx}g(x)\right) y(x)\ \frac{d^3}{dx^3}g(x) + 24\ (g(x) + G)\left(\frac{d}{dx}y(x)\right)\frac{d^3}{dx^3}g(x) + 15\left(\frac{d^2}{dx^2}g(x)\right)^2 y(x) + 48\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}y(x)\right)\frac{d^2}{dx^2}g(x) + 22\ (g(x) + G)^2\, y(x)\ \frac{d^2}{dx^2}g(x) + 28\ (g(x) + G)\, y(x)\left(\frac{d}{dx}g(x)\right)^2 + 12\ (g(x) + G)^2\left(\frac{d}{dx}y(x)\right)\frac{d}{dx}g(x) + (g(x) + G)^4\, y(x)$$

$$\ldots$$

*Remark.*The above expressions of the derivatives of the function y_n are finally dependent from $G = V_c - E$ which is dependent from the energy E.

–Based on the above mentioned remark it is easy for one to see that the expressions of the derivatives of the function y_n helps the formulae of the Local Truncation Error to be expressed as functions of the energy E. This is happened via its substitution in the formulae of the Local Truncation Error of the derivatives of the function y_n mentioned above.

–The study of the obtained via the above procedure formulae of the Local Truncation Errors contains two main cases in terms of the value of E :

1. $G = V_c - E \approx 0$. In this case the Energy is close to the potential. Therefore and since $G = 0$ and consequently G^n, $n = 1, 2, \ldots = 0$,all the terms of G in the formulae of the Local Truncation Error analysis are equal to zero. Therefore, only the terms of the formulae of the Local Truncation Errors which are free from G are considered. Thus, for these values of G, the methods are of **comparable accuracy**. The reason is explained below via the mentioned Remark.

   *Remark.*In the case of formulae of Local Truncation Errors for which $G = 0$, the behavior of the methods of the family are similar. This is due to the fact that for $G = 0$ for this family of methods the free from G terms of the polynomials are the same (and this for both of cases of methods of the family with constant coefficients or methods of the family with coefficients dependent from the frequency of the problem).

2. $G >> 0$ or $G << 0$. Then $|G|$ is a large number. In this case we take into account all the terms in the formulae of the Local Truncation Error analysis.

–Finally the asymptotic expansions of the Local Truncation Errors are computed

Based on the analysis presented above, the following asymptotic expansions of the Local Truncation Errors are produced :

4.5. Classical Method

$$LTE_{CL} = h^8\left(\frac{275}{4032}\, y(x)\ G^4 + \cdots\right) + O\left(h^{10}\right) \quad (23)$$

4.6. The Phase-Fitted Method Produced in [39]

$$LTE_{Linear\ Six\ Step\ PF} = h^8 \left(\frac{275}{1344} g(x) \right.$$
$$\left. y(x)\ G^3 + \cdots \right) + O\left(h^{10}\right) \quad (24)$$

4.7. The Method with Vanished Phase-Lag and its First Derivative Produced Obtained in [39]

$$LTE_{Six\ Step\ Linear} = h^8 \left[\left(\frac{275}{672} \left(\frac{d}{dx} g(x) \right) \right. \right.$$
$$\frac{d}{dx} y(x) + \frac{5225}{4032} \left(\frac{d^2}{dx^2} g(x) \right)$$
$$y(x) + \frac{275}{1344} (g(x))^2$$
$$\left. \left. y(x) \right) G^2 + \cdots \right] + O\left(h^{10}\right) \quad (25)$$

4.8. The New Proposed Method with Vanished Phase-Lag and its First and Second Derivatives Developed in Section 3

$$LTE_{Linear\ Six\ Step} = h^8 \left(\frac{275}{1008} \left(\frac{d^2}{dx^2} g(x) \right) \right.$$
$$\left. y(x)\ G^2 + \cdots \right) + O\left(h^{10}\right) \quad (26)$$

From the above equations we have the following theorem:

