

# ***A New Two–Step Obrechhoff 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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## **ABSTRACT**

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A new two–step implicit linear Obrechhoff 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.

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## **1. INTRODUCTION**

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

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

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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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 Obrechhoff 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], Ananthkrishnaiah [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 Obrechhoff methods of the form

$$\sum_{j=0}^k \alpha_j y_{n-j+1} = \sum_{i=1}^l h^{2i} \sum_{j=0}^k \beta_j y_{n-j+1}^{(2i)}, \quad (2)$$

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 (1), Lambert and Watson [14] introduced the scalar test equation. From the form (2) and without loss of generality we assume

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

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

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

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  $y(nh)$ ,  $n = 0, 1, 2, \dots$ . The characteristic equation associated with (4) is

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

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  $|\zeta_2| \leq 1$  for all values of  $\omega h$ .

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

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

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

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

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

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

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

and we can write

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

When  $m = 3$  we get

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

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

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

where its phase-lag is given by

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

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  $C(v^2)$  given by

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

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:

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

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

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

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  $|v|$  in the coefficients, are subject to heavy cancelations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} \beta_{10} = & \frac{229}{7788} + \frac{45469}{262829424}v^2 - \frac{24889175}{21492613318176}v^4 - \frac{678202459751}{17615223060643802880}v^6 \\ & + \frac{35019787379195}{1824591850710709359831552}v^8 + \frac{51820722922675986337}{1979239042857375626001274828800}v^{10} \\ & + \frac{640261689488085567511}{621981077741727283564653249884160}v^{12} \\ & + \frac{305831417285687021551777934669}{11073950059127779543752189341357114253312000}v^{14} + \dots \end{aligned}$$

$$\begin{aligned} \beta_{11} = & \frac{3665}{3894} - \frac{45469}{131414712}v^2 + \frac{24889175}{10746306659088}v^4 + \frac{678202459751}{8807611530321901440}v^6 \\ & - \frac{35019787379195}{91229592535354679915776}v^8 - \frac{51820722922675986337}{989619521428687813000637414400}v^{10} \\ & - \frac{640261689488085567511}{310990538870863641782326624942080}v^{12} \\ & - \frac{305831417285687021551777934669}{5536975029563889771876094670678557126656000}v^{14} - \dots \end{aligned}$$

$$\begin{aligned} \beta_{20} = & -\frac{1}{2360} - \frac{45469}{6021183168}v^2 - \frac{805517}{58616218140480}v^4 + \frac{441092244757}{134516248826734494720}v^6 \\ & + \frac{5333451495777199}{41799740579918068970686464}v^8 + \frac{1166381440358669133769}{352664411272768747905681696768000}v^{10} \\ & + \frac{73168428536999510080433}{1052844333413723819997622137531187200}v^{12} \\ & + \frac{37396229930111340972105463871}{30042725758494980867499958643777434361856000}v^{14} + \dots \end{aligned}$$

$$\beta_{21} = \frac{711}{12980} - \frac{5228935}{33116507424}v^2 + \frac{47774789}{40298649971580}v^4 + \frac{4726497723443}{147967873709407944192}v^6$$

$$- \frac{63080459663327759}{229898573189549379338775552}v^8 - \frac{2330989829190428205673}{387930852400045622696249866444800}v^{10}$$

$$- \frac{12281012353250799618959}{62941780801907402282466540830668800}v^{12}$$

$$- \frac{2468604944991863950283930434259}{627892968352545100130749135654948378162790400}v^{14} - \dots$$

$$\beta_{30} = \frac{127}{39251520} + \frac{45469}{305690837760}v^2 + \frac{5624977}{1289556799090560}v^4 + \frac{14566546103957}{143415016056810776678400}v^6$$

$$+ \frac{184980240090953987}{91959429275819751735510220800}v^8 + \frac{41313447360649468349}{1193633392000140377526922665984000}v^{10}$$

$$+ \frac{22457771382822810779232493}{43777267383342636435501128478546763776000}v^{12}$$

$$+ \frac{20012234957709499586085136211}{3219963940269462051952559670025376298270720000}v^{14} + \dots$$

