Iranian J. Math. Chem. 8(2) June (2017) 137−159

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

A New Two–Step Obrechkoff Method with Vanished Phase–Lag and some of its Derivatives for the Numerical Solution of Radial Schrödinger Equation and Related IVPs with Oscillating Solutions

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ARTICLE INFO

Article History:

Received 2 October 2016
Accepted 26 February 2017
Published online 22 March 2017
Academic Editor: Ivan Gutman

Keywords:

Schrödinger equation
Phase–lag
Ordinary differential equations
Symmetric multistep methods.

ABSTRACT

A new two–step implicit linear Obrechkoff twelfth algebraic order method with vanished phase–lag and its first, second, third and fourth derivatives is constructed in this paper. The purpose of this paper is to develop an efficient algorithm for the approximate solution of the one–dimensional radial Schrödinger equation and related problems. This algorithm belongs in the category of the multistep methods. In order to produce an efficient multistep method the phase–lag property and its derivatives are used. An error analysis and a stability analysis are also investigated and a comparison with other methods is also studied. The efficiency of the new methodology is proved via theoretical analysis and numerical applications.

1. INTRODUCTION

The radial time–independent Schrödinger equation can be written as:

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

The boundary conditions are $y(0) = 0$, and a second boundary condition, for large values of x, determined by physical considerations. Large research on the algorithmic development of numerical methods for the solution of the Schrödinger equation has been done in the last decades. The aim and scope of this research is the construction of fast and reliable algorithms for the solution of the Schrödinger equation and related problems.

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DOI: 10.22052/ijmc.2017.62671.1243

Mathematical models in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics etc. can be express via the above boundary value problem [1]. The numerical methods for the approximate solution of the Schrödinger equation and related problems can be divided into two main categories:

1. Methods with constant coefficients.
2. Methods with coefficients depending on the frequency of the problem.

The main result of this paper is the development of an efficient multistep method for the numerical solution of systems of ordinary differential equations with oscillating or periodical solutions. The reason of their efficiency, as the analysis proved, is that the phase–lag and its derivatives are eliminated. Another reason of the efficiency of the new obtained method is that it has high algebraic order. The purpose of this paper is to extend the methodology for the development of numerical methods for the approximate solution periodic initial–value problems. The new methodology is based on the requirement of the phase–lag and its derivatives vanishing. Based on this new methodology we will develop a method one will have phase–lag and its first, second, third and fourth derivatives vanishing. We will apply the new developed method on the numerical solution of the radial Schrödinger equation. We will study the efficiency of the new obtained methods via:

- A comparative error analysis,
- A comparative stability analysis and finally,
- The numerical results produced from the numerical solution of the radial Schrödinger with application to the specific potential.

More specifically, we will develop a family of implicit symmetric two–step Obrechkoff methods of twelfth algebraic order. The development of the new family of methods is based on the requirement of the phase–lag and its first, second, third and fourth derivatives vanishing. We will give a comparative error analysis and a comparative stability analysis in order to study the efficiency of new proposed method of the family. Finally, we will apply both methods to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation.

For several decades, there has been strong interest in searching for better numerical methods to integrate first order and second–order initial value problems, because these problems are usually encountered in celestial mechanics, quantum mechanical scattering theory, theoretical physics and chemistry, and electronics. Computational methods involving a parameter proposed by Gautschi [8], Jain et al. [13] and Steifel and Bettis [24] yield numerical solution of problems of class (1). Chawla et al. [3, 4], Ananthakrishnaiah [1], Shokri and et al. [17, 18,19], Dahlquist [5], Asadzadeh [2], Franco [6], Lambert and Watson [14], Simos and et al. [20, 21, 22], Saldanha and Achar [16], and Daele and Vanden Berghe [26] have developed methods to solve problems of class (2). Consider the class of Obrechkoff methods of the form

$$\sum_{j=0}^{k}\alpha_i y_{n-j+1}=\sum_{i=1}^{l}h^{2i}\sum_{j=0}^{k}\beta_i y^{(2i)}{}_{n-j+1,} \tag{2}$$

for the numerical integration of the problem (1). The method (2) is symmetric when $\alpha_j=\alpha_{k-j},\beta_j=\beta_{k-j}, j=0,1,2,k,$ and it is of order q if the truncation error associated with the linear difference operator is given as

$$TE=C_{q+2}h^{q+2}y^{(q+2)},\quad x_{n-k+1}<\eta<x_{n+1},$$

where C_{q+2} is a constant dependent on h. We have organized the paper as follows: In Section 2 we present the theory of the new methodology. In Section 3 we present the development of the new method. A comparative error analysis is presented in Section 4. Finally, the numerical results are presented in Section 5.

2. PRELIMINARIES

In order to define the interval of periodicity of a method the periodic stability analysis of this method is very important. The interval of periodicity defines the step size which can be used in order the approximation of the solution of problems with high oscillatory or periodic solution to be of the same order as the algebraic order of the method. It can be seen that when we have a large interval of periodicity then we can have a large step size for the same accuracy. To investigate the stability properties of methods for solving the initial value problem (l), Lambert and Watson [14] introduced the scalar test equation. From the form (2) and without loss of generality we assume

$$y''=-\omega^2 y,\quad \omega\in\mathbb{R}. \tag{3}$$

and the interval of periodicity, where w is defined as the frequency of the problem and may be a constant. When we apply a symmetric two–step method to the scalar test equation (3), we obtain a difference equation of the form

$$y_{n+1}-2C(v)y_n+y_{n-1}=0, \tag{4}$$

where $v=\omega h$, h is the step length, $C(v)=B(v)/A(v)$ where $A(v)$ and $B(v)$ are polynomials in v and y_n is the computed approximation to $y(nh), n=0,1,2,\ldots.$ The characteristic equation associated with (4) is

$$\zeta^2-2C(v)\zeta+1=0. \tag{5}$$

We have the following definitions.

Definition 2.1. (See [25]). The method of Eq. (4) with the characteristic Eq. (5) is unconditionally stable if $|\zeta_1| \leq 1$ and $|\zeta_1| \leq 1$ for all values of ωh.

Following Lambert and Watson [14], we say that the numerical method (4) has an interval of periodicity $(0, \nu_0^2)$, if for all $\nu \in (0, \nu_0^2)$, ζ_1 and ζ_2 satisfy $\zeta_1 = \exp(i\theta(\nu))$, and $\zeta_2 = \exp(-i\theta(\nu))$, where $\theta(\nu)$ is a real function of ν. For any method corresponding to the characteristic equation (4) the phase–lag is defined as the leading term in the expansion of

$$t = \nu - \theta(\nu) = \nu - \cos^{-1}[C(\nu)]. \tag{6}$$

If the quantity $t = O(\nu^{q+1})$ as $\nu \to 0$, the order of phase–lag is q.

