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ORIGINAL PAPER

A new optimized symmetric 8-step semi-embedded predictor–corrector method for the numerical solution of the radial Schrödinger equation and related orbital problems

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Abstract In this work we introduce a new predictor–corrector (PC) pair form (SEPCM) for the numerical integration of second-order initial-value problems and a new optimized eight-step symmetric predictor–corrector method with minimal phase-lag and algebraic order ten is constructed. The new method is based on the multistep symmetric method of Quinlan–Tremaine (Astron. J. 100(5):1694–1700, 1990), with eight steps and eighth algebraic order and 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 oscillatory solutions such as orbital problems. We compare the new method to some recently constructed optimized methods and other methods from the literature. We measure the efficiency of the methods and conclude that the new optimized method is the most efficient of all the compared methods and for all the problems solved.

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1 Introduction

We study the numerical integration of special second-order periodic initial-value problems of the form

$$\frac{d^2 y(x)}{dx^2} = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0 \tag{1}$$

with an oscillatory solutions (see [29]). These ordinary differential equations are of second order in which the derivative y' does not appear explicitly.

A well-known example of problems of form (1) is the one-dimensional Schrödinger equation that has the form:

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

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 $\bar{W}_i$. After this the problem (2) can be expressed by the approximation:

$$y''_i = (\bar{W} - E)\, y_i, \tag{3}$$

whose solution is:

$$\begin{aligned} &y_i(x) = A_i \exp\left(\sqrt{\bar{W} - E}\, x\right) + B_i \exp\left(-\sqrt{\bar{W} - E}\, x\right), \\ &A_i,\ B_i \in \mathbb{R}. \end{aligned} \tag{4}$$

Much research has been done the last decades on the construction of computationally efficient and reliable algorithms for the numerical solution of the one-dimensional Schrödinger equation and related problems (see for example [1–86]), which can be divided in the following categories:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge-Kutta and Runge-Kutta Nyström type have been obtained in [1–4].
- In [5–9] exponentially and trigonometrically fitted Runge-Kutta and Runge-Kutta Nyström methods are constructed.

– Multistep phase-fitted methods and multistep methods with minimal phase-lag are obtained in [10–30].
– Symplectic integrators are investigated in [31–47].
– Exponentially and trigonometrically multistep methods have been produced in [48–70].
– Nonlinear methods have been studied in [71] and [72]
– Review papers have been presented in [73–86]

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

$$y'' = f(x, y) \tag{5}$$

multistep methods of the form

$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \tag{6}$$

with m steps can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a, b]$ and $h = |x_{i+1} - x_i|$, $i = 0(1)m - 1$. If the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}$ $i = 0(1)\lfloor \frac{m}{2} \rfloor$.

Method (6) is associated with the operator

$$L(x) = \sum_{i=0}^{m} a_i u(x + ih) - h^2 \sum_{i=0}^{m} b_i u''(x + ih) \tag{7}$$

where $u \in C^2$.

Definition 1 The multistep method (6) is called algebraic of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{p+1}$.

If $u(x)$ has continuous derivatives of sufficiently high order then

$$L(x) = C_0 u(x) + C_1 u'(x) h + \cdots + C_q u^{(q)}(x) h^q + \cdots, \tag{8}$$

The coefficients C_q are given

$$C_0 = \sum_{i=0}^{m} a_i$$

$$C_1 = \sum_{i=0}^{m} i \cdot a_i$$

$$C_q = \frac{1}{q!} \sum_{i=0}^{m} i^q \cdot a_i - \frac{1}{(q-2)!} \sum_{i=0}^{m} i^{q-2} \cdot b_i, \quad q = 2, 3 \ldots. \tag{9}$$

The order p is the unique integer for which

$$C_0 = \cdots = C_{p+1} = 0,\ C_{p+2} \neq 0. \tag{10}$$

A method is said to be consistent if this order is at least 1, i.e., if

$$C_0 = C_1 = C_2 = 0. \tag{11}$$

In what follows we will assume that the method (6) is consistent.

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

$$y'' = -\omega^2 y \tag{12}$$

a difference equation of the form

$$\sum_{i=1}^{k} A_i(v)(y_{n+i} + y_{n-i}) + A_0(v) y_n = 0 \tag{13}$$

is obtained, where $v = \omega h$, h is the step length and $A_0(v)$, $A_1(v), \ldots,\ A_k(v)$ are polynomials of v.

The characteristic equation associated with (13) is

$$\sum_{i=1}^{k} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \tag{14}$$

From Lambert and Watson [83] we have the following definitions:

Definition 2 A symmetric $2k$-step method with characteristic equation given by (14) is said to have an interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots s_i, $i = 1(1)2k$ of Eq. (14) satisfy:

$$s_1 = e^{i\theta(v)}, s_2 = e^{-i\theta(v)}, \quad \text{and} \quad |s_i| \leq 1, \quad i = 3(1)2k \tag{15}$$

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

Definition 3 For any method corresponding to the characteristic equation(14) the phase-lag is defined as the leading term in the expansion of

$$t = v - \theta(v) \tag{16}$$

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

Theorem 1 [75] *The symmetric $2k$-step method with characteristic equation given by (14) has phase-lag order q and phase-lag constant c given by*

$$- cv^{q+2} + O(v^{q+4}) = \frac{2\sum_{j=1}^{k} A_j(v)\cos(jv) + A_0(v)}{2\sum_{j=1}^{k} j^2 A_j(v)} \tag{17}$$