$$\beta_{31} = \frac{2923}{3925152} - \frac{14231797}{1986990445440}v^2 + \frac{26183459}{257911359818112}v^4 - \frac{255261508015541}{932197604369270048409600}v^6$$

$$+ \frac{6643202390908931}{9195942927581975173551022080}v^8 - \frac{768504540290345312837}{7758617048000912453924997328896000}v^{10}$$

$$- \frac{2818055834584169721163}{1152033352193227274618450749435441152}v^{12}$$

$$- \frac{336906392707210170648185126081}{6976588537250501112563879285054981979586560000}v^{14} - \dots$$

hence

$$PL_{New} = \frac{31110884252198220240000327708149886656237506486999939597}{3706259298163314268929977306836020716126560618326079160070087321067278299400000}v^{30},$$

and

$$LTE_{New} = -\frac{45469}{1697361329664000} \left( 5\omega^8 y^{(6)} + 10\omega^4 y^{(10)} + 5\omega^2 y^{(12)} + y^{(14)} + 10\omega^6 y^{(8)} + \omega^{10} y^{(4)} \right) h^{14},$$

where  $\nu = \omega h$ ,  $\omega$  is the frequency and  $h$  is the step length. As  $\nu \rightarrow 0$ , 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  $H \rightarrow 0$ . The characteristic equation

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

has complex roots of unit magnitude when

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

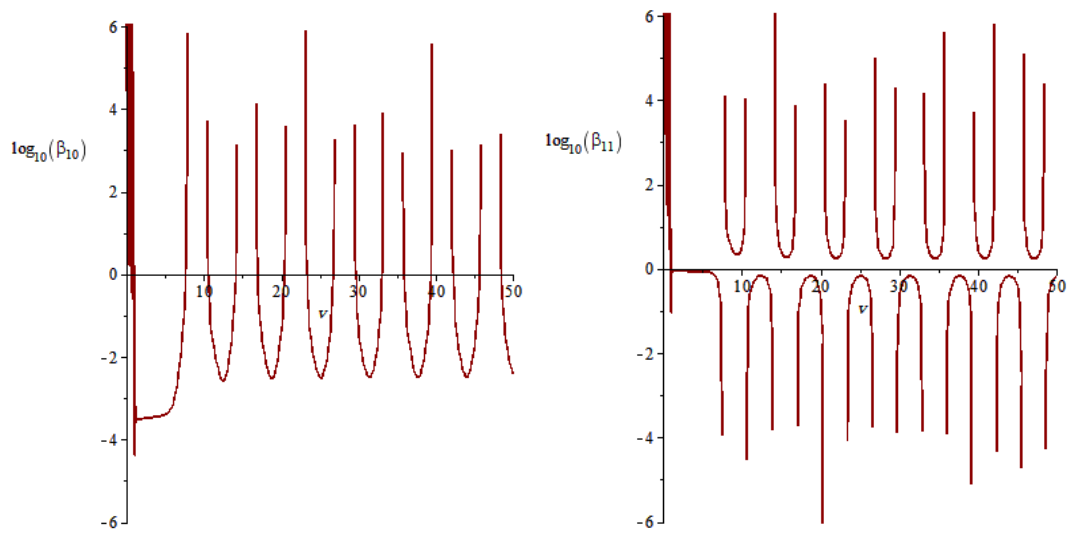
i.e. when  $A(\nu)^2 \pm B(\nu) > 0$ . Substituting for  $A(\nu)$  and  $B(\nu)$  for new method, the interval of periodicity of the classical Obrechhoff method, PL' and PL'' methods [18], the new method when  $\nu \rightarrow 0$  are obtained [0, 25.2004], [0,408.04], [0, 1428.84] and [0, 6593.44] respectively.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