Definition 2.2. Suppose (5) is the characteristic equation of (4), and

$$|C(\nu)| < 1, \ \forall \nu^2 \in (0, \nu_0^2).$$

Then the periodicity interval of the method is $(0, \nu_0^2)$.

Definition 2.2. The method (4) is said to be P–stable if its interval of periodicity is $(0, \infty)$.

Theorem 2.4. (See Ibraheem and Simos [10]) The phase–lag of a symmetric two–step method with characteristic equation given by (5) is the leading term in the expansion of

$$\frac{[C(\nu) - \cos(\nu)]}{\nu^2}.$$

3. DEVELOPMENT AND ANALYSIS

From the form (2) and without loss of generality we assume

$$\alpha_j = \alpha_{m-j}, \ \beta_{ij} = \beta_{i,m-j}, \quad j = 0(1)\left\lfloor \frac{m}{2} \right\rfloor,$$

and we can write

$$y_{n+1} - 2y_n + y_{n-1} = \sum_{i=1}^{m} h^{2i} \left[\beta_{i0} y_{n+1}^{(2i)} + \beta_{i1} y_n^{(2i)} + \beta_{i0} y_{n-1}^{(2i)} \right] \tag{7}$$

When $m = 3$ we get

$$y_{n+1}-2y_n+y_{n-1}=h^2\left[\beta_{10}(y_{n+1}^{(2)}+y_{n-1}^{(2)})+\beta_{11}y_n^{(2)}\right]$$
$$+h^4\left[\beta_{20}(y_{n+1}^{(4)}+y_{n-1}^{(4)})+\beta_{21}y_n^{(4)}\right] \tag{8}$$
$$+h^6\left[\beta_{30}(y_{n+1}^{(6)}+y_{n-1}^{(6)})+\beta_{31}y_n^{(6)}\right].$$

$M-3$ for method (8) is 11 so that if $P=-1$, $K=13$ we obtain classic method and the coefficients of this method are

$$\beta_{10}=\frac{229}{7788},\quad \beta_{11}=\frac{3665}{3894},\quad \beta_{20}=-\frac{1}{2360},$$
$$\beta_{21}=\frac{711}{12980},\quad \beta_{30}=\frac{127}{39251520},\quad \beta_{31}=\frac{2923}{3925152}, \tag{9}$$

where its phase–lag is given by

$$pl_{clas}=-\frac{45469}{3394722659328000}v^{12}+O\left(v^{14}\right),$$

and its local truncation error is given by

$$LTE_{clas}=-\frac{45469}{1697361329664000}y^{(14)}h^{14}+O(h^{16}).$$

If $P=6$, $K=-1$ then we obtain the method with zero phase–lag (*PL*), and the coefficients of this case are given in [16].

3.1. DEVELOPMENT

Application of the method (8) to the scalar test equation (3) leads to the difference equation (4) with $C\left(v^2\right)$ given by

$$C\left(v^2\right)=\frac{1-\frac{1}{2}\beta_{11}v^2+\frac{1}{2}\beta_{21}v^4-\frac{1}{2}\beta_{31}v^6}{1+\beta_{10}v^2-\beta_{20}v^4+\beta_{30}v^6}. \tag{10}$$

We require the above mentioned method to have the phase–lag and its derivatives vanished. Using the Eq. (10) and Theorem 2.4, and requiring the above method (8) to have the maximum algebraic order with five free parameters, the following relations are obtained:

$$\beta_{10}=\frac{1}{2}-\frac{1}{2}\beta_{11}.$$

So the phase–lag is equal to:

$$PL = \left(\frac{1 - \frac{1}{2}\beta_{11}\nu^2 + \frac{1}{2}\beta_{21}\nu^4 - \frac{1}{2}\beta_{31}\nu^6}{1 + \left(\frac{1}{2} - \frac{1}{2}\beta_{11}\right)\nu^2 - \beta_{20}\nu^4 + \beta_{30}\nu^6} - \cos(\nu) \right) \nu^{-2}.$$

We require the above mentioned method to have the phase–lag and some of its derivatives vanished. Hence we can write

$$PL^{(i)} = 0, \qquad i = 0,1,2,3,4.$$

Demanding the phase–lag and the first, second, third and fourth derivatives of the phase to vanish we can find of all coefficients. For small values of $|\nu|$ in the coefficients, are subject to heavy cancelations. In this case the following Taylor series expansions should be used:

$$\beta_{10} = \frac{229}{7788} + \frac{45469}{262829424}\nu^2 - \frac{24889175}{21492613318176}\nu^4 - \frac{678202459751}{17615223060643802880}\nu^6 + \frac{35019787379195}{1824591850710709359831552}\nu^8 + \frac{51820722922675986337}{197923904285737562600127482880}\nu^{10} + \frac{640261689488085567511}{6219810777417272835646532498841 60}\nu^{12} + \frac{3058314172856870215517779346 69}{1107395005912777954375218934135711425331 2000}\nu^{14} + \ldots$$

$$\beta_{11} = \frac{3665}{3894} - \frac{45469}{131414712}\nu^2 + \frac{24889175}{10746306659088}\nu^4 + \frac{678202459751}{8807611530321901440}\nu^6 - \frac{35019787379195}{9122959253553546799157 76}\nu^8 - \frac{51820722922675986337}{9896195214286878130006374144 00}\nu^{10} - \frac{640261689488085567511}{3109905388708636417823266249420 80}\nu^{12} - \frac{3058314172856870215517779346 69}{5536975029563889771876094670678557126656000}\nu^{14} - \ldots$$

$$\beta_{20} = -\frac{1}{2360} - \frac{45469}{6021183168}\nu^2 - \frac{805517}{58616218140480}\nu^4 + \frac{441092244757}{1345162488267344947 20}\nu^6 + \frac{5333451495777199}{4179974057991806897068646 4}\nu^8 + \frac{1166381440358669133769}{3526644112727687479056816967680 00}\nu^{10} + \frac{7316842853699951008043 3}{1052844333413723819997622137531187200}\nu^{12} + \frac{3739622993011134097210546387 1}{3004272575849498086749995864377743436185 6000}\nu^{14} + \ldots$$

$$\beta_{21} = \frac{711}{12980} - \frac{5228935}{33116507424}v^2 + \frac{47774789}{40298649971580}v^4 + \frac{4726497723443}{147967873709407944192}v^6 - \frac{63080459663327759}{22989857318954937933877552}v^8 - \frac{2330989829190428205673}{3879308524000456226962498664448800}v^{10} - \frac{12281012353250799618959}{629417808019074022824665408306688800}v^{12} - \frac{24686049449918639502839304342 59}{627892968352545100130749135654948378162790400}v^{14} - \ldots$$

