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ORIGINAL PAPER

Trigonometrically fitted high-order predictor–corrector method with phase-lag of order infinity for the numerical solution of radial Schrödinger equation

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Abstract In this paper, we present a new optimized symmetric ten-step predictor–corrector method with phase-lag of order infinity (phase-fitted). The method is based on the symmetric eight-step predictor–corrector method of Simos and et al, that is constructed to solve numerically the radial Schrödinger equation during the resonance problem with the use of the Woods–Saxon potential. It can also be used to integrate related IVPs with oscillating solutions such as orbital problems. We compare the new method to some recently constructed optimized methods from the literature. We measure the efficiency of the methods and conclude that the new method with infinite order of phase-lag is the most efficient of all the compared methods and for all the problems solved.

Keywords Orbital problems · Phase-lag · Initial value problems · Oscillating solution · Predictor–corrector · Symmetric multistep methods

1 Introduction

The radial time-independent Shorödinger equation can be written as

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

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where $\frac{l(l+1)}{x^2}$ is the centrifugal potential, $V(x)$ is the potential, E is the energy and $W(x) = \frac{l(l+1)}{x^2} + V(x)$ is the effective potential. It is valid that $\lim_{x\to\infty} V(x) = 0$ and therefore $\lim_{x\to\infty} W(x) = 0$. We consider $E > 0$ and divide $[0, \infty)$ into subintervals $[a_i, b_i)$ so that $W(x)$ is a constant with value $\overline{W}$. After this the problem (1) can be expressed by the approximation:

$$y_i'' = (\overline{W} - E)y_i,$$

whose theoretical solution is

$$y_i = A_i \exp(\sqrt{\overline{W} - E}x) + B_i \exp(\sqrt{\overline{W} - E}\, x), \quad A_i,\ B_i \in \mathbb{R},$$

Many numerical methods have been developed for the efficient solution of the Schrödinger equation and related problems [1–27,35–54,58–90]. For example Simos et al. [44], developed a symmetric eight-step predictor–corrector method of tenth algebraic order, Raptis and Allison have developed a two-step exponentially-fitted method of order four [50]. More recently Kalogiratou and Simos have constructed a two-step P-stable exponentially-fitted method of order four [22]. Some other notable multistep methods for the numerical solution of oscillating IVPs have been developed by Chawla and Rao [10], who produced a three-stage, two-step P-stable method with minimal phase-lag and order six and by Henrici [16], who produced a four-step symmetric method of order six. Also Anastassi and Simos have developed trigonometrically fitted six-step symmetric methods in [6]. In [49,75–78,82,86,87] some new multistep methods of several orders are developed for the numerical solution of Schrödinger equation by Vigo-Aguiar and et al. In [30–83] detailed reviews of the current research on the subject of this paper is presented.

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \tag{2}$$

multistep methods of the form

$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}), \tag{3}$$

with m steps can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a, b]$ and $h := |x_{i+1} - x_i|, \quad i = 0(1)m-1$.

If the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}, \quad i = 0(1)\lfloor \frac{m}{2} \rfloor$. Method (3) is associated with the operator

$$L(x) = \sum_{i=0}^{m} a_i\, u(x + ih) = h^2 \sum_{i=0}^{m} b_i\, u''(x + ih), \tag{4}$$

where $u \in \mathbb{C}^2$.

Definition 2.1 The multistep method (3) is called algebraic of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{p-1}$.

When a symmetric $2k$-step method, that is for $i = -k\,(1)\,k$, is applied to the scalar test equation

$$y'' = -\omega^2 y, \tag{5}$$

a difference equation of the form

$$A_k(\nu)y_{n+k} + \cdots + A_1(\nu)y_{n+1} + A_0(\nu)y_n + A_1(\nu)y_{n1} + \cdots + A_k(\nu)y_{nk} = 0, \tag{6}$$

is obtained, where $\nu = \omega h$, h is the step length and $A_0(\nu), A_1(\nu), \ldots, A_k(\nu)$ are polynomials of ν. The characteristic equation associated with (6) is

$$A_k(\nu)s^k + \cdots + A_1(\nu)s + A_0(\nu) + A_1(\nu)s^{-1} + \cdots + A_k(\nu)s^{-k} = 0. \tag{7}$$

From Lambert and Watson [29] we have the following definitions.

Definition 2.2 A symmetric $2k$-step method with characteristic equation given by (7) is said to have an interval of periodicity $(0, \nu_0^2)$ if, for all $\nu \in (0, \nu_0^2)$, the roots s_i, $i = 1(1)2k$ of Eq. (7) satisfy

$$s_1 = \exp(i\,\theta(\nu)), \quad s_2 = \exp(-i\,\theta(\nu)), \quad \textit{and} \quad |s_i| \leqslant 1, \qquad i = 3(1)2k, \tag{8}$$

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

Definition 2.3 For any method corresponding to the characteristic equation (7) the phase-lag is defined as the leading term in the expansion of

$$t = \nu - \theta(\nu).$$

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

Theorem 2.4 *The symmetric 2k-step method with characteristic equation given by* (7) *has phase-lag order q and phase-lag constant c given by*

$$-c\nu^{q+2} + O(\nu^{q+4}) = \frac{D_1}{D_2},$$

where

$$D_1 = \sum_{i=1}^{k} 2A_i(\nu)\cos(i\nu) + A_0(\nu),$$

and

$$D_2 = \sum_{i=1}^{k} 2k^2 A_k(\nu).$$

Proof See [11]. □

The formula proposed from the above theorem gives us a direct method to calculate the phase-lag of any symmetric $2k$-step method. In our case, the symmetric ten-step method has phase-lag order q and phase-lag constant c given by:

$$-c\nu^{q+2} + O(\nu^{q+4}) = \frac{pl_{num}}{pl_{den}},$$

where

$$pl_{num} = 2A_5(\nu)\cos(5\nu) + 2A_4(\nu)\cos(4\nu) + 2A_3(\nu)\cos(3\nu) + 2A_2(\nu)\cos(2\nu), \\ +2A_1(\nu)\cos(\nu) + A_0(\nu),$$

and

$$pl_{den} = 50A_5(\nu) + 34A_4(\nu) + 18A_3(\nu) + 8A_2(\nu) + 2A_1(\nu).$$

3 Construction of the new optimized predictor–corrector method

From the form (3) and without loss of generality we assume $a_m = 1$ and we can write

$$y_{n+m} + \sum_{i=0}^{m-1} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}), \tag{9}$$

hence

$$y_{n+m} = -\sum_{i=0}^{m-1} a_i y_{n+i} + h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}). \tag{10}$$

If the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}$, $i = 0(1)\lfloor \frac{m}{2} \rfloor$.