#### 4. COMPARATIVE ERROR ANALYSIS

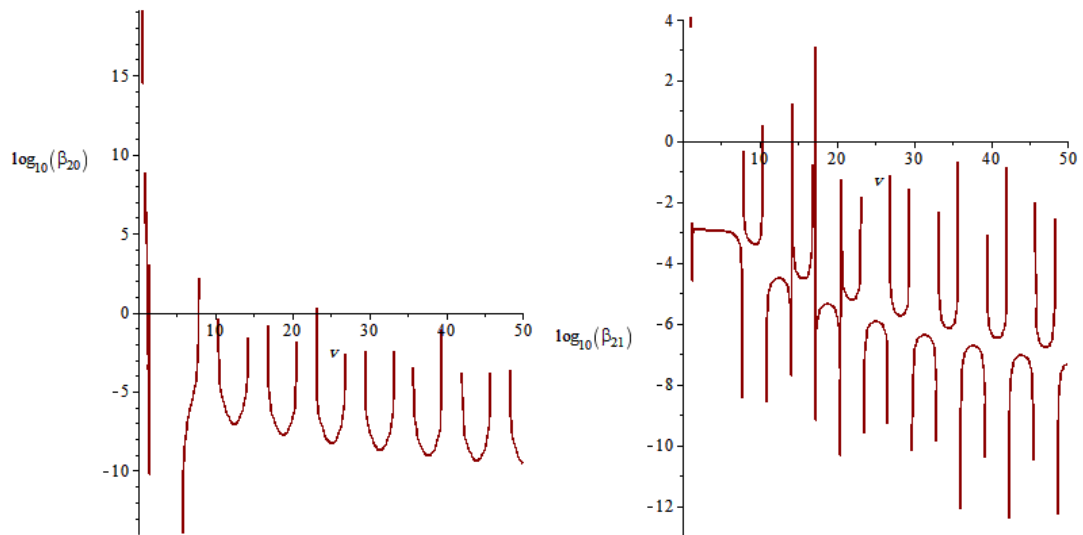
We will study the following methods:

- 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 Obrechhoff 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 Obrechhoff method with vanished phase-lag and its first, second, third and fourth derivatives obtained in this paper which is indicated as new.

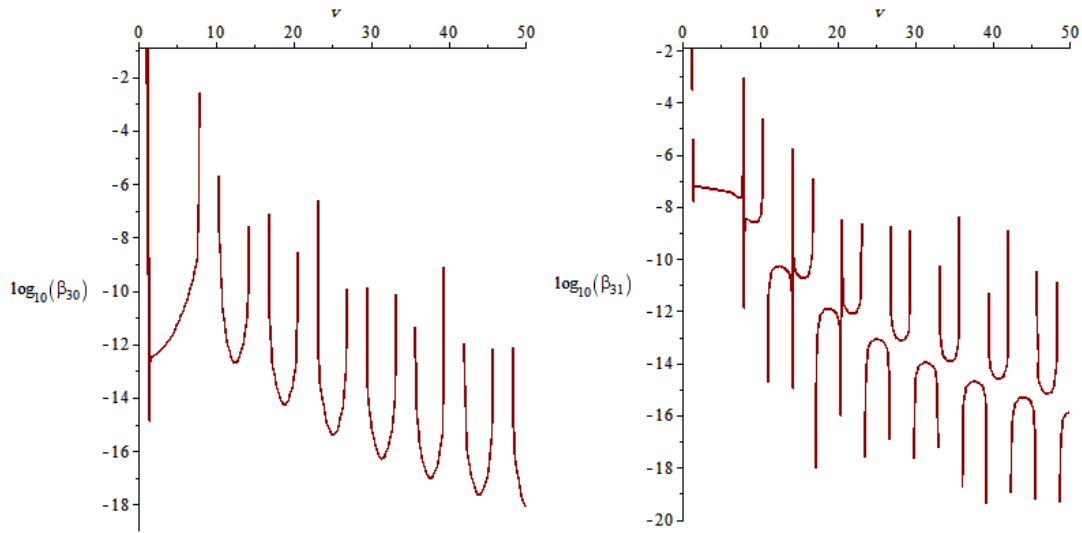




**Figure 1:** Behavior of the coefficients  $\beta_{10}$  and  $\beta_{11}$  in the new method.



**Figure 2:** Behavior of the coefficients  $\beta_{20}$  and  $\beta_{21}$  in the new method.



**Figure 3:** Behavior of the coefficients  $\beta_{30}$  and  $\beta_{31}$  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

$$y'' = f(x)y(x) \quad (12)$$

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  $y_n^{(i)}$ ,  $i = 2, 3, 4, \dots$  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:

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

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.  $G \gg$  or  $G \ll 0$ . 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]

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

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

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

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

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

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

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

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

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

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

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

- g. High phase-lag order trigonometrically fitted two-step Obrechhoff PL'' produced by Shokri [18] which is indicated as TFO

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

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

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

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

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

- 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.