$$\beta_{30} = \frac{127}{39251520} + \frac{45469}{305690837760}v^2 + \frac{5624977}{1289556799090560}v^4 + \frac{14566546103957}{1434150160568107766784000}v^6 + \frac{184980240090953987}{919594292758197517355102208000}v^8 + \frac{413134473606494683 49}{119363339200014037752692266598 4000}v^{10} + \frac{22457771382822810779232493}{43777267383342636435501128478546763776000}v^{12} + \frac{20012234957709499586085136211}{32199639402694620519525596700253762982707200 00}v^{14} + \ldots$$

$$\beta_{31} = \frac{2923}{3925152} - \frac{14231797}{1986990445440}v^2 + \frac{26183459}{257911359818112}v^4 - \frac{255261508015541}{93219760436927004840960 0}v^6 + \frac{6643202390908931}{919594292758197517355102208 0}v^8 - \frac{76850454029034531283 7}{77586170480009124539249973288960 00}v^{10} - \frac{28180558345841697211 63}{11520333521932272746184507494354411 52}v^{12} - \frac{33690639270721017064818512 6081}{69765885372505011125638792850549819795865600 00}v^{14} - \ldots$$

hence

$$PL_{New} = \frac{3111088424521982202400032770881498866535237506486999939597}{3706259298416331426189299773058360207161265606188326079161007008732110672782959400000}v^{30},$$

and

$$LTE_{New} = -\frac{45469}{1697361329\ 664000}\left(5\omega^8 y^{(6)} + 10\omega^4 y^{(10)} + 5\omega^2 y^{(12)} + y^{(14)} + 10\omega^6 y^{(8)} + \omega^{10} y^{(4)}\right)h^{14},$$

where $v = \omega h$, ω is the frequency and h is the step length. As $v \to 0$, the LTE of the method (8) with above derived coefficients, tends to

$$\frac{45469}{1697361329664000} h^{14} y^{(14)} + O(h^{16}),$$

which agrees with the LTE of the three methods due to Wang [27], Simos [20] and Daele [26], Achar [1], as $H \to 0$. The characteristic equation

$$\Omega\left(s;\nu^2\right) = A(\nu)s^2 - 2B(\nu)s + A(\nu) = 0$$

has complex roots of unit magnitude when

$$\left|\cos(\theta(\nu))\right| = \left|\frac{B(\nu)}{A(\nu)}\right| < 1,$$

i.e. when $A(\nu)^2 \pm B(\nu) > 0$. Substituting for $A(\nu)$ and $B(\nu)$ for new method, the interval of periodicity of the classical Obrechkoff method, PL′ and PL″ methods [18], the new method when $\nu \to 0$ are obtained [0, 25.2004], [0,408.04], [0, 1428.84] and [0, 6593.44] respectively. The behaviors of the coefficients are given in Figures 1, 2 and 3.

4. COMPARATIVE ERROR ANALYSIS

We will study the following methods:

- The ten–step tenth algebraic order method developed by Quinlan and Tremaine [15] which is indicated as QT10.
- The twelve–step twelfth algebraic order method developed by Quinlan and Tremaine [15] which is indicated as QT12.
- The classical two–step method of the family of methods mentioned in Section 3 of this paper which is indicated as CL2.
- The classical ten–step method of the family of methods mentioned in paragraph 3 of [9] which is indicated as CL10
- The method with vanished phase–lag produced by Alolyan and Simos [10] which is indicated as PF.
- The ten–step predictor–corrector method produced by Shokri [17] which is indicated as PC.
- High phase–lag order trigonometrically fitted two–step Obrechkoff produced by Shokri [18] which is indicated as TFO.
- The method with vanished phase–lag and its first derivative produced by Alolyan and Simos [10] which is indicated as PFDF.
- The ten–step method with phase–lag and its first and second derivatives equal to zero produced by Alolyan and Simos [9] which is indicated as PFDF12.
- The ten–step method with phase–lag and its first, second and third derivatives equal to zero produced by Alolyan and Simos [9] which is indicated as PFDF123.
- The new developed two–step Obrechkoff method with vanished phase–lag and its first, second, third and fourth derivatives obtained in this paper which is indicated as new.

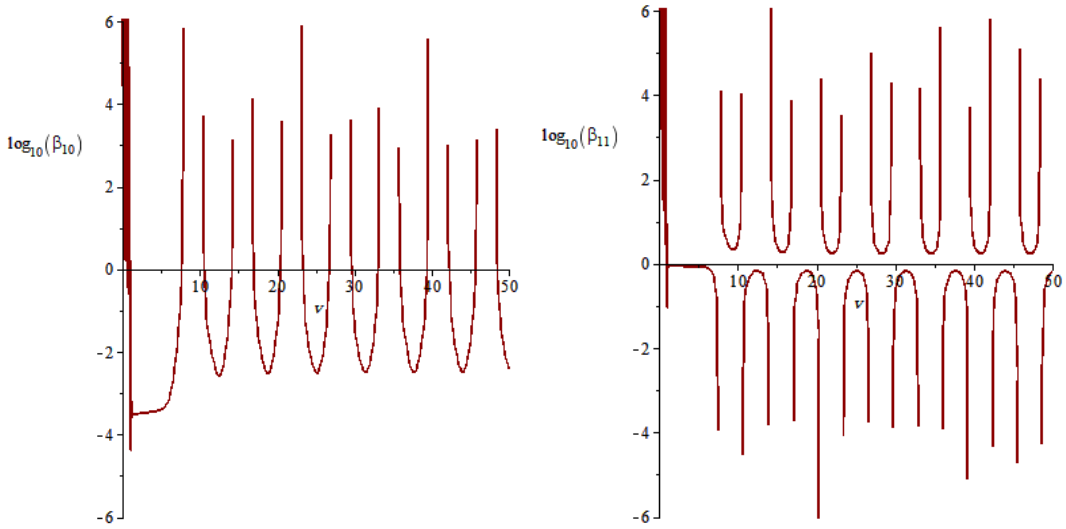

Figure 1: Behavior of the coefficients β_{10} and β_{11} in the new method.