The approach of Panopoulos and Simos

The main aim of this paper is the extension of the method presented in the paper: A symmetric eight-step predictor–corrector method for the numerical solution of the radial Schrödinger equation and related IVPs with oscillating solutions, by mathematicians Panopoulos, Anastassi, and Simos which published in [44]. In the mentioned paper, the authors provied a new optimized symmetric eight-step predictor–corrector method of order ten and infinite order of phase-lag (phase-fitted). Also their method has an interval of periodicity $(0, v_0^2)$ where $v_0^2 = 5.63$. The local truncation of their method is

$$LTE_{[44]} = \frac{12506213339}{5794003353600} h^{12} \left(y_n^{(12)} + y_n^{(10)} \omega^2 \right) + O\left(h^{14}\right).$$

Their method is based on the symmetric multistep method of Quinlan–Tremaine, with eight steps and eighth algebraic order and is constructed to solve numerically the radial time-independent Schrödinger equation during the resonance problem with the use of the Woods–Saxon potential. It can also be used to integrate related IVPs with oscillating solutions such as orbital problems.

3.1 The new explicit method with phase-lag of order infinite (phase-fitted)

From the form (10) with $m = 10$ we get the form of the explicit symmetric ten-step methods

$$\begin{aligned} y_5 = &-(y_{-5} + a_4(y_4 + y_{-4}) + a_3(y_3+y_{-3})+a_2(y_2 + y_{-2}) + a_1(y_1 + y_{-1})+a_0 y_0) \\ &+h^2(b_4(f_4 + f_{-4}) + b_3(f_3 + f_{-3}) + b_2(f_2 + f_{-2})) + b_1(f_1 + f_{-1}) + b_0 f_0). \end{aligned} \tag{11}$$

The characteristic equation (7) becomes

$$A_5(\nu)s^5 + \cdots + A_1(\nu)s + A_0(\nu) + A_1(\nu)s^{-1} + \cdots + A_5(\nu)s^{-5} = 0, \tag{12}$$

where

$$A_i(\nu) = a_i + \nu^2 b_i\,, \quad i = 0(1)5\,, \quad a_5 = 1. \tag{13}$$

From (11) with

$$\begin{aligned} &a_4 = -2, \quad a_3 = 2, \quad a_2 = -1, \quad a_1 = 0, \quad a_0 = 0, \\ &b_0 = \frac{187585}{10368}, \quad b_1 = -\frac{1725439}{129600}, \quad b_2 = \frac{1195787}{129600}, \\ &b_3 = -\frac{395137}{129600}, \quad b_4 = \frac{823931}{518400}, \\ &y_i = y(x + ih)\,, \quad f_i = f(x + ih, y(x + ih)), \end{aligned}$$

we obtain the symmetric multistep method, like Quinlan and Tremaine method [48], with ten step and tenth algebraic order. This method has an interval of periodicity $(0, \nu_0^2)$ where $\nu_0^2 = 0.1681$. From (11) and by keeping the same a_i coefficients and by nullifying the phase-lag, we get

$$\begin{aligned} &a_4 = -2, \quad a_3 = 2, \quad a_2 = -1, \quad a_1 = 0, \quad a_0 = 0, \\ &b_0 = -\frac{201233}{2160} + 70\, b_4, \quad b_1 = \frac{217991}{2880} - 56\, b_4, \quad b_2 = -\frac{50797}{1440} + 28\, b_4, \\ &b_3 = -8\, b_4 + \frac{16703}{1728}, \quad b_4 = \frac{b_{4\,,\,num}}{17280\, v^2\, (\cos(v) - 1)^4}, \end{aligned} \tag{14}$$

where

$$b_{4,num} = -34560\ (\cos(v))^5 + 34560\ (\cos(v))^4 + 25920\ (\cos(v))^3$$
$$-83515\ (\cos(v))^3\, v^2 - 30240\ (\cos(v))^2 + 152391\ (\cos(v))^2\, v^2$$
$$-100857\, v^2 \cos(v) + 2160\ \cos(v) + 2160 + 24421\, v^2,$$
$$y_i = y(x + ih), \qquad f_i = f(x + ih, y(x + ih)),$$

where $v = \omega h$, ω is the frequency and h is the step length. For small values of v the above formulae are subject to heavy cancelations. In this case the following Taylor series expansion must be used

$$b_0 = \frac{187585}{10368} - \frac{9450497}{2280960}\, v^2 + \frac{58886839}{242611200}\, v^4 - \frac{10906937}{4269957120}\, v^6 + \frac{448351349}{10888390656000}\, v^8 - \frac{54990688271}{52133614460928000}\, v^{10} - \frac{1448007761}{32769700518297600}\, v^{12} - \frac{6319150661}{3365819319582720000}\, v^{14} - \frac{651455797942379}{10370351857541287772160000}\, v^{16} - \frac{53443646514719}{29629576735832250777600000}\, v^{18} - \frac{518135205550103}{12029608154747893815705600000}\, v^{20},$$

$$b_1 = -\frac{1725439}{129600} + \frac{9450497}{2851200}\, v^2 - \frac{58886839}{303264000}\, v^4 + \frac{10906937}{5337446400}\, v^6 - \frac{448351349}{13610488320000}\, v^8 + \frac{54990688271}{65167018076160000}\, v^{10} + \frac{1448007761}{40962125647872000}\, v^{12} + \frac{6319150661}{4207274149478400000}\, v^{14} + \frac{651455797942379}{12962939821926609715200000}\, v^{16} + \frac{53443646514719}{37036970919790313472000000}\, v^{18} + \frac{518135205550103}{15037010193434867269632000000}\, v^{20},$$

$$b_2 = \frac{1195787}{129600} - \frac{9450497}{5702400}\, v^2 + \frac{58886839}{606528000}\, v^4 - \frac{10906937}{10674892800}\, v^6 + \frac{448351349}{27220976640000}\, v^8 - \frac{54990688271}{130334036152320000}\, v^{10} - \frac{1448007761}{81924251295744000}\, v^{12} - \frac{6319150661}{8414548298956800000}\, v^{14} - \frac{651455797942379}{25925879643853219430400000}\, v^{16} - \frac{53443646514719}{74073941839580626944000000}\, v^{18} - \frac{518135205550103}{30074020386869734539264000000}\, v^{20},$$

$$b_3 = -\frac{395137}{129600} + \frac{1350071}{2851200}\, v^2 - \frac{58886839}{2122848000}\, v^4 + \frac{10906937}{37362124800}\, v^6 - \frac{448351349}{95273418240000}\, v^8 + \frac{54990688271}{456169126533120000}\, v^{10} + \frac{1448007761}{286734879535104000}\, v^{12} + \frac{6319150661}{29450919046348800000}\, v^{14} + \frac{651455797942379}{90740578753486268006400000}\, v^{16}$$