Theorem 2.*For the Classical Linear Six-Step Explicit Method, the error increases as the four power of G. For the Linear Six-Step Explicit Phase-Fitted Method developed in [39] , the error increases as the third power of G. For the Linear Six-Step Explicit Method with Vanished Phase-lag and its First Derivative which is developed in [39], the error increases as the second power of G. Finally, for the Linear Six-Step Explicit Method with Vanished Phase-lag and its First and Second Derivatives which is developed in Section 3, the error increases as the second power of G but with lower coefficient than the error the Linear Six-Step Explicit Method with Vanished Phase-lag and its First Derivative which is developed in [39]. So, for the numerical solution of the time independent radial Schrödinger equation the New Developed Method with Vanished Phase-Lag and its First and Second Derivative is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.*

5. Stability Analysis

In this section we will investigate the stability (interval of periodicity) of the new methods. The main idea is that the scalar test equation which we will use for the stability analysis will have different frequency than the scalar test equation used for the phase-lag analysis (mentioned in Section 2). Therefore, we apply the new obtained method to the scalar test equation:

$$y'' = -\phi^2 y. \quad (27)$$

where $\phi \neq \omega$.

The above mentioned application leads to the following difference equation :

$$A_3(s,v)\ (y_{n+3} + y_{n-3}) + A_2(s,v)\ (y_{n+2} + y_{n-2})$$
$$+A_1(s,v)\ (y_{n+1} + y_{n-1}) + A_0(s,v)\ y_n = 0 \quad (28)$$

where

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

$$\begin{aligned} A_3(s,v) &= 1, \\ A_2(s,v) &= -2 + \frac{T_8}{3v^4 \sin(v) - v^4 \sin(3v)}, \\ A_1(s,v) &= \frac{T_9}{\sin(v)(\cos(v)+1)v^4} \\ A_0(s,v) &= -\frac{1}{2} \frac{T_{10}}{\sin(v)(\cos(v)+1)v^4} \end{aligned} \quad (29)$$

where

$$\begin{aligned} T_8 &= s^2 \left(6v^2 \sin(v) - 6v^2 \sin(2v) \right. \\ &+3v^2 \sin(4v) - 2v^2 \sin(3v) + 12 \cos(v) v \\ &+5v \cos(4v) - 6v \cos(3v) - 5v \cos(2v) \\ &\left. -3 \sin(2v) - 3 \sin(4v) + 6 \sin(3v) - 6v \right) \\ T_9 &= 12 \sin(v) (\cos(v))^3 s^2 v^2 \\ &+12 \sin(v) (\cos(v))^2 s^2 v^2 \\ &+32 s^2 v (\cos(v))^4 - 24 \sin(v) \\ &(\cos(v))^3 s^2 + \sin(v) \cos(v) s^2 v^2 \\ &+2 \sin(v) \cos(v) v^4 + 16 s^2 v (\cos(v))^3 \\ &+ \sin(v) s^2 v^2 + 2v^4 \sin(v) - 24 s^2 v (\cos(v))^2 \\ &+6 \sin(v) \cos(v) s^2 - 4 \cos(v) s^2 v - 2 s^2 v \end{aligned}$$

$$
\begin{aligned}
T_{10} \;=\; & 12\,\sin(v)\,(\cos(v))^2\,s^2v^2 \\
& +8\,\sin(v)\cos(v)\,s^2v^2+4\,\sin(v)\cos(v)\,v^4 \\
& +20\,s^2v\,(\cos(v))^3-12\,\sin(v) \\
& (\cos(v))^2\,s^2-4\,\sin(v)\,s^2v^2 \\
& +4\,v^4\sin(v)+8\,s^2v\,(\cos(v))^2 \\
& -17\,\cos(v)\,s^2v+3\,\sin(v)\,s^2-2\,s^2v
\end{aligned}
$$

and $s = \phi\, h$.

*Remark.*The investigation of the stability is based on the scalar test equation (27) with frequency of the , ϕ, which is not equal with the frequency of the scalar test equation (4), ω, of the phase-lag analysis i.e. $\omega \neq \phi$.

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

Definition 5.*(see [13]) A method is called P-stable if its interval of periodicity is equal to* $(0, \infty)$.

Definition 6.*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 lag analysis is the same as the frequency of the stability analysis, i.e.* $s = v$.

In Figure 2 we present the $s - w$ plane for the method developed in Section 3 (Method with Vanished Phase-lag and its First and Second Derivative).

*Remark.*The white area denotes the $s - v$ region where the method is unstable while the shadowed area denotes the $s - v$ region where the method is stable.