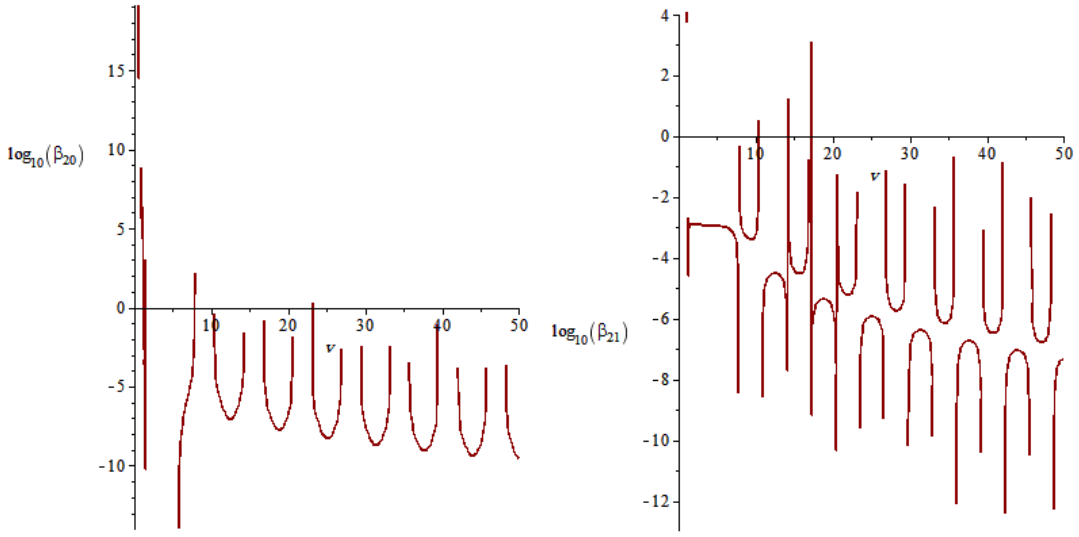

Figure 2: Behavior of the coefficients β_{20} and β_{21} in the new method.

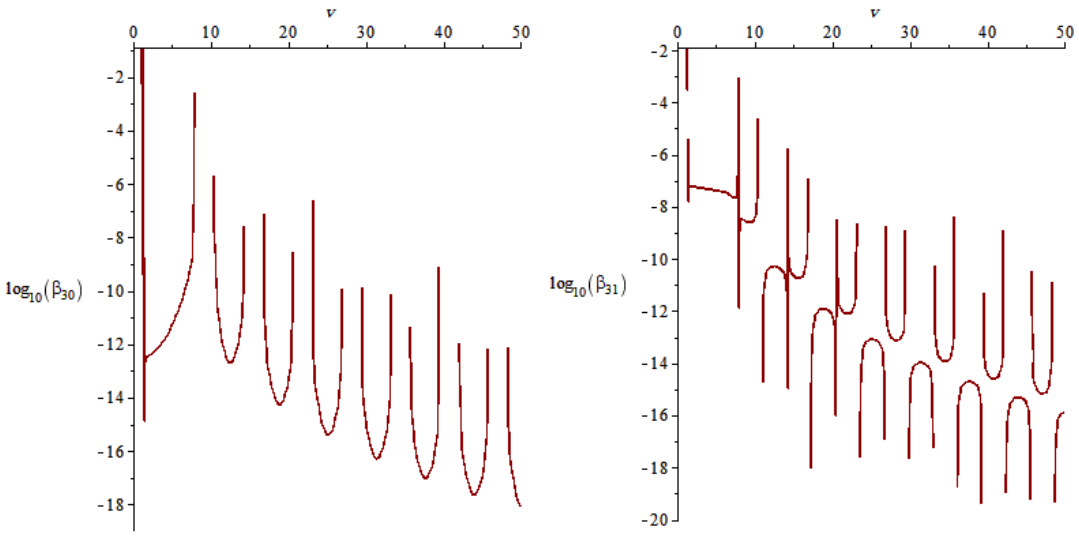

Figure 3: Behavior of the coefficients β_{30} and β_{31} in the new method.

From the above equations we have the following theorem:

Theorem 4.1. For the numerical solution of the time independent radial Schrödinger equation the new proposed method produced in this paper is the most accurate method, especially for large values of $|G|=|V_C - E|$.

Proof. The radial time independent Schrödinger equation is of the form

$$y'' = f(x)y(x) \tag{12}$$

Based on the paper of Ixaru and Rizea [12], the function $f(x)$ can be written in the form $f(x) = g(x) + G$, where $g(x) = V(x) - V_C = g$, and V_C is the constant approximation of the potential and $G = \nu^2 = V_C - E$. We express the derivatives $y_n^{(i)}$, $i = 2,3,4,...$ which are terms of the local truncation error formulae, in terms of Eq. (12). The expressions are presented as polynomials of G. Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae. We use the procedure mentioned above and the formulae:

$$
\begin{aligned}
y_n^{(2)} &= \left(V(x)-V_C+G\right)y(x),\\
y_n^{(4)} &= \left(\frac{d^2}{dx^2}V(x)\right)y(x)+2\left(\frac{d}{dx}V(x)\right)\left(\frac{d}{dx}y(x)\right)+\left(V(x)-V_C+G\right)\left(\frac{d^2}{dx^2}y(x)\right),\\
y_n^{(6)} &= \left(\frac{d^4}{dx^4}V(x)\right)y(x)+4\left(\frac{d^3}{dx^3}V(x)\right)\left(\frac{d}{dx}y(x)\right)+3\left(\frac{d^2}{dx^2}V(x)\right)\left(\frac{d^2}{dx^2y(x)}\right)\\
&\quad +4\left(\frac{d}{dx}V(x)\right)^2 y(x)+6\left(V(x)-V_C+G\right)\left(\frac{d}{dx}V(x)\right)\left(\frac{d}{dx}y(x)\right)\\
&\quad +4\left(V(x)-V_C+G\right)\left(\frac{d^2}{dx^2}V(x)\right)y(x)+\left(V(x)-V_C+G\right)^2\left(\frac{d^2}{dx^2}y(x)\right)
\end{aligned}
\tag{13}
$$

We consider two cases in terms of the value of E:

1. The energy is close to the potential, i.e. $G=V_C-E\approx 0$. So only the free terms of the polynomials in G are considered. Thus for these values of G, the methods are of comparable accuracy. This is because the free terms of the polynomials in G, are the same for the cases of the classical method and of the new developed methods.
2. $G>>$ or $G<<0$. Then $|G|$ is a large number.