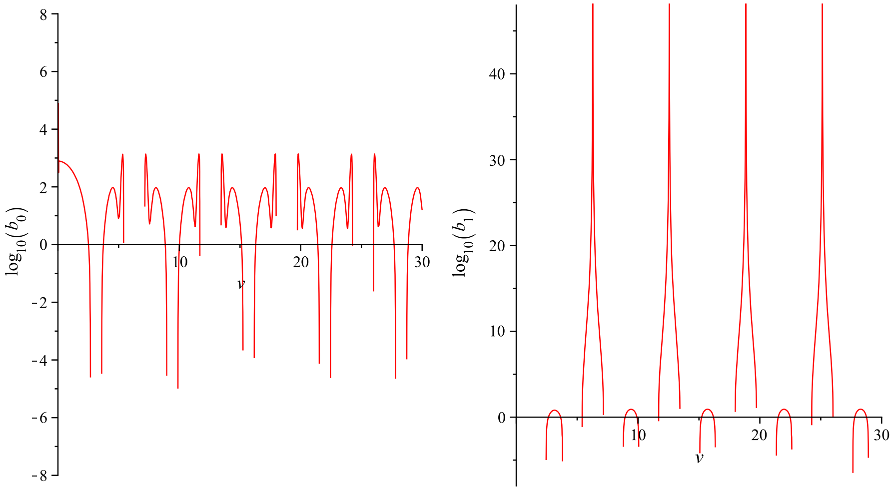


Fig. 1 Behavior of the coefficients b_0 and b_1 in new method

$$+\frac{53443646514719}{25925879643853219430400000}v^{18}+\frac{518135205550103}{105259071354044070887424000000}v^{20},$$

$$b_4=\frac{823931}{518400}-\frac{1350071}{22809600}v^2+\frac{58886839}{16982784000}v^4-\frac{10906937}{298896998400}v^6$$
$$+\frac{448351349}{762187345920000}v^8-\frac{54990688271}{3649353012264960000}v^{10}-\frac{1448007761}{2293879036280832000}v^{12}$$
$$-\frac{6319150661}{2356073523707904000000}v^{14}-\frac{651455797942379}{7259246300278901440512000000}v^{16}$$
$$-\frac{53443646514719}{2074070371508257554432000000}v^{18}-\frac{518135205550103}{842072570832352567099392000000}v^{20}.$$

The explicit symmetric ten-step method (11) with coefficients (14), has an interval of periodicity $(0, v_0^2)$ where $v_0^2 = 0.1764$ and the behavior of the coefficients of the predictor method are shown in Figs. 1, 2 and 3. In order to find the local truncation error (LTE), we express $y_{\pm i}$, $i = 1(1)5$ and $f_{\pm j}$, $j = 0(1)5$ via Taylor series and we substitute in (11). Based on this procedure we obtain the following expansion for the LTE:

$$LTE=\frac{1350071}{22809600}\left(y_n^{(12)}+\omega^2 y_n^{(10)}\right)h^{12}+O\left(h^{14}\right).$$

The new optimized explicit symmetric multistep method has ten steps, tenth algebraic order and infinite order of phase-lag (phase-fitted).

3.2 The new implicit method with phase-lag of order infinite (phase-fitted)

From the form (10) with $m = 10$, we get the form of the implicit symmetric ten-step methods

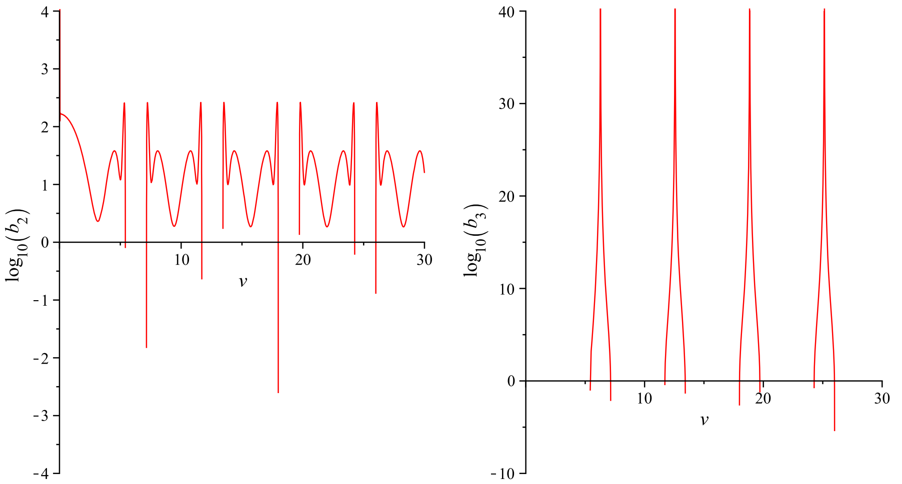
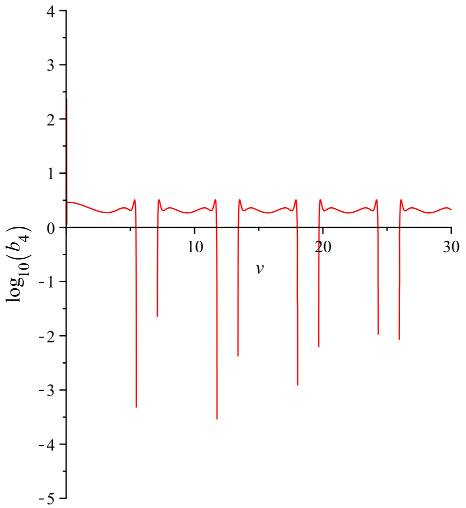


Fig. 2 Behavior of the coefficients b_2 and b_3 in new method

Fig. 3 Behavior of the coefficient b_4 in new method



$$y_5 = -(y_{-5} + \alpha_4(y_4 + y_{-4}) + \alpha_3(y_3 + y_{-3}) + \alpha_2(y_2 + y_{-2}) + \alpha_1(y_1 + y_{-1}) + \alpha_0 y_0) + h^2(\beta_5(f_5 + f_{-5}) + \beta_4(f_4 + f_{-4}) + \beta_3(f_3 + f_{-3}) + \beta_2(f_2 + f_{-2})) + b_1(f_1 + f_{-1}) + b_0 f_0) \tag{15}$$