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 8-step method has phase-lag order q and phase-lag constant c given by:

$$\begin{aligned} &-cv^{q+2} + O(v^{q+4}) \\ &= \frac{2A_4(v)\cos(4v) + 2A_3(v)\cos(3v) + 2A_2(v)\cos(2v) + 2A_1(v)\cos(v) + A_0(v)}{32A_4(v) + 18A_3(v) + 8A_2(v) + 2A_1(v)} \end{aligned} \tag{18}$$

3 Construction of the new optimized predictor–corrector method

From the form (6) and without loss of generality we assume $a_m = 1$ and we can write

$$y_{n+m} + \sum_{i=0}^{m-1} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}), \tag{19}$$

finally we get

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

where $|a_0| + |b_0| \neq 0$. If the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}$ $i = 0(1)\lfloor \frac{m}{2} \rfloor$.

3.1 The implicit method phase-lag order infinity (phase-fitted)

From (20) for $m = 8$, we get the form of the symmetric implicit eight-step method:

$$\begin{aligned} y_4 = &-(y_{-4} + \alpha_3(y_3 + y_{-3}) + \alpha_2(y_2 + y_{-2}) + \alpha_1(y_1 + y_{-1}) + \alpha_0 y_0) \\ &+h^2(\beta_4(f_4+f_{-4}) + \beta_3(f_3+f_{-3}) + \beta_2(f_2+f_{-2}) + \beta_1(f_1+f_{-1}) + \beta_0 f_0). \end{aligned} \tag{21}$$

The characteristic equation (14) becomes

$$\sum_{i=1}^{4} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \tag{22}$$

where

$$A_i(v) = \alpha_i + v^2\, \beta_i, \qquad i = 0(1)4, \qquad \alpha_4 = 1.$$

We take

$$\alpha_4 = 1, \qquad \alpha_3 = -2, \qquad \alpha_2 = 2, \qquad \alpha_1 = -1, \qquad \alpha_0 = 0, \tag{23}$$

and we want the implicit method to have infinite order of phase-lag, that is the phase-lag will be nullified using β_4 coefficient. We satisfy as many algebraic equations as possible, but we keep β_4 free. After achieving 10th algebraic order, the coefficients depend now on β_4:

$$\begin{aligned}
&\beta_0 = 70 \quad \beta_4 - \frac{12629}{3024}, \quad \beta_1 = -56 \quad \beta_4 + \frac{20483}{4032}, \quad \beta_2 = 28 \quad \beta_4 - \frac{3937}{2016}, \\
&\quad \beta_3 = -8 \quad \beta_4 + \frac{17671}{12096}
\end{aligned} \tag{24}$$

and the phase-lag becomes:

$$\begin{aligned}
PL &= \frac{1}{1260}\frac{A}{B}, \qquad \text{where} \\
A &= 24192\,(\cos(v))^4 + 24192\,(\cos(v))^4\, v^2\beta_4 + 17671\,(\cos(v))^3\, v^2 \\
&\quad -96768\,(\cos(v))^3\, v^2\beta_4 - 24192\,(\cos(v))^3 + 14152\,(\cos(v))^2\, v^2\beta_4 \\
&\quad -12096\,(\cos(v))^2 - 11811\,(\cos(v))^2\, v^2 + 2109\cos(v)\, v^2 + 15120\cos(v) \\
&\quad -96768\cos(v)\, v^2\beta_4 - 409v^2 + 24192v^2\beta_4 - 3024 \quad \text{and} \\
&\quad B = 12 + 25v^2
\end{aligned}$$

so by satisfying $PL = 0$, we derive

$$\begin{aligned}
\beta_4 &= -\frac{1}{24192}\,\frac{C}{D}, \qquad \text{where} \\
C &= 24192\,(\cos(v))^4 + \left(17671\,v^2 - 24192\right)(\cos(v))^3 \\
&\quad - \left(12096 + 11811v^2\right)(\cos(v))^2 + \left(15120 + 2109\,v^2\right)\cos(v) - 409\,v^2 - 3024 \\
D &= v^2\,(\cos(v) - 1)^4
\end{aligned} \tag{25}$$

where $v = \omega\, h,\ \omega$ 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:

$$\beta_4 = \frac{45767}{725760} + \frac{58061}{31933440}v^2 + \frac{2399921}{261534873600}v^4 - \frac{602311}{298896998400}v^6 - \frac{1067953}{7904165068800}v^8 - \frac{29376529643}{5109094217170944000}v^{10} - \frac{3029692489}{16057153253965824000}v^{12} - \frac{89043304369}{18801466719189073920000}v^{14} - \frac{9809592400337}{14518492600557802881024000}v^{16} + \frac{47323386203}{30565247580121690275840000}v^{18}, \tag{26}$$

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

From (21), (23) and (24) an optimized symmetric eight-step implicit method with infinite order of phase-lag (phase-fitted) obtained (see [70]):

$$y_4 = -y_{-4} + 2(y_3 + y_{-3}) - 2(y_2 + y_{-2}) + (y_1 + y_{-1}) + h^2 \left(\beta_4(v)(f_4 + f_{-4}) + \left(\frac{17671}{12096} - 8\beta_4(v) \right)(f_3 + f_{-3}) + \left(28\beta_4(v) - \frac{3937}{2016} \right)(f_2 + f_{-2}) + \left(\frac{20483}{4032} - 56\beta_4(v) \right)(f_1 + f_{-1}) + \left(70\beta_4(v) - \frac{12629}{3024} \right) f_0 \right) \tag{27}$$

where $y_i = y(x + ih),\ f_i = f(x + ih, y(x + ih)),\ i = -4(1)4,$

$$\beta_4(v) = \frac{-24192(\cos(v))^4 - (17671v^2 - 24192)(\cos(v))^3 + (12096 + 11811v^2)(\cos(v))^2 - (15120 + 2109v^2)\cos(v) + 409v^2 + 3024}{24192\ v^2\ (\cos(v) - 1)^4},$$