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

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

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

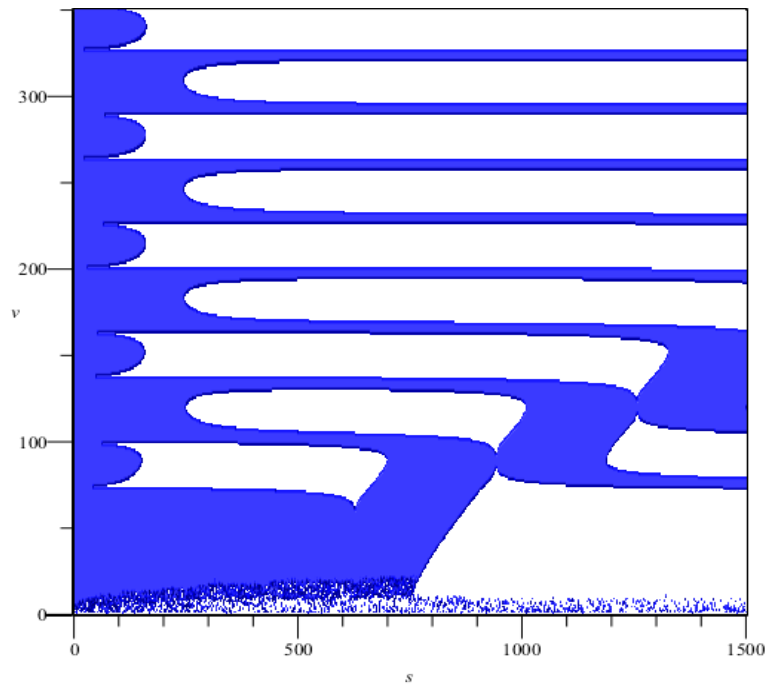
Based on the analysis presented above, we studied the interval of periodicity of the eight methods mentioned in the previous paragraph. The results are presented in Table 1.

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 Obrechhoff methods, the error increases as the seventh power of  $G$ . For the classical ten-step methods, the error increases as the seventh power of  $G$ . For the method with vanished phase-lag produced by Alolyan and Simos [10], the error increases as the sixth power of  $G$ . For ten-step predictor-corrector method produced by Shokri [17], the error increases as the sixth power of  $G$ . For two-step twelfth order Obrechhoff method produced by Shokri [18], the error increases 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 first and second derivatives 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 first, second and third derivatives produced by Alolyan and Simos [9], the error increases as the fourth power of  $G$ . For the new two-step Obrechhoff method with vanished phase-lag and its first, second, third and fourth derivatives obtained in this paper, the error increases as the fourth power of  $G$  but it has lower coefficient than the method developed in [9]. So, for the numerical solution of the time-independent radial Schrödinger equation the new obtained two-step Obrechhoff method with vanished phase-lag and its derivatives is the most accurate ones, especially for large values of  $|G| = |V_c - E|$ . ■

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

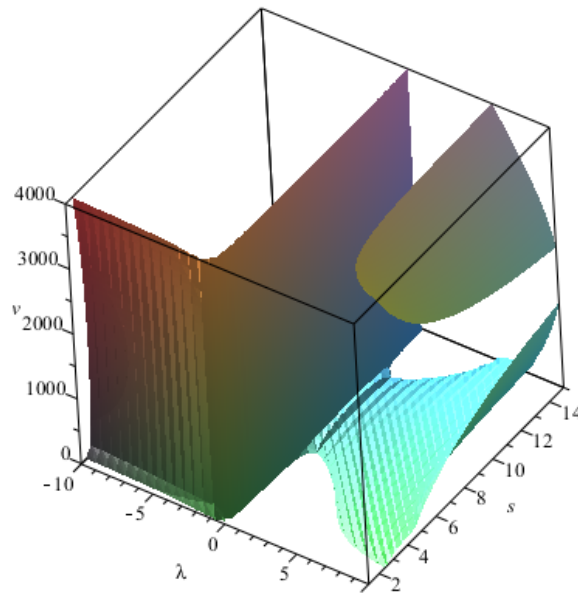
## 5. NUMERICAL RESULTS

### 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 Obrechhoff 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  $\omega$  is needed. For every problem of the one-dimensional Schrödinger equation given by (1) the parameter  $\omega$  is given by