The characteristic equation (7) becomes

$$A_5(v)s^5 + \cdots + A_1(v)s + A_0(v) + A_1(v)s^{-1} + \cdots + A_5(v)s^{-5} = 0, \tag{16}$$

where

$$A_i(v) = \alpha_i + v^2 \beta_i, \qquad i = 0(1)5, \quad \alpha_5 = 1. \tag{17}$$

From (15) and by keeping the same α_i coefficients and by nullifying the phase-lag, we get

$$\begin{aligned}
&\alpha_4 = -2\,, \quad \alpha_3 = 2\,, \quad \alpha_2 = -1, \quad \alpha_1 = 0\,, \quad \alpha_0 = 0\,, \\
&\beta_0 = \frac{187585}{10368} - 252\,\beta_5,\ \beta_1 = -\frac{1725439}{129600} + 210\,\beta_5\,,\ \beta_2 = \frac{1195787}{129600} - 120\,\beta_5, \\
&\beta_3 = -\frac{395137}{129600} + 45\,\beta_5\,, \quad \beta_4 = -10\,\beta_5 + \frac{823931}{518400}, \\
&\beta_5 = \frac{\beta_{5\,,\,num}}{1036800\,v^2\,(\cos(v)-1)^5},
\end{aligned} \tag{18}$$

where

$$\begin{aligned}
\beta_{5\,,\,num} = {} & -1036800\,(\cos(v))^5 + 1036800\,(\cos(v))^4 - 823931\,(\cos(v))^4\,v^2 \\
& +777600\,(\cos(v))^3 + 790274\,(\cos(v))^3\,v^2 - 371856\,(\cos(v))^2\,v^2 \\
& -907200\,(\cos(v))^2 + 270014\,v^2\cos(v) + 64800\,\cos(v) \\
& -91301\,v^2 + 64800,
\end{aligned}$$

where $v = \omega h$, ω is the frequency and h is the step length.

For small values of v the above formulae are subject to heavy cancelations. In this case the following Taylor series expansion must be used

$$\begin{aligned}
\beta_0 = {} & \frac{18117277}{5702400} - \frac{547336457}{1482624000}\,v^2 + \frac{13099127}{8895744000}\,v^4 + \frac{1122215903}{2016368640000}\,v^6 \\
& + \frac{411284674673}{14481559572480000}\,v^8 + \frac{1674319402961}{1911565863567360000}\,v^{10} \\
& + \frac{54172151741}{41872395106713600000}\,v^{12} - \frac{406647992425891}{872925240533778432000000}\,v^{14} \\
& - \frac{1769796744884513}{34567839525137625907200000}\,v^{16} - \frac{650688266276051}{227316858555326791680000000}\,v^{18} \\
& - \frac{3621430254757757 2541}{287146746653832225380892672000000}\,v^{20} \\
& - \frac{281261578491373371 0991}{585779363173817739777021050880000000}\,v^{22} + \cdots,
\end{aligned}$$

$$\begin{aligned}
\beta_1 = {} & -\frac{10081177}{11404800} + \frac{547336457}{1779148800}\,v^2 - \frac{13099127}{10674892800}\,v^4 - \frac{1122215903}{2419642368000}\,v^6 \\
& - \frac{411284674673}{17377871486976000}\,v^8 - \frac{1674319402961}{2293879036280832000}\,v^{10} \\
& - \frac{54172151741}{50246874128056320000}\,v^{12} + \frac{406647992425891}{1047510288640534118400000}\,v^{14} \\
& + \frac{1769796744884513}{41481407430165151088640000}\,v^{16} + \frac{650688266276051}{272780230266392150016000000}\,v^{18}
\end{aligned}$$

$$+\frac{3621430254757757 2541}{3445760959845986704570712064000000}v^{20}$$
$$+\frac{28126157849137337 10991}{702935235808581287732425261056000000}v^{22}+\cdots,$$

$$\beta_2=\frac{6056249}{2851200}-\frac{547336457}{3113510400}v^2+\frac{13099127}{18681062400}v^4+\frac{1122215903}{4234374144000}v^6$$
$$+\frac{411284674673}{30411275102208000}v^8+\frac{1674319402961}{4014288313491456000}v^{10}$$
$$+\frac{54172151741}{8793202972409856000}v^{12}-\frac{406647992425891}{18331430051209347072000000}v^{14}$$
$$-\frac{1769796744884513}{725924630027890144051200000}v^{16}-\frac{650688266276051}{4773654029661862625280000000}v^{18}$$
$$-\frac{3621430254757757 2541}{6030081679730476732998746112000000}v^{20}$$
$$-\frac{28126157849137337 10991}{1230136662665017253531744206848000000}v^{22}+\cdots,$$

$$\beta_3=-\frac{8790917}{22809600}+\frac{547336457}{8302694400}v^2-\frac{13099127}{49816166400}v^4-\frac{1122215903}{11291664384000}v^6$$
$$-\frac{411284674673}{81096733605888000}v^8-\frac{1674319402961}{10704768835977216000}v^{10}$$
$$-\frac{54172151741}{23448541259759616000}v^{12}+\frac{406647992425891}{48883813469891592192000000}v^{14}$$
$$+\frac{1769796744884513}{1935799013407707050803200000}v^{16}+\frac{650688266276051}{12729744079098300334080000000}v^{18}$$
$$+\frac{3621430254757757 2541}{16080217812614604621329989632000000}v^{20}$$
$$+\frac{28126157849137337 10991}{3280364433773379342751317884928000000}v^{22}+\cdots,$$

$$\beta_4=\frac{11376127}{11404800}-\frac{547336457}{37362124800}v^2+\frac{13099127}{224172748800}v^4+\frac{1122215903}{50812489728000}v^6$$
$$+\frac{411284674673}{364935301226496000}v^8+\frac{1674319402961}{48171459761897472000}v^{10}$$
$$+\frac{54172151741}{105518435668918272000}v^{12}-\frac{406647992425891}{219977160614512164864000000}v^{14}$$
$$-\frac{1769796744884513}{8711095560334681728614400000}v^{16}-\frac{650688266276051}{57283848355942351503360000000}v^{18}$$
$$-\frac{3621430254757757 2541}{72360980156765720795984953344000000}v^{20}$$
$$-\frac{28126157849137337 10991}{14761639951980207042380930482176000000}v^{22}+\cdots,$$