So, we have the following asymptotic expansions of the equations produced from the Local Truncation Errors and based on the above procedure:

a. The ten–step tenth algebraic order method developed by Quinlan and Tremaine [15], for the analysis of the local truncation error see [11]

$$LTE_{QT10}=h^{12}\left[-\frac{52559}{912384}y(x)G^6+...\right]. \tag{14}$$

b. The twelve–step twelfth algebraic order method developed by Quinlan and Tremaine [15], for the analysis of the local truncation error see [11]

$$LTE_{QT14}=h^{14}\left[-\frac{16301796103}{290594304000}y(x)G^7+...\right]. \tag{15}$$

c. The classical two–step Obrechkoff method with $m=3$ which is indicated as CL2

$$LTE_{CL2}=h^{14}\left[-\frac{45469}{1697361329664000}y(x)G^7+...\right]. \tag{16}$$

d. The classical ten–step method of the family 1, [9] which is indicated as CL10

$$LTE_{CL10}=h^{14}\left[-\frac{547336457}{373621248000}y(x)G^7+...\right]. \tag{17}$$

e. The method with vanished phase–lag produced by Alolyan and Simos [10] which is indicated as PF

$$LTE_{PF} = h^{14}\left[-\frac{547336457}{373621248000}g(x)y(x)G^{6}+...\right]. \quad (18)$$

f. The ten–step predictor–corrector method produced by Shokri [17] which is indicated as PC

$$LTE_{PC} = h^{14}\left[-\frac{96506469327691}{47345284546560000}g(x)y(x)G^{6}+...\right]. \quad (19)$$

g. High phase–lag order trigonometrically fitted two–step Obrechkoff PL″ produced by Shokri [18] which is indicated as TFO

$$LTE_{TFO} = h^{14}\left[-\frac{45469}{1697361329664000}g(x)y(x)G^{6}+...\right]. \quad (20)$$

h. The method with vanished phase–lag and its first derivative produced by Alolyan and Simos [9] which is indicated as PFDF

$$LTE_{PFDF} = h^{14}\left[\left[\begin{array}{l}\left(-\frac{547336457}{17791488000}\left(\frac{d^{2}}{dx^{2}}g(x)\right)y(x)-\frac{547336457}{373621248000}(g(x))^{2}y(x)\right)\\ +\left(-\frac{547336457}{186810624000}\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}y(x)\right)\end{array}\right]G^{5}+...\right]. \quad (21)$$

i. The method with vanished phase–lag and its first and second derivatives produced by Alolyan and Simos [9] which is indicated as PFDF12.

$$LTE_{PFDF12} = h^{14}\left[-\frac{547336457}{17791488000}\left(\frac{d^{2}}{dx^{2}}g(x)\right)y(x)G^{5}+...\right]. \quad (22)$$

j. The method with vanished phase–lag and its first, second and third derivatives produced by Alolyan and Simos [9] which is indicated as PFDF123.

$$LTE_{PFDF123} = h^{14}\left[\left[\begin{array}{l}\left(-\frac{547336457}{17791488000}\left(\frac{d^{4}}{dx^{4}}g(x)\right)y(x)-\frac{547336457}{373621248000}\left(\frac{d^{3}}{dx^{3}}g(x)\right)\frac{d}{dx}y(x)\right)\\ +\left(-\frac{547336457}{31135104000}\left(\frac{d}{dx}g(x)\right)^{2}y(x)-\frac{547336457}{23351328000}g(x)y(x)\frac{d^{2}}{dx^{2}}g(x)\right)\end{array}\right]G^{4}+...\right]. \quad (23)$$

k. The new two–step Obrechkoff method with phase–lag and its first, second, third and fourth derivatives equal to zero obtained in this paper which is indicated as new:

$$LTE_{New} = h^{14}\left[-\frac{45469}{106085083104000}\left(\frac{d^{4}}{dx^{4}}g(x)\right)y(x)G^{4}+...\right]. \quad (24)$$

Based on the analysis presented above, we studied the interval ofperiodicity of the eight methods mentioned in the previousparagraph. The results are presented in Table 1.

Method	Interval of periodicity
QT10	(0,0.17)
QT12	(0,0.046)
CL2	(0,25.2004)
CL12	(0,0.8)
PF(see [10])	(0,1.2)
PC (see [17])	(0,9.89)
TFO (see PL" in [18])	(0,1428.84)
PFDF (see [9])	(0,1.5)
PFDF12(see [9])	(0,6.6)
PFDF (see [9])	(0,3.6)
New method	(0,65559993.44)

Table 1: Comparative interval of periodicity for the methods mentioned in Section 4.

Hence for the classical two–step Obrechkoff methods, the errorincreases as the seventh power of G. For the classical ten–stepmethods, the error increases as the seventh power of G. For themethod with vanished phase–lag produced by Alolyan and Simos [10], the error increases as the sixth power of G. Forten–step predictor–corrector method produced by Shokri [17], the error increases as the sixth power of G. For two–step twelfthorder Obrechkoff method produced by Shokri [18], the errorincreases as the sixth power of G. For twelfth order method with vanished phase–lag and its first derivative produced by Alolyan and Simos [9], the error increases as the fifth power of G. For ten-step twelfth order method with vanished phase–lag and its firstand second derivatives produced by Alolyan and Simos [9], theerror increases as the fifth power of G. For ten–step twelfthorder method with vanished phase–lag and its first, second and thirdderivatives produced by Alolyan and Simos [9], the errorincreases as the fourth power of G. For the new two–step Obrechkoff method with vanished phase–lag and its first, second,third and fourth derivatives obtained in this paper, the errorincreases as the fourth power of G but it has lower coefficientsthan the method developed in [9]. So, for the numericalsolution of the time–independent radial Schrödinger equation thenew obtained two–step Obrechkoff method with vanished phase–lag andits derivatives is the most accurate ones, especially for largevalues of $|G| = |V_C - E|$. ■

Remark 4.2. In Figures 4, 5, we present the $s - \nu$ plane and behavior of stability polynomial (respectively) for the method developed in this paper (s is frequency of test problem and ν is frequency of method).

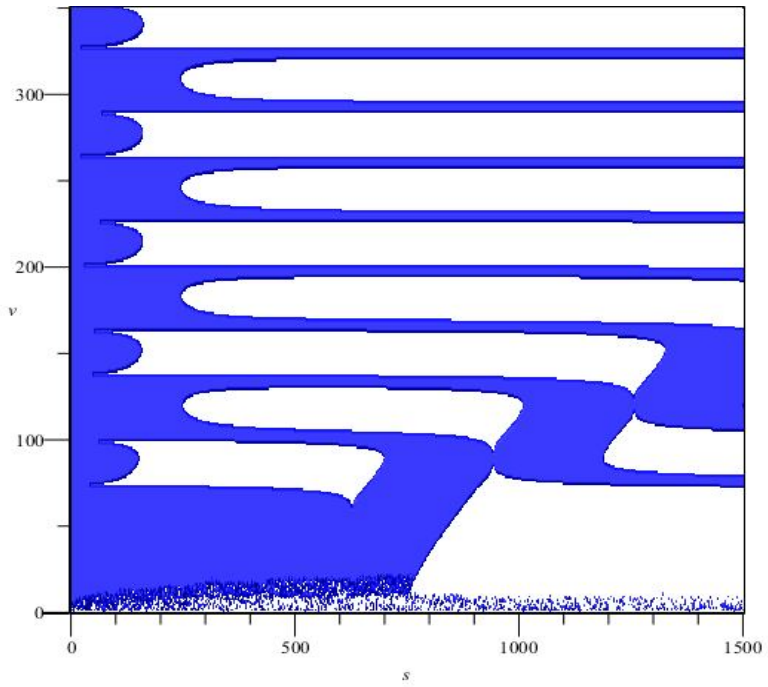

Figure 4: The stability region for the new method.