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

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

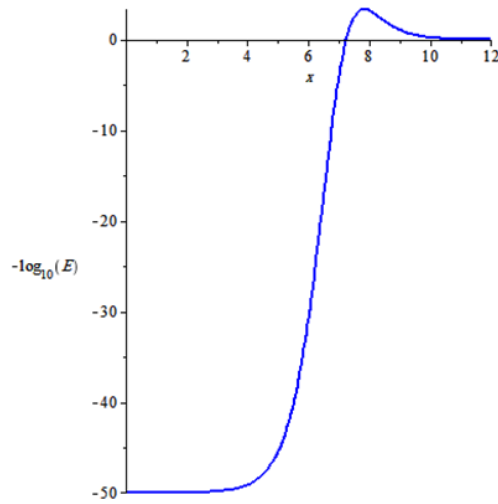
**Example 5.1.** We consider the Schrödinger equation resonance problem. We will integrate problem (1) with  $l = 0$  at the interval  $[0,15]$  using the well-known Woods-Saxon potential

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

where  $u_0 = 50$ ,  $a = 0.6$ ,  $x_0 = 7$ ,  $u_1 = -\frac{u_0}{a}$ . The behavior of the Woods-Saxon potential 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  $x \rightarrow \infty$  the solution 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  $\delta_l$  is called *scattering phase shift* and it is calculated 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 the phase 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  $\omega$  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  $\omega$  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

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

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

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

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

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

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

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

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

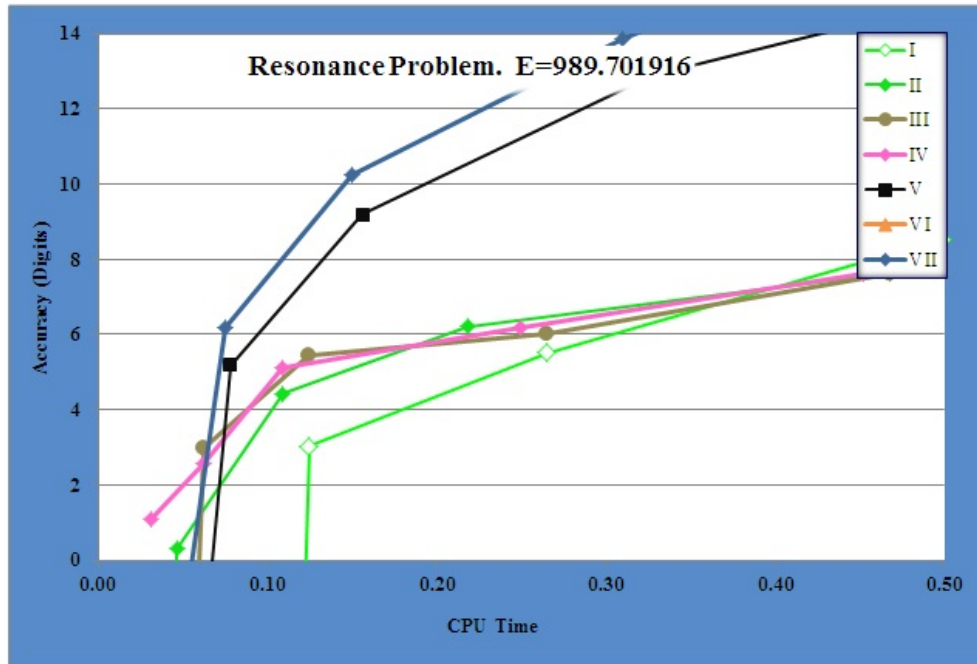
**Example 5.5.** We consider the nonlinear undamped **Duffing equation**

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

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  $E = 989:701916$ .