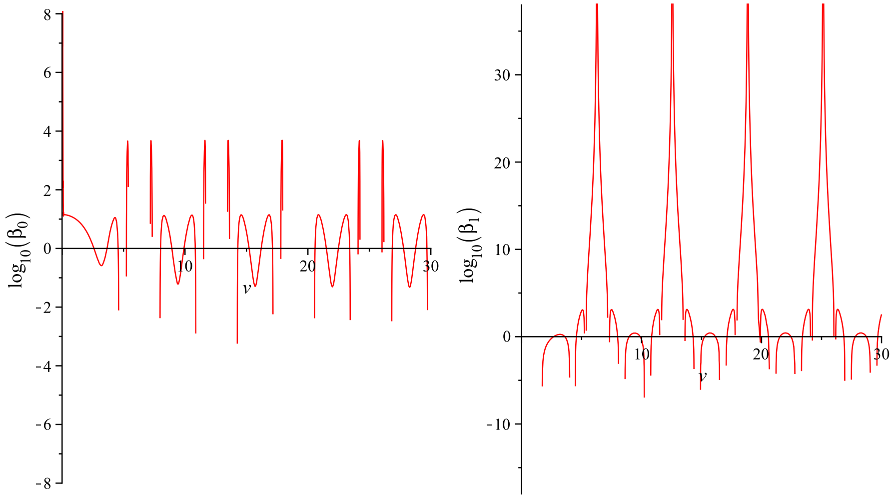


Fig. 4 Behavior of the coefficients β_0 and β_1 in new method

$$\beta_5 = \frac{1350071}{22809600} + \frac{547336457}{373621248000}v^2 - \frac{13099127}{2241727488000}v^4 - \frac{1122215903}{508124897280000}v^6 - \frac{411284674673}{3649353012264960000}v^8 - \frac{1674319402961}{481714597618974720000}v^{10} - \frac{54172151741}{1055184356689182720000}v^{12} + \frac{406647992425891}{21997716061451216486400000}v^{14} + \frac{1769796744884513}{871109556033468172861440000}v^{16} + \frac{650688266276051}{5728384835594235150336000000}v^{18} + \frac{36214302547577572541}{72360980156765720795984953344000000}v^{20} + \frac{28126157849137337 10991}{1476163995198020704238093048217600000000}v^{22} + \cdots .$$

The implicit symmetric ten-step method (15) with coefficients (18), has an interval of periodicity $(0, v_0^2)$ where $v_0^2 = 1.210$ and the behavior of the coefficients of the predictor method are shown in Figs. 4, 5 and 6. The LTE of the above method is given by

$$LTE = -\frac{547336457}{373621248000}\left(y^{(14)} + \omega^2 y^{(12)}\right)h^{14}.$$

The new optimized implicit symmetric multistep method has ten steps, twelve algebraic order and infinite order of phase-lag (phase-fitted).

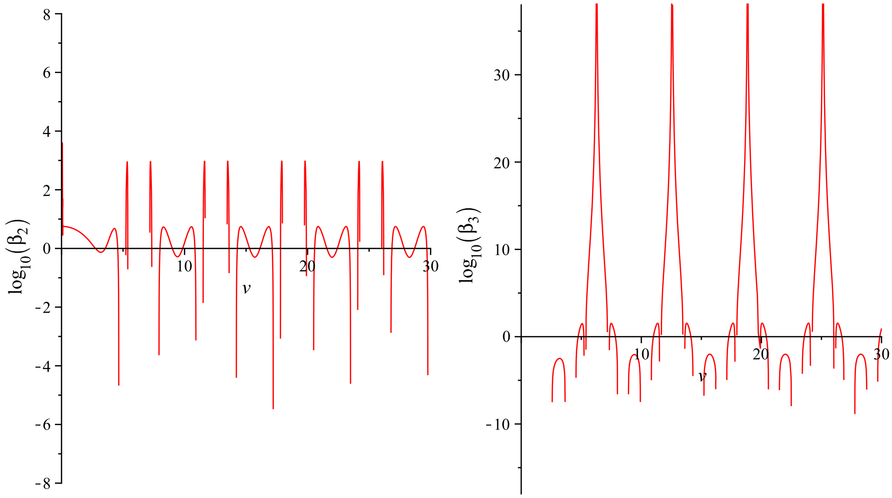


Fig. 5 Behavior of the coefficients β_2 and β_3 in new method

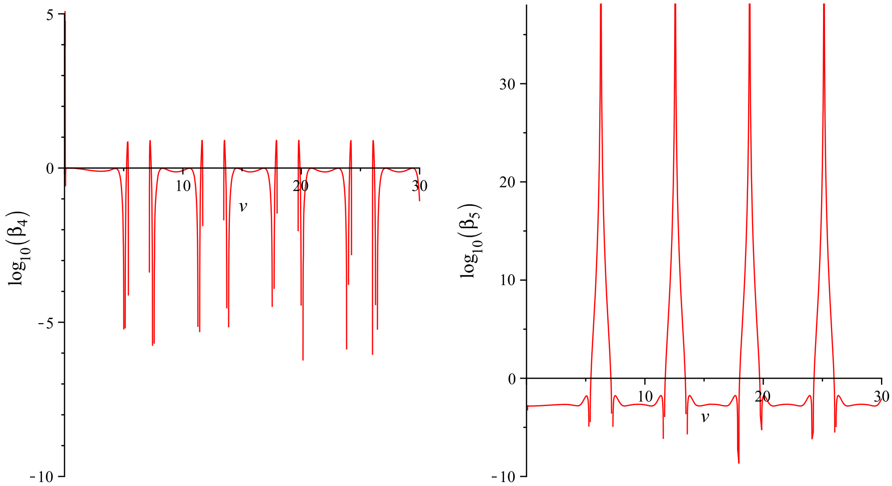


Fig. 6 Behavior of the coefficients β_4 and β_5 in new method

4 The new predictor–corrector method

From Lambert [28], we have that the general k-step predictor–corrector or PC pair is

$$\sum_{j=0}^{m} a_j^* y_{n+j} = h \sum_{j=0}^{m-1} b_j^* f_{n+j},$$
$$\sum_{j=0}^{m} a_j y_{n+j} = h \sum_{j=0}^{m} b_j f_{n+j}. \tag{19}$$

Let the predictor and corrector defined by (20) have orders p^* and $\lambda \leqslant p - p^* - 1$, respectively. The order of a PC method depend on the gap between p^* and p and on λ, the number of times the corrector is called. If $p^* < p$, the order of the PC method is $p^* + \lambda(< p)$ [28]. We consider the pair of linear multistep methods