*Remark.*For many real problems the frequency of the phase-lag analysis is equal to the frequency of the stability analysis. For these kind of of real problems it is necessary to observe **the surroundings of the first diagonal of the** $s - v$ **plane**. In these problems and in order to apply a method with frequency dependent coefficients, it is necessary to define one frequency of the problem (because the frequency of the phase-lag analysis is equal to the frequency of the stability analysis). In this category of problems belong many problems in sciences and engineering (for example the time independent Schrödinger equation).

For the problems of the above mentioned remark we study now the case where the frequency of the stability analysis is equal with the frequency of phase-lag analysis, i.e. we investigate the case where $s = v$ (more specifically we investigate the case seeing the surroundings of the first diagonal of the $s - v$ plane). From this investigation we have that the interval of periodicity of the new method is equal to: $(0, 4.4)$.

The above study leads to the following theorem:

Theorem 3.*The method developed in this paper (Section 3):*

[1] where S is a set of distinct points

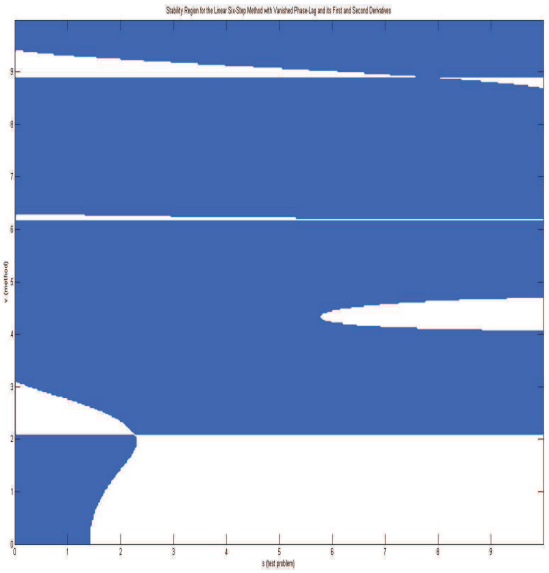

Figure 2 $s - v$ plane of the the new obtained method with vanished phase-lag and its first and second derivatives

–is of six algebraic order,
–has the phase-lag and its first and second derivatives equal to zero
–have an interval of periodicity equal to $(0, 4.4)$*, when the frequency of the stability analysis is equal with the frequency of phase-lag analysis.*

6. Numerical results

The application of the new obtained linear explicit six-step methods to the numerical solution of the radial time-independent Schrödinger equation is the study of its efficiency.

We can write the model of the radial time independent Schrödinger equation as :

$$y''(r) = [l(l+1)/r^2 + V(r) - k^2]y(r). \tag{30}$$

This is a boundary value problem with the following boundary conditions :

$$y(0) = 0 \tag{31}$$

and another boundary condition, for large values of r, determined by physical considerations.

The following definitions help us to understand the details of the mathematical model :

1.The function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(r) \to 0$ as $r \to \infty$,

2.The quantity k^2 is a real number denoting *the energy*,
3.The quantity l is a given integer representing the *angular momentum*,
4.V is a given function which denotes the *potential*.

The new obtained algorithm is belonged into the category of numerical methods with coefficients dependent on the frequency of the problem. For this, it is necessary to define the value of the parameter ω. The determination of the above mentioned parameter is dependent from the problem we have to solve. For the specific case of the the radial time independent Schrödinger equation the parameter ω is given by (for $l = 0$) :

$$\omega = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{32}$$

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

6.1. Woods-Saxon potential

In order to solve the radial time independent Schrödinger equation, we have to determine the potential which we will use in the mathematical model. For the purpose of the numerical tests of this paper we will use the well known Woods-Saxon potential. The Woods-Saxon potential can be written as :

$$V(r) = \frac{u_0}{1+q} - \frac{u_0\, q}{a\,(1+q)^2} \tag{33}$$

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

The behavior of Woods-Saxon potential is shown in Figure 5.