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

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

$$\beta_4(v) = \frac{45767}{725760} + \frac{58061}{31933440}v^2 + \frac{2399921}{261534873600}v^4 - \frac{602311}{298896998400}v^6 - \frac{1067953}{7904165068800}v^8 - \frac{29376529643}{5109094217170944000}v^{10} - \frac{3029692489}{16057153253965824000}v^{12} - \frac{89043304369}{18801466719189073920000}v^{14} - \frac{9809592400337}{14518492600557802881024000}v^{16} + \frac{47323386203}{30565247580121690275840000}v^{18},$$

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

The implicit symmetric multistep method (27) has an interval of periodicity $(0, v_0^2)$ where $v_0^2 = 3.57524404$.

The local truncation error of the above method is given by:

$$L.T.E. = -\frac{58061}{31933440} \quad h^{12}\left(y_n^{(12)} + y_n^{(10)}\omega^2\right) + O(h^{14}) \tag{28}$$

The above implicit symmetric multistep method, has eight steps 10th algebraic order and infinite order of phase-lag (phase-fitted).

3.2 The explicit method

From the form (20) with $m = 8$ and $b_8 = 0$ we get the form of the eight-step symmetric explicit methods:

$$\begin{aligned} y_4 = &-\left(y_{-4} + a_3\left(y_3 + y_{-3}\right) + a_2\left(y_2 + y_{-2}\right) + a_1\left(y_1 + y_{-1}\right) + a_0 y_0\right) \\ &+h^2\left(b_3\left(f_3 + f_{-3}\right) + b_2\left(f_2 + f_{-2}\right) + b_1\left(f_1 + f_{-1}\right) + b_0 f_0\right). \end{aligned} \tag{29}$$

The characteristic equation (14) becomes

$$\sum_{i=1}^{4} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \tag{30}$$

where

$$A_i(v) = a_i + v^2 b_i, \qquad i = 0(1)4, \qquad a_4 = 1, \qquad b_4 = 0.$$

From (27) with $\beta_4(v) = 0$, the explicit symmetric method of Quinlan–Tremaine [78], with eight steps and eighth algebraic order, obtained:

$$\begin{aligned} y_4 = &-\Big(y_{-4} - 2(y_3 + y_{-3}) + 2(y_2 + y_{-2}) - (y_1 + y_{-1})\Big) \\ &+h^2\Big(\frac{17671}{12096}(f_3 + f_{-3}) - \frac{23622}{12096}(f_2 + f_{-2}) + \frac{61449}{12096}(f_1 + f_{-1}) - \frac{50516}{12096} f_0\Big) \end{aligned} \tag{31}$$

where $y_i = y(x + ih)$, $f_i = f(x + ih, y(x + ih))$, $i = -4(1)3$.

(We see that: $a_3 = -2$, $a_2 = 2$, $a_1 = -1$, $a_0 = 0$, $b_3 = \frac{17671}{12096}$, $b_2 = -\frac{23622}{12096} = -\frac{3937}{2016}$, $b_1 = \frac{61449}{12096} = \frac{20483}{4032}$, $b_0 = -\frac{50516}{12096} = -\frac{12629}{3024}$.)

This method has an interval of periodicity $(0, v_0^2)$ where $v_0^2 = 0.52$, eighth algebraic order and eighth order of phase-lag (see [28]).

The local truncation error of the above method is given by:

$$L.T.E. = \frac{45767}{725760} \quad y_n^{(10)} h^{10} + O(h^{12}) \tag{32}$$

3.3 The general m-step predictor–corrector pair form

From J.D. Lambert [87] we have that the general m-step predictor–corrector or PC pair is:

$$\begin{aligned} \sum_{j=0}^{m} a_j^* \, y_{n+j} &= h \sum_{j=0}^{m-1} b_j^* \, f_{n+j} \\ \sum_{j=0}^{m} a_j \, y_{n+j} &= h \sum_{j=0}^{m} b_j \, f_{n+j} \end{aligned} \tag{33}$$

Let the predictor and corrector defined by (33) have orders p^* and p 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 $p^* < p$ and $\lambda =< p - p^* - 1$, the order of the PC method is $p^* + \lambda (< p)$ [83].

We consider the pair of linear multistep methods:

$$\left.\begin{aligned} \sum_{i=0}^{m} a_i y_{n+i} &= h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \\ \sum_{i=0}^{m} \alpha_i y_{n+i} &= h^2 \sum_{i=0}^{m} \beta_i(v) f(x_{n+i}, y_{n+i}) \end{aligned}\right\}$$

where $|a_0| + |b_0| \neq 0, \ |\alpha_0| + |\beta_0(v)| \neq 0, \ v = \omega h, \ \omega$ is the frequency and h is the step length.

In this case the coefficients $\beta_i(v)$, of the second method, depend on v (where $i = 0(1)m, \ v = \omega h$, ω is the frequency and h is the step length).