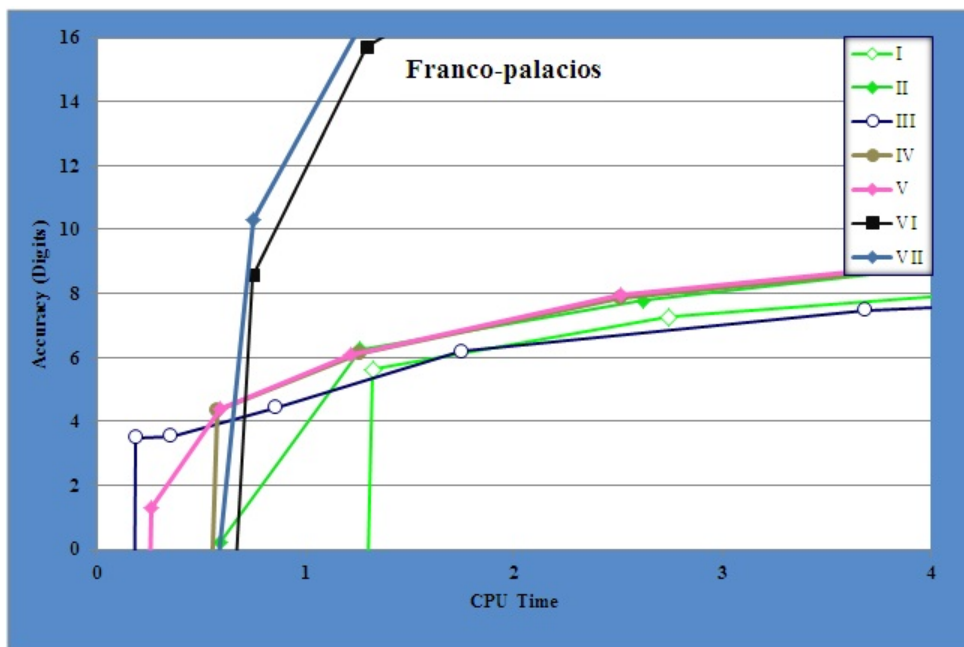


Figure 8: Efficiency for the Franco and Palacios equation.

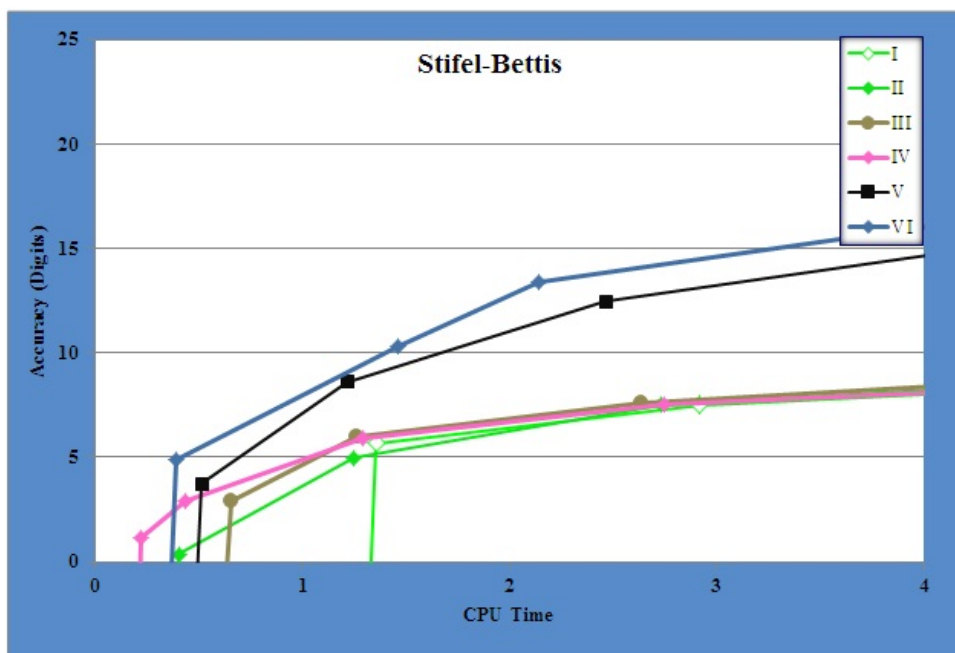


Figure 9: Efficiency for the orbital problem by Stiefel and Bettis.