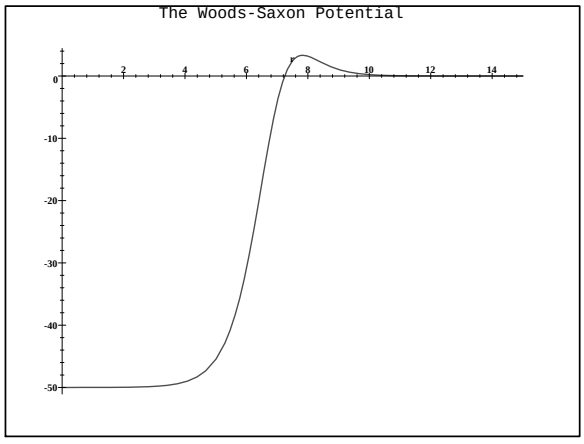

Figure 3 The Woods-Saxon potential.

The discrete approximation of a potential is an important subject of the research literature (see [101] and [102] and references therein).

*Remark.*A discrete approximation of a potential is an approximation of this potential via determination of critical points of this potential.

It is critical for the form of the picture of the potential the accurate knowledge of the points of the discrete approximation.

For the specific numerical example we chose the discrete approximation of the parameter ω. Based on [100] we determine the critical points for the Woods-Saxon potential. Therefore, we choose ω as follows (see for details [101] and [102]):

$$\phi = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{34}$$

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 $r = 6.5 - 3\,h$, the value of ϕ is equal to: $\sqrt{-50+E}$, etc.

6.2. Radial Schrödinger Equation - The Resonance Problem

The investigation of the efficiency of the new obtained method is taken place via the application of the new developed method to the numerical solution of the radial time independent Schrödinger equation (30) using the Woods-Saxon potential (33).

Since the approximate solution of the radial time independent Schrödinger equation (30) is a problem with infinite interval of integration and in order to apply the new produced method, we have to replace this infinite interval of integration with a finite one. For the purposes of our numerical investigations we select as interval of integration, the interval $[0, 15]$.

We study the equation (30) for a large domain of energies, i.e., $E \in [1, 1000]$.

For our numerical experiments, we investigate the case of positive energies. In this case we have that $E = k^2$ and the potential decays faster than the term $\frac{l(l+1)}{r^2}$. In such cases the radial Schrödinger equation effectively reduces to

$$y''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) y(r) = 0 \tag{35}$$

for r greater than some value R.

The above mentioned problem 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 asymptotic form of the solution of equation (30) (when $r \to \infty$) is given by:

$$y(r) \approx Akrj_l(kr) - Bkrn_l(kr)$$
$$\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \quad (36)$$

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

$$\tan\delta_l = \frac{y(r_2)S(r_1) - y(r_1)S(r_2)}{y(r_1)C(r_1) - y(r_2)C(r_2)} \quad (37)$$

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 $C(r) = -krn_l(kr)$. The problem we consider in our experiments is treated as an initial-value problem. In this caswe we must define $y_j,\ j = 0(1)5$ in order to begin the application of a six-step method. From the initial condition, we obtain y_0. The values $y_i,\ i = 1(1)5$ are obtained by using high order Runge-Kutta-Nyström methods(see [18] and [19]). Based on these starting values, we can evaluate the phase shift δ_l at r_2 of the asymptotic region.

The resonance problem is defined for positive energies. This problem consists either

–of finding the phase-shift δ_l or
–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:

$$y(0) = 0,\ y(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \quad (38)$$

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

–The eighth order multi-step method developed by Quinlan and Tremaine [2], which is indicated as **Method QT8**.
–The tenth order multi-step method developed by Quinlan and Tremaine [2], which is indicated as **Method QT10**.
–The twelfth order multi-step method developed by Quinlan and Tremaine [2], which is indicated as **Method QT12**.
–The fourth algebraic order method of Chawla and Rao with minimal phase-lag [104], which is indicated as **Method MCR4**
–The exponentially-fitted method of Raptis and Allison [103], which is indicated as **Method MRA**
–The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [105], which is indicated as **Method MCR6**
–The classical form of the sixth algebraic order six-step method developed in Section 4, which is indicated as **Method NMCL6** [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 Phase-Fitted Method developed in [39], which is indicated as **Method N6SMPF**
–The Method with vanished phase-lag and its first derivative developed in [39], which is indicated as **Method N6SMPFD**
–The New Obtained Method with vanished phase-lag and its first and second derivatives developed in Section 3, which is indicated as **Method N6SMPFDD**