$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m-1} b_i(\nu) f(x_{n+i}, y_{n+i}),$$
$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m-1} \beta_i(\nu) f(x_{n+i}, y_{n+i}), \tag{20}$$

where $|a_0| + |b_0(\nu)| \neq 0,\ |a_0| + |\beta_0(\nu)| \neq 0,\ \nu = \omega h,\ \omega$ is the frequency and h is the step length. Without loss of generality we assume that $a_m = 1$ and we can write

$$y_{n+m} + \sum_{i=0}^{m-1} a_i y_{n+i} = h^2 \sum_{i=0}^{m-1} b_i(\nu) f(x_{n+i}, y_{n+i}),$$
$$y_{n+m} + \sum_{i=0}^{m-1} a_i y_{n+i} = h^2 \Big(\beta_m(\nu) f(x_{n+i}, y_{n+i}) \sum_{i=0}^{m-1} \beta_i(\nu) f(x_{n+i}, y_{n+i})\Big),$$

and we have

$$y_{n+m} = -\sum_{i=0}^{m-1} a_i y_{n+i} + h^2 \sum_{i=0}^{m-1} b_i(\nu) f(x_{n+i}, y_{n+i}),$$
$$y_{n+m} = -\sum_{i=0}^{m-1} a_i y_{n+i} + h^2 \Big(\beta_m(\nu) f(x_{n+i}, y_{n+i}) \sum_{i=0}^{m-1} \beta_i(\nu) f(x_{n+i}, y_{n+i})\Big).$$

If we call $A_n = -\sum_{i=0}^{m-1} a_i y_{n+i}$ we can write

$$y_{n+m} = A_n + h^2 \sum_{i=0}^{m-1} b_i(\nu) f(x_{n+i}, y_{n+i}),$$
$$y_{n+m} = A_n + h^2 \Big(\beta_m(\nu) f(x_{n+i}, y_{n+i}) \sum_{i=0}^{m-1} \beta_i(\nu) f(x_{n+i}, y_{n+i})\Big).$$

From this pair, a new predictor–corrector (PC) pair form, is formally defined as follows

$$y^*_{n+m} = A_n + h^2 \sum_{i=0}^{m-1} b_i(\nu) f(x_{n+i}, y_{n+i}),$$
$$y_{n+m} = A_n + h^2 \beta_m(\nu) f(x_{n+i}, y^*_{n+i}) + h^2 \sum_{i=0}^{m-1} \beta_i(\nu) f(x_{n+i}, y_{n+i}), \tag{21}$$

where $A_n = -\sum_{i=0}^{m-1} a_i\, y_{n+i}$, $\mid a_0 \mid + \mid b_0(\nu) \mid \neq 0$, $\mid a_0 \mid + \mid \beta_0(\nu) \mid \neq 0$, $\nu = \omega\, h$, ω is the frequency and h is the step length. If the method is symmetric then $a_i = a_{m-i}$, $b_i(\nu) = b_{m-i}(\nu)$, $i = 0(1)\lfloor \frac{m}{2} \rfloor$. From (21), (11) and (15) a new symmetric ten-step predictor–corrector method with phase-lag of order infinite (phase-fitted) obtained

$$\begin{aligned}
y_5^* &= A + h^2\Bigg(b_4(\nu)(f_4 + f_{-4}) + \left(-8\, b_4(\nu) + \frac{16703}{1728}\right)(f_3 + f_{-3}) \\
&\quad + \left(-\frac{50797}{1440} + 28\, b_4(\nu)\right)(f_2 + f_{-2}) + \left(\frac{217991}{2880} - 56\, b_4(\nu)\right)(f_1 + f_{-1}) \\
&\quad + \left(-\frac{201233}{2160} + 70\, b_4(\nu)\right) f_0\Bigg), \\
y_5 &= A + h^2\Bigg(\beta_5(\nu)(f_5^* + f_{-5}) + \left(-10\, \beta_5(\nu) + \frac{823931}{518400}\right)(f_4 + f_{-4}) \\
&\quad + \left(-\frac{395137}{129600} + 45\, \beta_5(\nu)\right)(f_3 + f_{-3}) + \left(\frac{1195787}{129600} - 120\, \beta_5(\nu)\right)(f_2 + f_{-2}) \\
&\quad + \left(-\frac{1725439}{129600} + 210\, \beta_5(\nu)\right)(f_1 + f_{-1}) \\
&\quad + \left(\frac{187585}{10368} - 252\, \beta_5(\nu)\right) f_0\Bigg), \qquad (22)
\end{aligned}$$

where

$$\begin{aligned}
A &= -y_{-5} + (y_4 + y_{-4}) - 10(y_3 + y_{-3}) + 10(y_2 + y_{-2}), \\
b_4(\nu) &= \frac{b_{4\,,\,num}}{17280\, v^2\, (\cos(v) - 1)^4}, \quad \beta_5(\nu) = \frac{\beta_{5\,,\,num}}{1036800\, v^2\, (\cos(v) - 1)^5},
\end{aligned}$$

and

$$\begin{aligned}
b_{4\,,\,num} &= -34560\, (\cos(v))^5 + 34560\, (\cos(v))^4 + 25920\, (\cos(v))^3 \\
&\quad -83515\, (\cos(v))^3\, v^2 - 30240\, (\cos(v))^2 + 152391\, (\cos(v))^2\, v^2 \\
&\quad -100857\, v^2 \cos(v) + 2160\, \cos(v) + 2160 + 24421\, v^2, \\
\beta_{5\,,\,num} &= -1036800\, (\cos(v))^5 + 1036800\, (\cos(v))^4 - 823931\, (\cos(v))^4\, v^2 \\
&\quad +777600\, (\cos(v))^3 + 790274\, (\cos(v))^3\, v^2 - 371856\, (\cos(v))^2\, v^2 \\
&\quad -907200\, (\cos(v))^2 + 270014\, v^2 \cos(v) + 64800\, \cos(v) \\
&\quad -91301\, v^2 + 64800, \\
y_i &= y(x + ih), \quad f_i = f(x + ih, y(x + ih)),
\end{aligned}$$

ω is the frequency and h is the step length.