Without loss of generality we assume $a_m = 1$ and $\alpha_m = 1$ we can write

$$\left.\begin{aligned} y_{n+m} + \sum_{i=0}^{m-1} a_i y_{n+i} &= h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \\ y_{n+m} + \sum_{i=0}^{m-1} \alpha_i y_{n+i} &= h^2 \Big(\beta_m(v) f(x_{n+m}, y_{n+m}) + \sum_{i=0}^{m-1} \beta_i(v) f(x_{n+i}, y_{n+i}) \Big) \end{aligned}\right\}$$

and we have

$$\left.\begin{aligned} y_{n+m} &= - \sum_{i=0}^{m-1} a_i y_{n+i} + h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \\ y_{n+m} &= - \sum_{i=0}^{m-1} \alpha_i y_{n+i} + h^2 \beta_m(v) f(x_{n+m}, y_{n+m}) + h^2 \sum_{i=0}^{m-1} \beta_i(v) f(x_{n+i}, y_{n+i}) \end{aligned}\right\} \tag{34}$$

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

$$\left.\begin{aligned} y_{n+m}^* &= - \sum_{i=0}^{m-1} a_i y_{n+i} + h^2 \sum_{i=0}^{m-1} b_i f(x_{n+i}, y_{n+i}) \\ y_{n+m} &= - \sum_{i=0}^{m-1} \alpha_i y_{n+i} + h^2 \beta_m(v) f(x_{n+m}, y_{n+m}^*) + h^2 \sum_{i=0}^{m-1} \beta_i(v) f(x_{n+i}, y_{n+i}) \end{aligned}\right\} \tag{35}$$

where $|a_0| + |b_0| \neq 0, \ |\alpha_0| + |\beta_0(v)| \neq 0, \ v = \omega h, \ \omega$ is the frequency and h is the step length.

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

From (35) for $m = 8$, we get the form of the symmetric predictor–corrector eight-step method:

$$\left.\begin{aligned} y_4^* = &-(y_{-4} + a_3(y_3 + y_{-3}) + a_2(y_2 + y_{-2}) + a_1(y_1 + y_{-1}) + a_0 y_0) \\ &+h^2(b_3(f_3 + f_{-3}) + b_2(f_2 + f_{-2}) + b_1(f_1 + f_{-1}) + b_0 f_0) \\ y_4 = &-(y_{-4} + \alpha_3(y_3 + y_{-3}) + \alpha_2(y_2 + y_{-2}) + \alpha_1(y_1 + y_{-1}) + \alpha_0 y_0) \\ &+h^2(\beta_4(v)(f_4 + f_{-4}) + \beta_3(v)(f_3 + f_{-3}) + \beta_2(v)(f_2 + f_{-2}) \\ &+\beta_1(v)(f_1 + f_{-1}) + \beta_0(v) f_0) \end{aligned}\right\} \tag{36}$$

where $y_i = y(x + ih)$, $f_i = f(x + ih, y(x + ih))$, $i = -4(1)3$, $f_4 = f(x + 4h, y_4^*)$, $v = \omega h$, ω is the frequency and h is the step length.

The characteristic equation (14) becomes

$$\sum_{i=1}^{4} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \tag{37}$$

where

$$\begin{gathered} A_i(v) = \alpha_i + v^2(\beta_i(v) - a_i\,\beta_4(v)) - v^4\, b_i\,\beta_4(v), \\ i = 0(1)4, \qquad \alpha_4 = a_4 = 1, \qquad b_4 = 0. \end{gathered} \tag{38}$$

3.4 The new predictor–corrector pair form (SEPCM)

From (34) for $\alpha_i = a_i$, $i = 0(1)m$, we get:

$$\left.\begin{aligned} y_{n+m} &= -\sum_{i=0}^{m-1} a_i\, y_{n+i} + h^2 \sum_{i=0}^{m} b_i\, f(x_{n+i}, y_{n+i}) \\ y_{n+m} &= -\sum_{i=0}^{m-1} a_i\, y_{n+i} + h^2 \beta_m(v) f(x_{n+m}, y_{n+m}) + h^2 \sum_{i=0}^{m-1} \beta_i(v) f(x_{n+i}, y_{n+i}) \end{aligned}\right\}$$

If we call:

$$A_n = -\sum_{i=0}^{m-1} a_i\, y_{n+i},$$

we can write

$$\left.\begin{aligned} y_{n+m} &= A_n + h^2 \sum_{i=0}^{m-1} b_i\, f(x_{n+i}, y_{n+i}) \\ y_{n+m} &= A_n + h^2 \beta_m(v) f(x_{n+m}, y_{n+m}) + h^2 \sum_{i=0}^{m-1} \beta_i(v) f(x_{n+i}, y_{n+i}) \end{aligned}\right\}$$

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

$$\left.\begin{aligned} y^*_{n+m} &= A_n + h^2 \sum_{i=0}^{m-1} b_i\, f(x_{n+i}, y_{n+i}) \\ y_{n+m} &= A_n + h^2 \beta_m(v) f(x_{n+m}, y^*_{n+m}) + h^2 \sum_{i=0}^{m-1} \beta_i(v) f(x_{n+i}, y_{n+i}) \end{aligned}\right\} \tag{39}$$

where $A_n = -\sum_{i=0}^{m-1} a_i y_{n+i}$, $|a_0| + |b_0| \neq 0$, $|a_0| + |\beta_0(v)| \neq 0$, $v = \omega h$, ω is the frequency and h is the step length.