For the solution of the Schrödinger equation the frequency of the exponential fitting is equal to the frequency of the scalar test equation. So, it is necessary to observe the surroundings of the first diagonal of the $s-v$ plane.

5. NUMERICAL RESULTS

5.1 THE METHODS

We have used several multistep methods for the integration of the five test problems. These methods are

- The ten–step tenth algebraic order method developed by Quinlan and Tremaine [15] which is indicated as Method I.
- The twelve–step twelfth algebraic order method developed by Quinlan and Tremaine [15] which is indicated as Method II.
- The ten–step method with phase–lag and its first and second derivatives equal to zero obtained in [9] which is indicated as Method III.
- The ten–step method with phase–lag and its first, second and third derivatives equal to zero obtained in [9] which is indicated as Method IV.
- The ten–step predictor–corrector method produced by Shokri [17], which is indicated as Method V.

- The new method obtained in this paper which is indicated as VI.

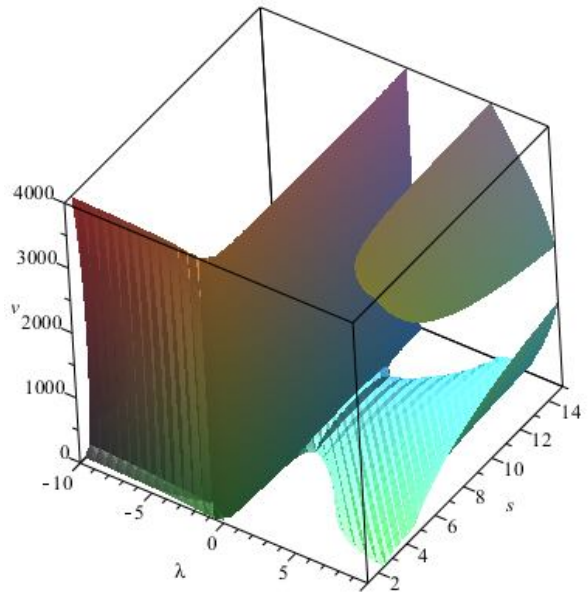

Figure 5: Behavior of the stability polynomial for the new method.

5.2. THE PROBLEMS

The efficiency of the new symmetric two–step Obrechkoff method will be measured through the integration of five initial value problems with oscillating solution. In order to apply the new method to the radial Schrödinger equation the value of parameter ω is needed. For every problem of the one-dimensional Schrödinger equation given by (1) the parameter ω is given by

$$\omega = \sqrt{|q(x)|} = \sqrt{|V(x) - E|}\,, \tag{25}$$

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

Example 5.1. We consider the Schrödinger equation resonance problem. We will integrate problem (1) with $l = 0$ at the interval $[0,15]$ using the well–known Woods–Saxon potential

$$V(x) = \frac{u_0}{(1+q)} + \frac{u_1 q}{(1+q)^2}, \qquad q = \exp\left(\frac{x - x_0}{a}\right),$$

where $u_0 = 50$, $a = 0.6$, $x_0 = 7$, $u_1 = -\dfrac{u_0}{a}$. The behavior of the Woods–Saxonpotential is shown in Figure 6 and with boundary condition $y(0) = 0$. The potential $V(x)$ decays more

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

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

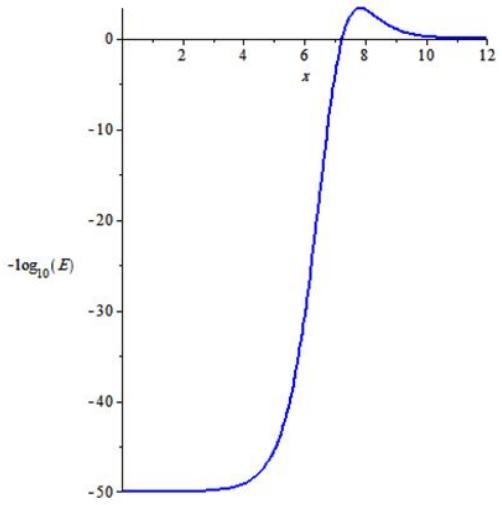

Figure 6: The Woods-Saxon potential.

The last equation has two linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where j_l and n_l are the spherical Bessel and Neumann functions respectively. When $x \to \infty$ thesolution of Schrödinger has the asymptotic form

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

where δ_l is called *scattering phase shift* and it iscalculated by the following expression:

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

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

We will use for the energy the value $E = 989.701916$. For some well–known potentials, such as the Woods–Saxon potential, the definition of parameter ω is not given as a function of x but based on some critical points which have been defined from the

study of the appropriate potential (see for details [12]). For the purpose of obtaining our numerical results it is appropriate to choose ω as follows (see for details [12]):

$$\omega = \begin{cases} \sqrt{E+50} & , \quad x \in [0,6.5], \\ \sqrt{E} & , \quad x \in [6.5,15]. \end{cases}$$

Example 5.2. The almost periodic orbital problem studied by Franco and Palacios [7], can be described by

$$y''+y = \varepsilon \exp(i\psi x), \qquad y(0)=1, \quad y'(0)=i, \quad y \in C$$

or equivalently by

$$\begin{cases} u''+u = \varepsilon \cos(i\psi x), & u(0)=1, \quad u'(0)=0 \\ v''+v = \varepsilon \sin(\psi x), & u(0)=0, \quad v'(0)=1 \end{cases}$$

where $\varepsilon = 0.001$ and $\psi = 0.01$. The theoretical solution of this problem is given by

$$y(x) = u(x) + iv(x), \qquad x \in R, \tag{26}$$

where

$$u(x) = \frac{1-\varepsilon-\psi^2}{1-\psi^2}\cos(x) + \frac{\varepsilon}{1-\psi^2}\cos(\psi x),$$

$$v(x) = \frac{1-\varepsilon\psi-\psi^2}{-\psi^2}\sin(x) + \frac{\varepsilon}{1-\psi^2}\sin(\psi x).$$

This system of equations has been solved for $x \in [0,1000\pi]$. For this problem we use $\omega = 1$.