For small values of v the following Taylor series expansions must be used:

$$b_4(\nu) = \frac{823931}{518400} - \frac{1350071}{22809600}\, v^2 + \frac{58886839}{16982784000}\, v^4 - \frac{10906937}{298896998400}\, v^6$$

$$
\begin{aligned}
&+\frac{448351349}{762187345920000}v^{8}-\frac{54990688271}{3649353012264960000}v^{10}\\
&-\frac{1448007761}{2293879036280832000}v^{12}-\frac{6319150661}{2356073523707904000 0}v^{14}\\
&-\frac{651455797942379}{72592463002789014405120000 0}v^{16}-\frac{53443646514719}{20740703715082575544320000 00}v^{18}\\
&-\frac{518135205550103}{84207257083235256709939200 0000}v^{20}\\
&+\cdots,\\
\beta_5(v)=&\frac{1350071}{22809600}+\frac{547336457}{373621248000}v^{2}-\frac{13099127}{2241727488000}v^{4}\\
&-\frac{1122215903}{508124897280000}v^{6}-\frac{411284674673}{3649353012264960000}v^{8}\\
&-\frac{1674319402961}{481714597618974720000}v^{10}-\frac{54172151741}{105518435668918272000 0}v^{12}\\
&+\frac{406647992425891}{21997716061451216486400000 0}v^{14}+\frac{1769796744884513}{87110955603346817286144000 00}v^{16}\\
&+\frac{650688266276051}{57283848355942351503360000000}v^{18}+\frac{36214302547577572541}{7236098015676572079598495334400000 0}v^{20}\\
&+\frac{28126157849137337 10991}{1476163995198020704238093048217600000 00}v^{22}+\cdots.
\end{aligned}
$$

The characteristic equation (7) becomes

$$A_5(v)s^5+\cdots+A_1(v)s+A_0(v)+A_1(v)s^{-1}+\cdots+A_5(v)s^{-5}=0, \tag{23}$$

where

$$A_i(v)=\alpha_i+v^2\left(\beta_i(v)-a_i\beta_5(v)\right)-v^4 b_i\beta_5(v),\quad i=0(1)5, \tag{24}$$

$$b_5=0,\quad a_5=\alpha_5=1. \tag{25}$$

The new optimized symmetric ten-step predictor–corrector method (22) has an interval of periodicity $(0, v_0^2)$ where $v_0^2 = 9.89$. The LTE of the above method is given by

$$LTE_{PC}=\frac{96506469327691}{47345284546560000}\left(y^{(14)}+\omega^2 y^{(12)}\right)h^{14}+O\left(h^{16}\right).$$

The new optimized symmetric ten-step predictor–corrector method (22) has ten steps, twelve algebraic order and infinite order of phase-lag (phase-fitted).

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 Numerovs method which is indicated as Method I.

- The Exponentially-fitted two-step method developed by Raptis and Allison [50] which is indicated as Method II.
- The Exponentially-fitted four-step method developed by Raptis [51] which is indicated as Method III.
- The eight-step ninth algebraic order method developed by Quinlan and Tremaine [48] which is indicated as Method IV.
- The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [48] which is indicated as Method V.
- The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [48] which is indicated as Method VI.
- The eight-step method with phase-lag and its first derivative equal to zero obtained in [18] which is indicated as Method VII.
- The eight-step method with phase-lag and its first and second derivative equal to zero obtained in [19] which is indicated as Method VIII.
- The ten-step method with phase-lag and its first and second derivatives equal to zero obtained in [17] which is indicated as Method IX.
- The ten-step method with phase-lag and its first, second and third derivatives equal to zero obtained in [17] which is indicated as Method X.
- The new developed ten-step predictor–corrector method which is indicated as Method XI.
- An exponentially-fitted eight-order method obtained in [77] which is indicated as XII.

5.2 The problems

The efficiency of the new optimized symmetric ten-step predictor–corrector 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

$$\omega = \sqrt{|q(x)|} = \sqrt{|V(x) - E|}, \tag{26}$$

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 behaviour of the Woods–Saxon potential is shown in Fig. 7 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

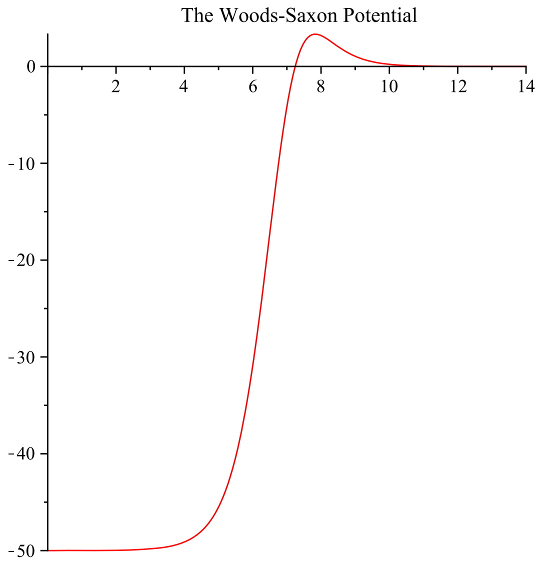


Fig. 7 The Woods–Saxon potential

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

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 $x \to \infty$ the solution of Eq. (1) 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 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 $x_i < x_i + 1$ and 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 $E = 341.495874$. 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 [20]). For the purpose of obtaining our numerical results it is appropriate to choose ω as follows (see for details [20]):

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

Example 5.2 The "almost" by *Franco and Palacios* [14], can be described by

$$y'' + y = \epsilon e^{i\psi x}, \quad y(0) = 1, \quad y'(0) = i, \quad y \in \mathbb{C}$$

or equivalently by

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

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

$$y(x) = u(x) + i v(x), \quad u, v \in \mathbb{R}, \tag{27}$$

where

$$\begin{aligned} u(x) &= \frac{1 - \epsilon - \psi^2}{1 - \psi^2} \cos(x) + \frac{\epsilon}{1 - \psi^2} \cos(\psi x), \\ v(x) &= \frac{1 - \epsilon\psi - \psi^2}{-\psi^2} \sin(x) + \frac{\epsilon}{1 - \psi^2} \sin(\psi x). \end{aligned}$$

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* [81], can be described by

$$y'' + y = 0.001 e^{ix}, \quad y(0) = 1, \quad y'(0) = 0.9995i, \quad y \in \mathbb{C},$$

or equivalently by

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

The theoretical solution of this problem is given by $y(x) = u(x) + i v(x)$, where $u, v \in \mathbb{R}$ and

$$\begin{aligned} u(x) &= \cos(x) + 0.0005 \sin(x), \\ v(x) &= \sin(x) - 0.0005 x \cos(x). \end{aligned}$$

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

Example 5.4 (Inhomogeneous Equation) Consider the initial value problem

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

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

Example 5.5 We consider the nonlinear undamped *Duffing equation*

$$y'' = -y - y^3 + B\cos(\omega x), \quad y(0) = 0.200426728067, \quad y'(0) = 0, \tag{28}$$

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 (28) from [33],

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

where

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

5.3 Comparison

For the problems that the theoretical solution is known the NFE is the Number of Function Evaluations.