In this pair form the coefficients $\beta_i(v)$, of the corrector method, depend on v (where $i = 0(1)m$, $v = \omega h$, ω is the frequency and h is the step length).

We call the above method Semi-Embedded Predictor–Corrector Method (SEPCM), in the sense that a part of the predictor method is contained in the corrector method.

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

From (39) for $m = 8$, we get the form of the symmetric semi-embedded predictor–corrector method (SEPCM) with eight-steps:

$$\left.\begin{aligned} A &= -\left(y_{-4} + a_3 (y_3 + y_{-3}) + a_2 (y_2 + y_{-2}) + a_1 (y_1 + y_{-1}) + a_0 y_0\right) \\ y^*_4 &= A + h^2 \left(b_3 (f_3 + f_{-3}) + b_2 (f_2 + f_{-2}) + b_1 (f_1 + f_{-1}) + b_0 f_0\right) \\ y_4 &= A + h^2 \Big(\beta_4(v) (f_4 + f_{-4}) + \beta_3(v) (f_3 + f_{-3}) \\ &\qquad + \beta_2(v) (f_2 + f_{-2}) + \beta_1(v) (f_1 + f_{-1}) + \beta_0(v) f_0\Big) \end{aligned}\right\} \tag{40}$$

where $y_i = y(x + ih)$, $f_i = f(x + ih, y(x + ih))$, $i = -4(1)3$, $f_4 = f(x + 4h, y^*_4)$, $v = \omega h$, ω is the frequency and h is the step length.

The characteristic equation (14) becomes

$$\sum_{i=1}^{4} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \tag{41}$$

where

$$\begin{aligned} A_i(v) = a_i + v^2(\beta_i(v) - a_i\, \beta_4(v)) - v^4\, b_i\, \beta_4(v), \\ i = 0(1)4, \qquad a_4 = 1, \qquad b_4 = 0. \end{aligned} \tag{42}$$

3.5 The new optimized symmetric semi-embedded predictor–corrector method

From (40), (31) and (26) a new optimized symmetric eight-step semi-embedded predictor–corrector method (SEPCM) with minimal phase-lag obtained:

$$\left.\begin{array}{l} A = -y_{-4} + 2(y_3 + y_{-3}) - 2(y_2 + y_{-2}) + (y_1 + y_{-1}) \\ y_4^* = A + h^2\left(\frac{17671}{12096}(f_3 + f_{-3}) - \frac{23622}{12096}(f_2 + f_{-2}) + \frac{61449}{12096}(f_1 + f_{-1}) - \frac{50516}{12096} f_0\right) \\ y_4 = A + h^2\Big(\beta_4(v)(f_4^* + f_{-4}) + \left(\frac{17671}{12096} - 8\beta_4(v)\right)(f_3 + f_{-3}) \\ \quad +(28\beta_4(v) - \frac{3937}{2016})(f_2 + f_{-2}) + \left(\frac{20483}{4032} - 56\beta_4(v)\right)(f_1 + f_{-1}) \\ \quad +(70\beta_4(v) - \frac{12629}{3024}) f_0\Big) \end{array}\right\} \tag{43}$$

where $y_i = y(x+ih),\ f_i = f(x+ih, y(x+ih)),\ i = -4(1)3,\ f_4^* = f(x+4h, y_4^*)$,

$$\beta_4(v) = \frac{-24192(\cos(v))^4 - (17671v^2 - 24192)(\cos(v))^3 + (12096 + 11811v^2)(\cos(v))^2 - (15120 + 2109v^2)\cos(v) + 409v^2 + 3024}{24192\ v^2\ (\cos(v) - 1)^4},$$

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

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

$$\begin{aligned} \beta_4(v) = {} & \frac{45767}{725760} + \frac{58061}{31933440} v^2 + \frac{2399921}{261534873600} v^4 - \frac{602311}{298896998400} v^6 \\ & - \frac{1067953}{7904165068800} v^8 - \frac{29376529643}{5109094217170944000} v^{10} - \frac{3029692489}{16057153253965824000} v^{12} \\ & - \frac{89043304369}{18801466719189073920000} v^{14} - \frac{9809592400337}{14518492600557802881024000 0} v^{16} \\ & + \frac{47323386203}{305652475801216902758400000} v^{18}, \end{aligned}$$

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

The new optimized symmetric eight-step semi-embedded predictor–corrector method (43) has an interval of periodicity $(0, v_0^2)$ where $v_0^2 = 0.9758918$.

The local truncation error of the above method is given by:

$$L.T.E. = \left(\frac{12506213339}{5794003353600} y_n^{(12)} - \frac{58061}{31933440} y_n^{(10)} \omega^2\right) h^{12} + O(h^{14}) \tag{44}$$

The new optimized symmetric eight-step semi-embedded predictor–corrector method, has eight steps 10th algebraic order and 10th order of phase-lag.

4 Numerical results

4.1 The problems

The efficiency of the new optimized symmetric eight-step semi-embedded predictor–corrector method will be measured through the integration of seven initial value problems with oscillating solution.