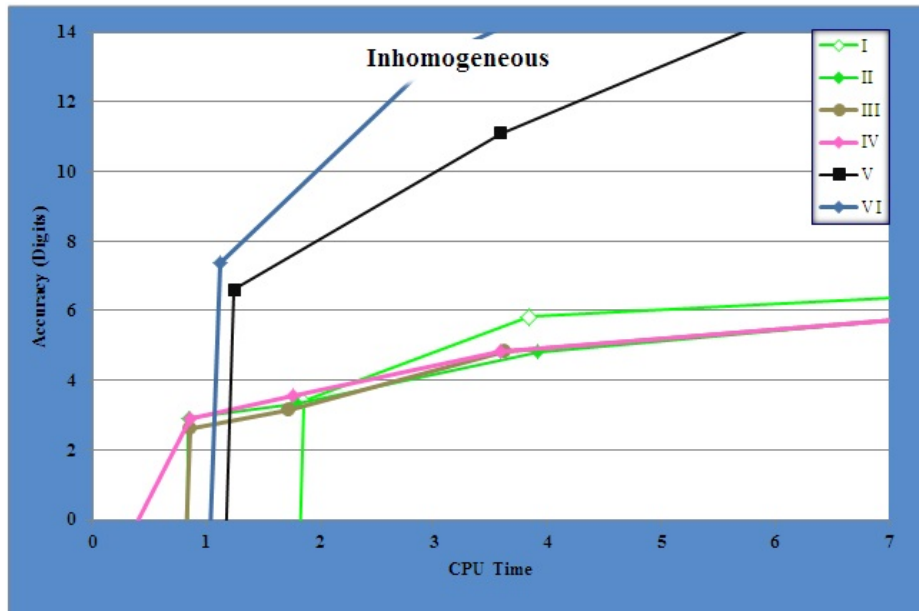


Figure 10: Efficiency for the inhomogeneous equation.

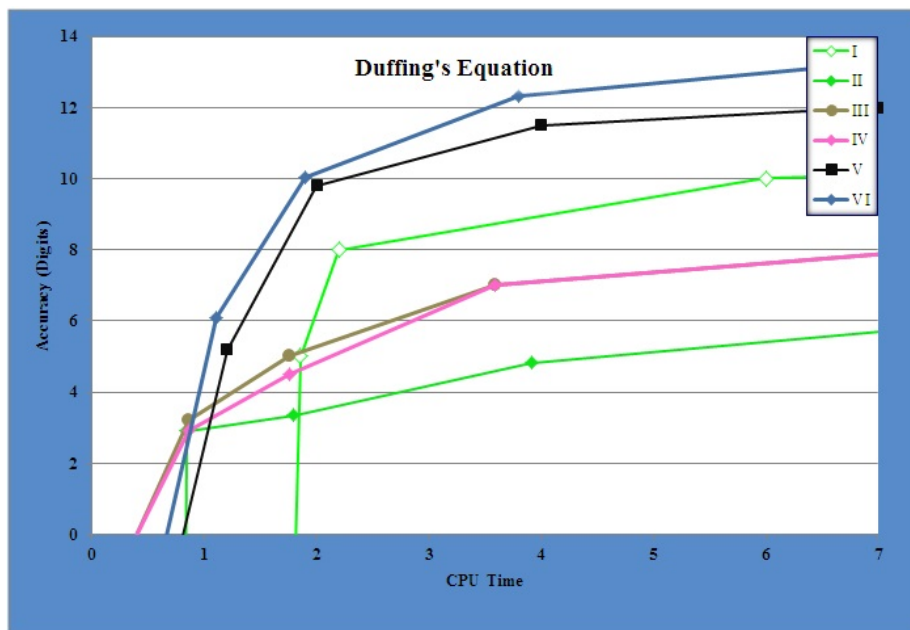


Figure 11: Efficiency for the Duffing Equation.

## 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 Obrechhoff method with twelfth algebraic order and vanished some of its derivatives was the most efficient.

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