Example 5.3. The almost periodic orbital problem studied by **Stiefel and Bettis** [24], can be described by

$$y''+y = 0.001\exp(ix), \qquad y(0)=1, \quad y'(0)=0.9995i, \quad y \in C$$

or equivalently by

$$\begin{cases} u''+u = 0.001\cos(\psi x), & u(0)=1, \quad u'(0)=0, \\ v''+v = 0.001\sin(\psi x), & u(0)=0, \quad v'(0)=0.9995i. \end{cases}$$

The theoretical solution of this problem is given by $y(x) = u(x) + iv(x)$, $u, v \in R$ and

$$u(x) = \cos(x) + 0.0005\cos(x),$$

$$v(x) = \sin(x) + 0.0005x\cos(x).$$

This system of equations has been solved for $x \in [0,1000\pi]$. For this problem we use $\omega = 1$.

Example 5.4. (**Inhomogeneous Equation**) Consider the initial value problem

$$y'' = -100y + 99\sin(x), \qquad y(0)=1, \qquad y'(0)=11, \qquad t \in [0,1000\pi].$$

With the exact solution $y(t) = \sin(t) + \sin(10t) + \cos(10t)$. For this problem we use $\omega = 1$.

Example 5.5. We consider the nonlinear undamped **Duffing equation**

$$y'' = -y - y^3 + B\cos(\omega x), \qquad y(0) = 0.200426728067, \quad y'(0) = 0, \tag{12}$$

where $B = 0.002$, $\omega = 1.01$ and $x \in \left[0, \frac{40.5\pi}{1.01}\right]$. We use the following exact solution for (27), from [23],

$$g(x) = \sum_{i=0}^{3} K_{2i+1} \cos((2i+1)\omega x),$$

where $\{K_1, K_3, K_5, K_7\} = \{0.200179477536, 0.246946143 \times 10^{-3}, 0.304016 \times 10^{-6}, 0.374 \times 10^{-9}\}$.

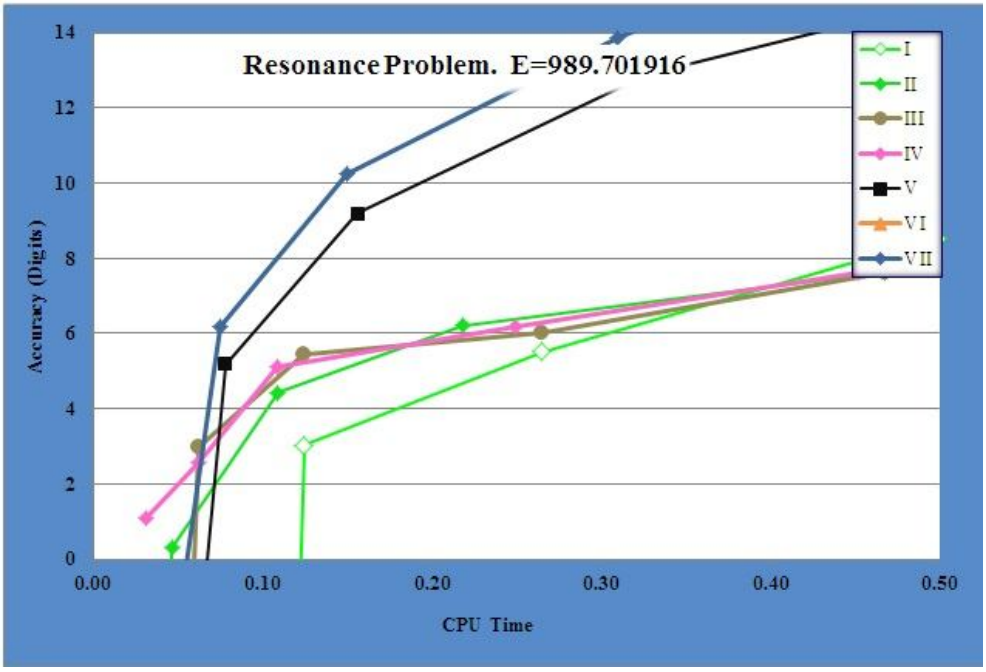

Figure 7: Efficiency for the resonance problem using E = 989:701916.

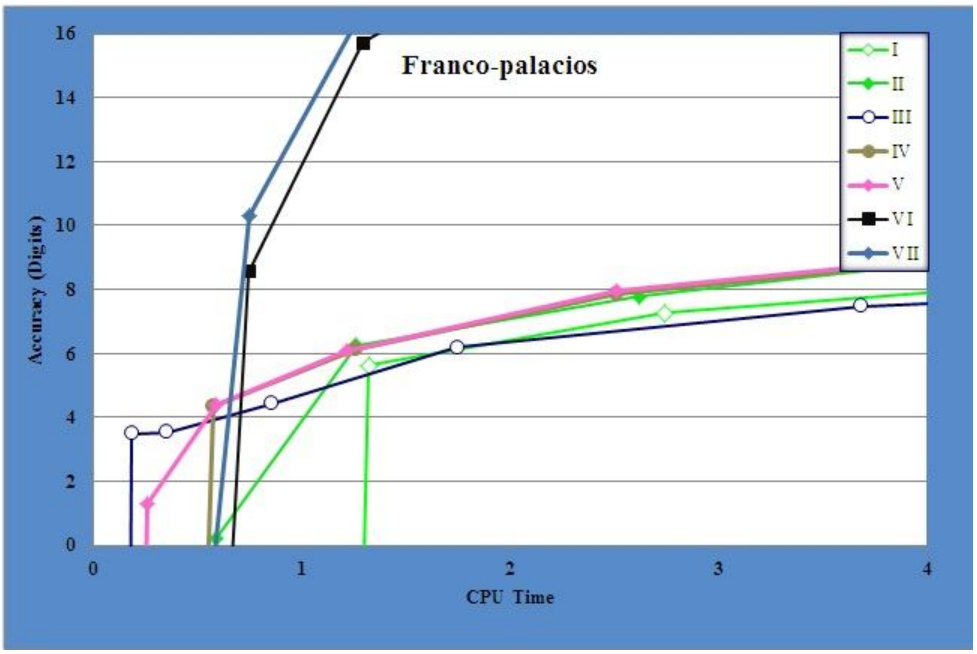

Figure 8: Efficiency for the Franco and Palacios equation.