4.1.1 Orbital problem by Stiefel and Bettis

The "almost" periodic orbital problem studied by [81] can be described by

$$y'' + y = 0.001\, e^{i\,x}, \quad y(0) = 1, \quad y'(0) = 0.9995\, i, \quad y \in \mathcal{C}, \tag{45}$$

or equivalently by

$$\begin{aligned} u'' + u &= 0.001\, \cos(x), \quad u(0) = 1, \quad u'(0) = 0, \\ v'' + v &= 0.001\, \sin(x), \quad v(0) = 0, \quad v'(0) = 0.9995. \end{aligned} \tag{46}$$

The theoretical solution of the problem (45) is given below:

$$\begin{aligned} y(x) &= u(x) + i\, v(x), \quad u, v \in \mathcal{R} \\ u(x) &= \cos(x) + 0.0005\, x\, \sin(x), \\ v(x) &= \sin(x) - 0.0005\, x\, \cos(x). \end{aligned}$$

The system of equations (46) has been solved for $x \in [0, 1000\,\pi]$. Estimated frequency: $w = 1$.

4.1.2 Nonlinear equation

$$y'' = -100y + \sin(y), \quad \text{with} \quad y(0) = 0, y'(0) = 1, \quad t \in [0, 20\pi].$$

The theoretical solution is not known, but we use $y(20\,\pi) = 3.92823991 \cdot 10^{-4}$. Estimated frequency: $w = 10$.

4.1.3 Inhomogeneous equation

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

Theoretical solution: $y(t) = \sin(t) + \sin(10\,t) + \cos(10\,t)$. Estimated frequency: $w = 10$.

4.1.4 Orbital problem by Franco and Palacios

The "almost" periodic orbital problem studied by [80] can be described by

$$y'' + y = \epsilon e^{i\psi x}, \quad y(0) = 1, \quad y'(0) = i, \quad y \in \mathcal{C}, \tag{47}$$

or equivalently by

$$\begin{aligned} u'' + u &= \epsilon \cos(\psi x), \quad u(0) = 1, \quad u'(0) = 0, \\ v'' + v &= \epsilon \sin(\psi x), \quad v(0) = 0, \quad v'(0) = 1, \end{aligned} \tag{48}$$

where $\epsilon = 0.001$ and $\psi = 0.01$. The theoretical solution of the problem (47) is given below:

$$\begin{aligned} y(x) &= u(x) + i\, v(x), \quad u, v \in \mathcal{R} \\ u(x) &= \tfrac{1-\epsilon-\psi^2}{1-\psi^2}\, \cos(x) + \tfrac{\epsilon}{1-\psi^2}\, \cos(\psi\, x) \\ v(x) &= \tfrac{1-\epsilon\psi-\psi^2}{1-\psi^2}\, \sin(x) + \tfrac{\epsilon}{1-\psi^2}\, \sin(\psi\, x) \end{aligned}$$

The system of equations (48) has been solved for $x \in [0, 1000\,\pi]$. The estimated frequency is $w = 1$.

4.1.5 Duffing equation

$$y'' = -y - y^3 + 0.002\cos(1.01\,t), \tag{49}$$

with $y(0) = 0.200426728067$, $y'(0) = 0$, $\quad t \in [0, 1000\,\pi]$.

Theoretical solution:

$y(t) = 0.200179477536\cos(1.01\,t) + 2.46946143 \cdot 10^{-4}\cos(3.03\,t) + 3.04014 \cdot 10^{-7}\cos(5.05\,t) + 3.74 \cdot 10^{-10}\cos(7.07\,t) + \cdots$

Estimated frequency: $w = 1$.

4.1.6 Two-body problem

$$y'' = -\frac{y}{(y^2+z^2)^{\frac{3}{2}}}, \quad z'' = -\frac{z}{(y^2+z^2)^{\frac{3}{2}}}, \tag{50}$$

with $y(0) = 1$, $y'(0) = 0$, $z(0) = 0$, $z'(0) = 1, t \in [0, 1000\,\pi]$. Theoretical solution: $y(t) = \cos(t)$ and $z(t) = \sin(t)$.

We used the estimation $w = \frac{1}{(y^2+z^2)^{\frac{3}{4}}}$ as frequency of the problem.

4.1.7 Schrödinger equation: resonance problem

We will integrate problem (2) with $l = 0$ at the interval [0, 15] using the well-known Woods-Saxon potential

$$V(x) = \frac{u_0}{1+q} + \frac{u_1\, q}{(1+q)^2}, \qquad q = \exp\left(\frac{x-x_0}{a}\right), \quad \text{where}$$
$$u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a} \tag{51}$$

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 (2) becomes

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \tag{52}$$

The last equation has two linearly independent solutions $k\,x\,j_l(k\,x)$ and $k\,x\,n_l(k\,x)$, where j_l and n_l are the *spherical Bessel* and *Neumann* functions. When $x \to \infty$ the solution takes the asymptotic form

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos(k\,x - \pi\,l/2)], \end{aligned} \tag{53}$$

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

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{54}$$

where $S(x) = k\,x\,j_l(k\,x)$, $C(x) = k\,x\,n_l(k\,x)$ 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: $E = 989.701916$. As for the frequency ω we will use the suggestion of Ixaru and Rizea [77]:

$$\omega = \begin{cases} \sqrt{E+50}, & x \in [0,\ 6.5] \\ \sqrt{E}, & x \in [6.5,\ 15] \end{cases} \tag{55}$$

4.2 The methods

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

- The new optimized symmetric eight-step semi-embedded predictor–corrector method with 10th algebraic order and minimal phase-lag(43) (New SEPCM)
- The symmetric 10-step method of Quinlan–Tremaine of order ten [78] (Q–T 10 step)
- The symmetric 8-step method of Quinlan–Tremaine of order eight [78] (Q–T 8 step)
- The 8-step, predictor–corrector method Störmer–Cowell of order eight [83] (S–C 8 step)
- The symmetric 6-step method of Jenkins of order six [79] (Jenkins 8 step)
- The 2-step, 3-stage exponentially-fitted predictor–corrector method of Simos and Williams of algebraic order six [69] (W–S EF1)
- The 3-step, 3-stage exponentially-fitted predictor–corrector method (EF2) of Psihoyios and Simos of algebraic order five [64] (P-S EF2)
- The 4-step predictor–corrector method Adams-Bashforth—Moulton of order four (PC ABM 4 step)
- The 4-step predictor–corrector method Milne–Simpson of order four. (PC M–S)