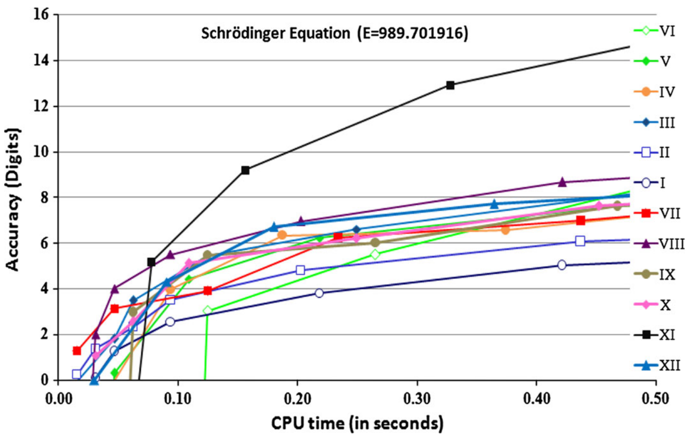


Fig. 8 Efficiency for the resonance problem using $E = 989.701916$

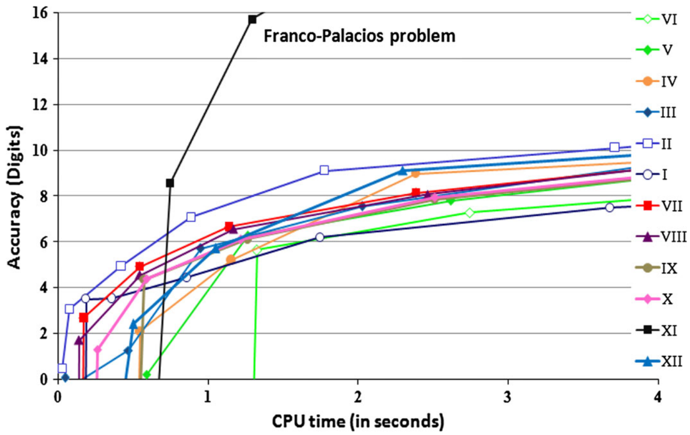


Fig. 9 Efficiency for the Franco and Palacios equation

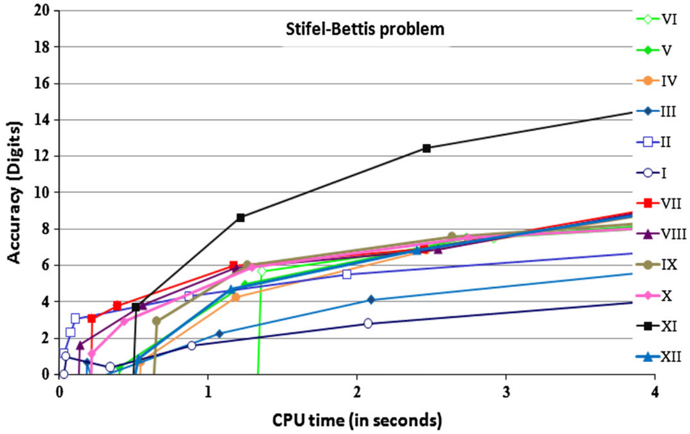


Fig. 10 Efficiency for the orbital problem by Stiefel and Bettis

In Fig. 8, we see the results for the resonance problem for energy $E = 989.495874$. In Fig. 9, we see the results for the Franco–Palacios almost periodic problem, in Fig. 10, the results for the Stiefel–Bettis almost periodic problem are present, in Fig. 11, the results for the inhomogeneous equation are present and finally in Fig. 12, we see the results for the Duffing equation.

Among all the methods used, the new optimized symmetric ten-step predictor–corrector method with twelfth algebraic order and infinite phase-lag order (phase-fitted) was the most efficient.

5.4 Conclusions

We have constructed a new predictor–corrector (PC) pair form (21) and from this form the new optimized symmetric ten-step predictor–corrector method with twelfth

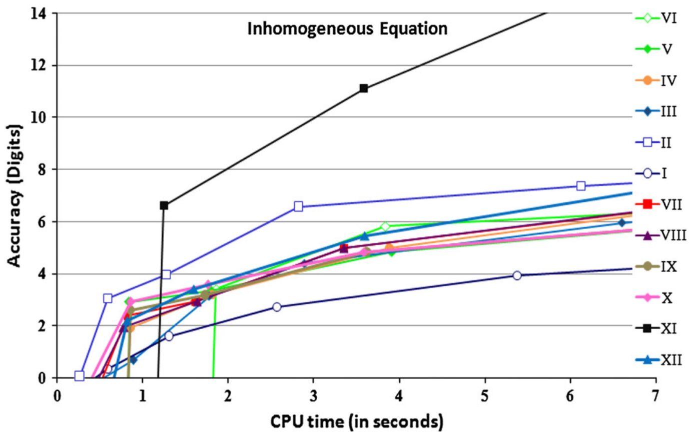


Fig. 11 Efficiency for the inhomogeneous equation

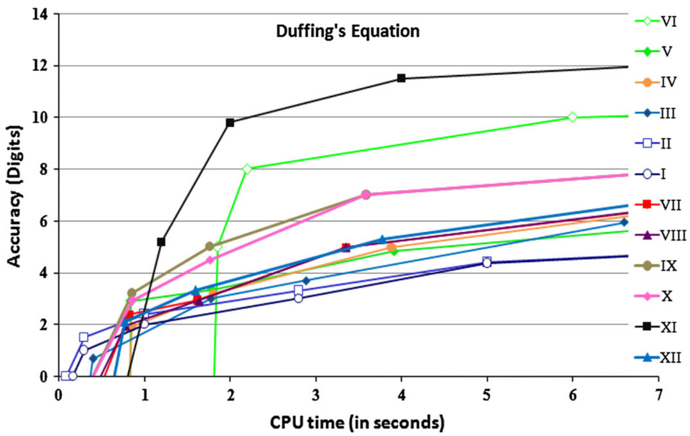


Fig. 12 Efficiency for the Duffing equation

algebraic order and infinite phase-lag order (phase-fitted) (22). We concluded that the new method are highly efficient compared to other optimized methods which also reveals the importance of phase-lag when solving ordinary differential equations with oscillating solutions.

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