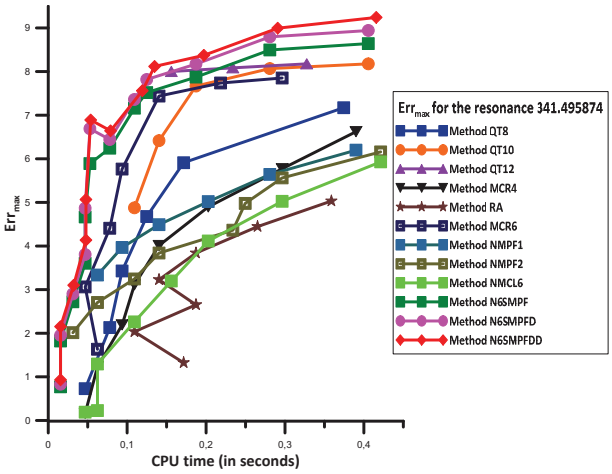

Figure 4 Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

We compare the computationally obtained eigenenergies with the reference values [3]. In Figures 5 and 6, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \quad (39)$$

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 4 with constant coefficients

[3] we define as reference values the computed using the well known two-step method of Chawla and Rao [105] with small step size for the integration

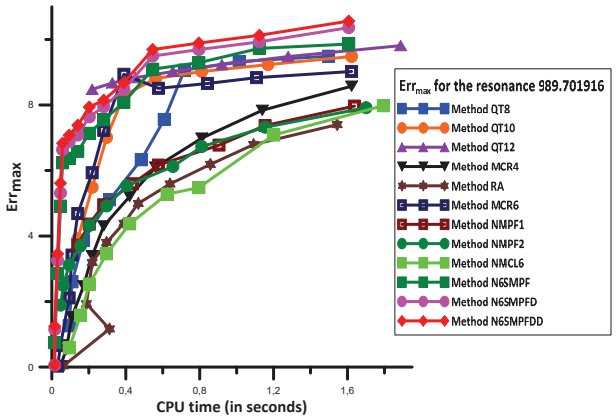

Figure 5 Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

7. Conclusions

The development of an explicit linear sixth algebraic order six-step method is investigated in this paper. More specifically we studied the following

1.Construction of the methods. The main requirements are:
   – The algebraic order of the new six-step method to be maximized
   – The phase-lag of the new six-step method to be vanished
   – The first derivative of the phase-lag of the new six-step method to be also vanished
   – Finally, the second derivative of the phase-lag of the new six-step method to be also equal to zero (i.e. vanished).
2.Theoretical study of the new obtained method. This consists of:
   – Comparative Local Truncation Error Analysis (for comparison reason we use the corresponding methods of the literature)
   – Stability Analysis (using a scalar test equation with frequency which is different than the frequency of the scalar test equation for phase-lag analysis)
3.Identification of the theoretical study. This was taken place via the numerical approximation of the resonance problem of the radial time independent Schrödinger equation and related problems.

From the obtained numerical experiments presented on the figures mentioned above , we can make the following remarks:

1.The classical form of the sixth algebraic order six-step method developed in Section 4, which is indicated as **Method NMCL6** has approximately the same efficiency than the the exponentially-fitted method of Raptis and Allison [103], which is indicated as **Method MRA**.
2.The tenth algebraic order multistep method developed by Quinlan and Tremaine [2], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [104], 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 [2], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [105], which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.
3.The twelfth algebraic order multistep method developed by Quinlan and Tremaine [2], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [2], which is indicated as **Method QT10**
4.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 NMCL6**, the exponentially-fitted method of Raptis and Allison [103] and the Phase-Fitted Method (Case 2) developed in [1], which is indicated as **Method NMPF2**
5.The Linear Six-Step Eight Algebraic Order Phase-Fitted Method developed in [39], which is indicated as **Method N6SMPF** is more efficient than all the methods mentioned above
6.The Linear Six-Step Eight Algebraic Order Method with Vanished Phase-Lag and its First Derivative which developed in [39] and is indicated as **Method N6SMPFD** is more efficient than all the methods mentioned above.
7.Finally, the new obtained Linear Six-Step Eight Algebraic Order Method with Vanished Phase-Lag and its First and Second Derivatives which developed in Section 3 and is indicated as **Method N6SMPFDD** 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).

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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).