Table 1 Comparison of the new optimized 8-step SEPC-method and Quinlan–Tremaine 8-step method

Test problem	Method	Accuracy (digits)	CPU time	Step length	Maximum error
Stiefel–Bettis	Q–T 8 step	10.65397472	26.8945724	0.03093733	2.22E-11
	New SEPCM	11.71347307	16.3021045	0.06187404	1.93E-12
Nonlinear equation	Q–T 8 step	11.63199947	4.3680280	0.00386705	2.33E-12
	New SEPCM	12.62431118	2.7144174	0.00773410	2.38E-13
Inhomogeneous equation	Q–T 8 step	9.725565257	284.2650222	0.00300000	1.88E-10
	New SEPCM	10.72760342	167.6542747	0.00600000	1.87E-11
Franco–Palacios	Q–T 8 step	10.86822149	27.0973737	0.02999993	1.35E-11
	New SEPCM	11.88458887	16.0057026	0.05999986	1.30E-12
Buffing’s equation	Q–T 8 step	10.53180999	14.6016936	0.06187500	2.94E-11
	New SEPCM	10.25603121	8.8452567	0.12375000	5.55E-11
Two-body problem e = 0.4	Q–T 8 step	7.282026611	251.3644113	0.00386718	5.22E-08
	New SEPCM	7.414240786	143.8173219	0.00773437	3.85E-08
Schrodinger’s equation E = 989.701916	Q–T 8 step	8.427376708	1.6692107	0.00250000	3.74E-09
	New SEPCM	8.341404916	1.1544074	0.00500000	4.56E-09

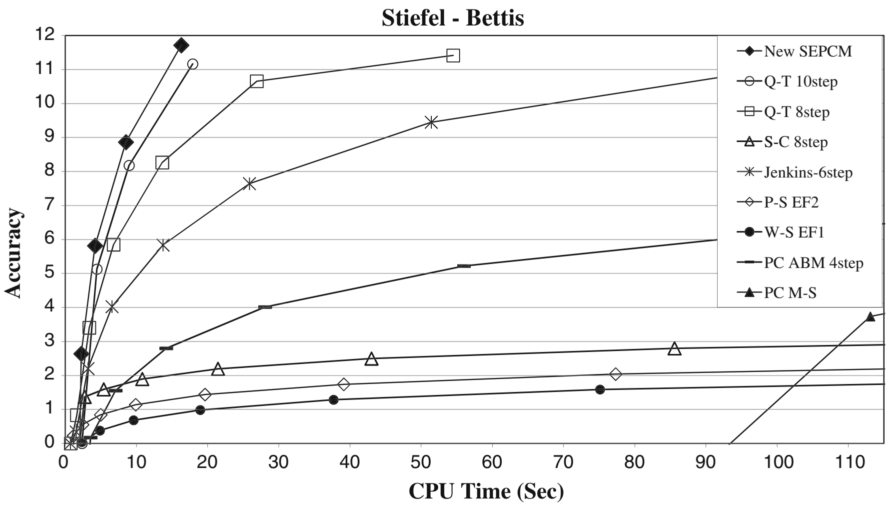

Fig. 1 Efficiency for the orbital problem by Stiefel and Bettis

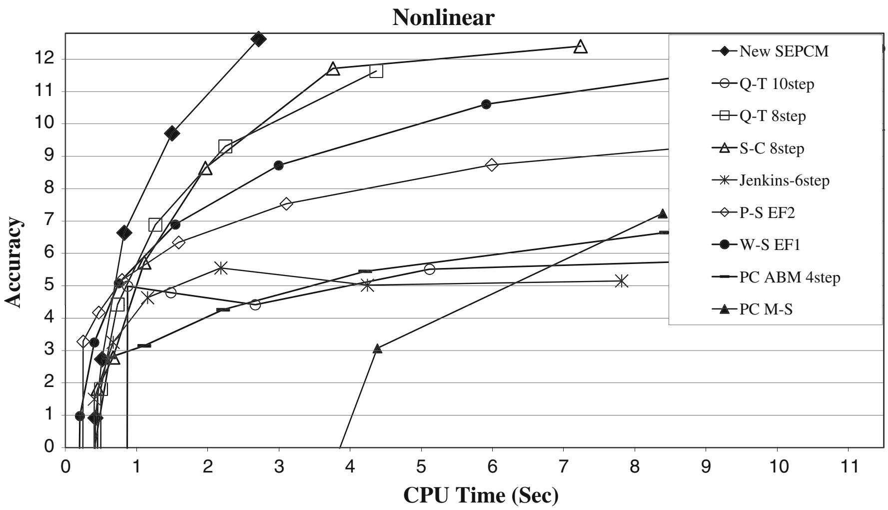

Fig. 2 Efficiency for the nonlinear equation

4.3 Comparison

We present the **accuracy** of the tested methods expressed by the $-\log_{10}$ (max. error over interval) or $-\log_{10}$(error at the end point), depending on whether we know the theoretical solution or not, versus the CPU time.