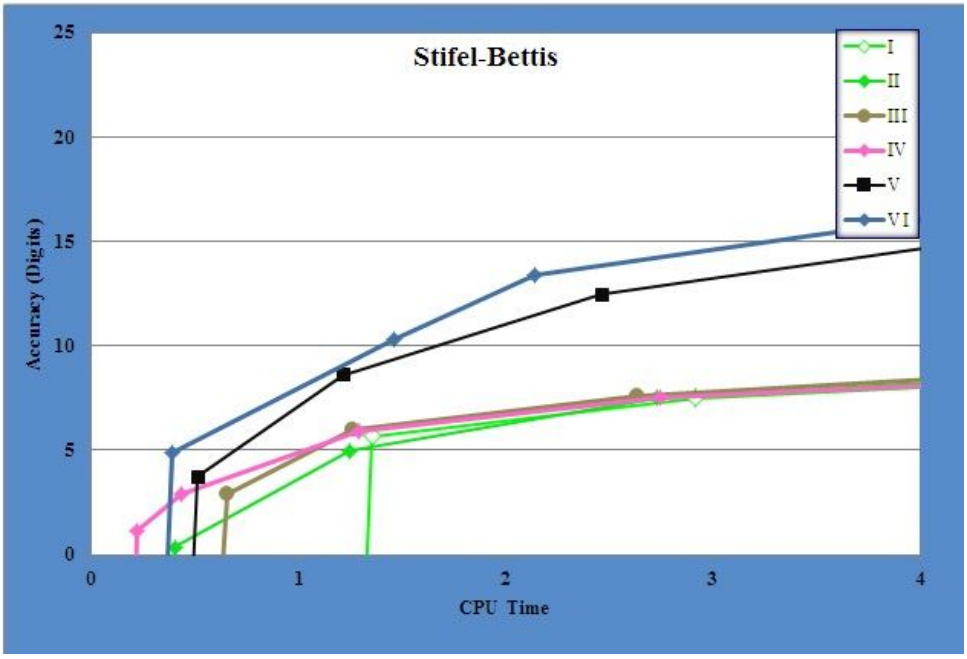

Figure 9: Efficiency for the orbital problem by Stiefel and Bettis.

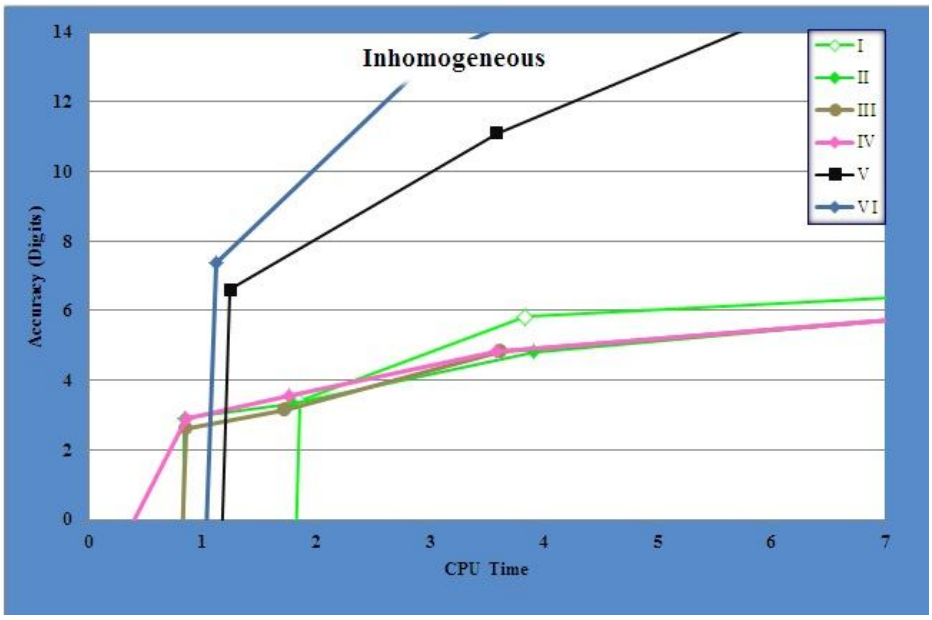

Figure 10: Efficiency for the inhomogeneous equation.

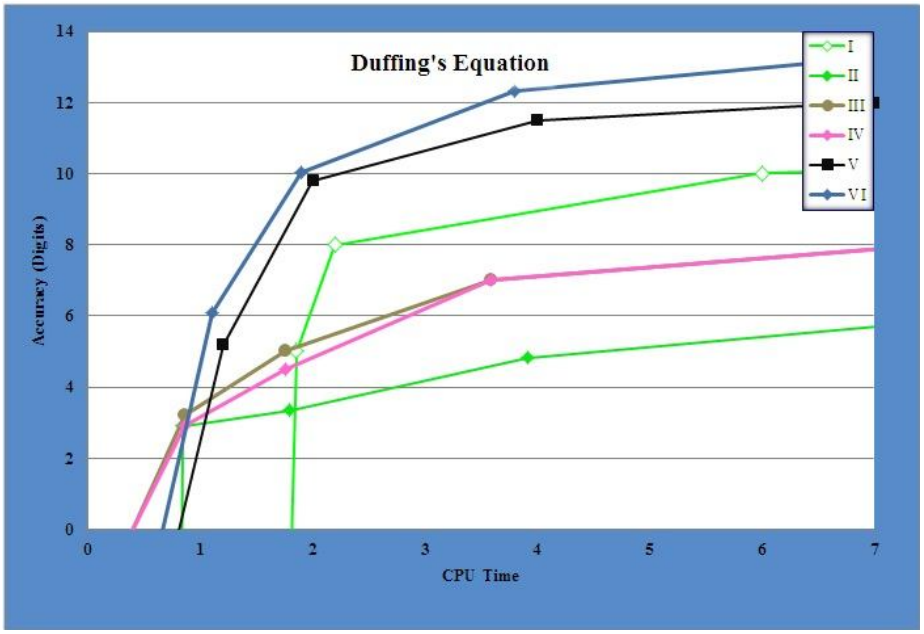

Figure 11: Efficiency for the Duffing Equation.

4. CONCLUSIONS

In Figure 7, we see the results for the resonance problem for energy $E = 989.495874$. In Figure 8, we see the results for the Franco–Palacios almost periodic problem, in Figure 9, the results for the Stiefel–Bettis almost periodic problem are present, in Figure 10, the results for the inhomogeneous equation are present and finally in Figure 11, we see the results for the Duffing equation.

Among all the methods used the new symmetric two–step Obrechkoff method with twelfth algebraic order and vanished some of its derivatives was the most efficient.

Acknowledgments. The authors wish to thank the anonymous referees for their careful reading of the manuscript and their fruitful comments and suggestions.

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