In Table 1 we see the comparison of the new optimized symmetric eight-step semi-embedded predictor–corrector method with 10th algebraic order and minimal phase-lag (43) and the multistep symmetric method of Quinlan–Tremaine [78] with eight steps and eighth algebraic order for all the problems solved.

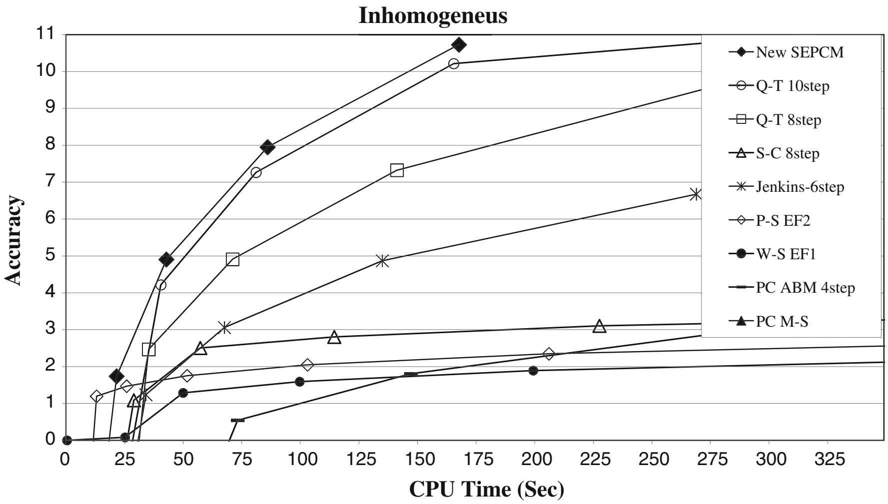

Fig. 3 Efficiency for the inhomogeneous equation

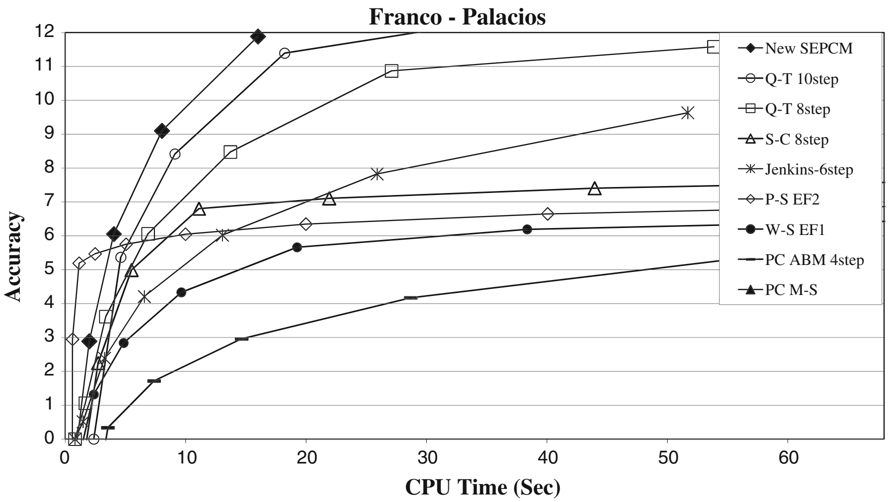

Fig. 4 Efficiency for the orbital problem by Franco and Palacios

In Fig. 1 we see the results for the Stiefel–Bettis almost periodic problem, in Fig. 2 the results for the Nonlinear equation, in Fig. 3 the results for the Inhomogeneous equation, in Fig. 4 the results for the Franco–Palacios almost periodic problem, in Fig. 5 the results for the Duffing equation, in Fig. 6 the results for the Two-body problem for eccentricity e = 0.4, in Fig. 7 the results for the resonance problem for energy $E = 989.701916$ and in Fig. 8 we see the results for the resonance problem for energy $E = 341.495874$.

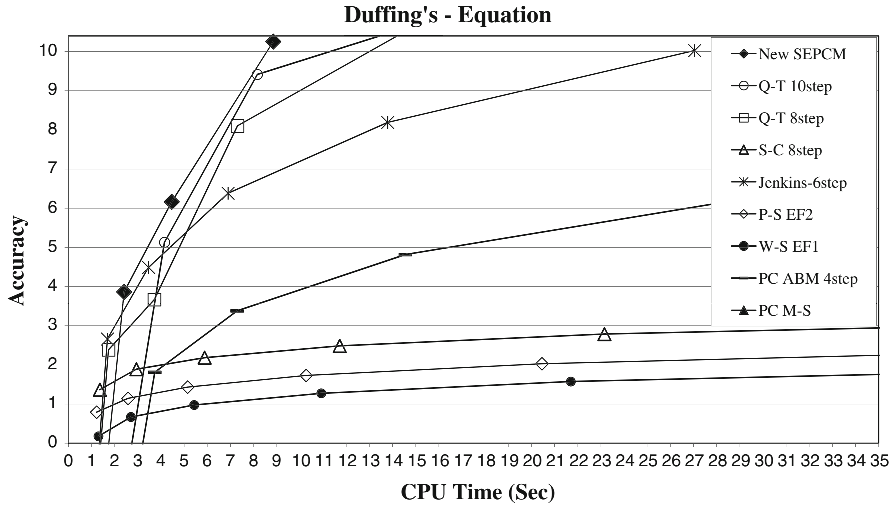

Fig. 5 Efficiency for the duffing equation

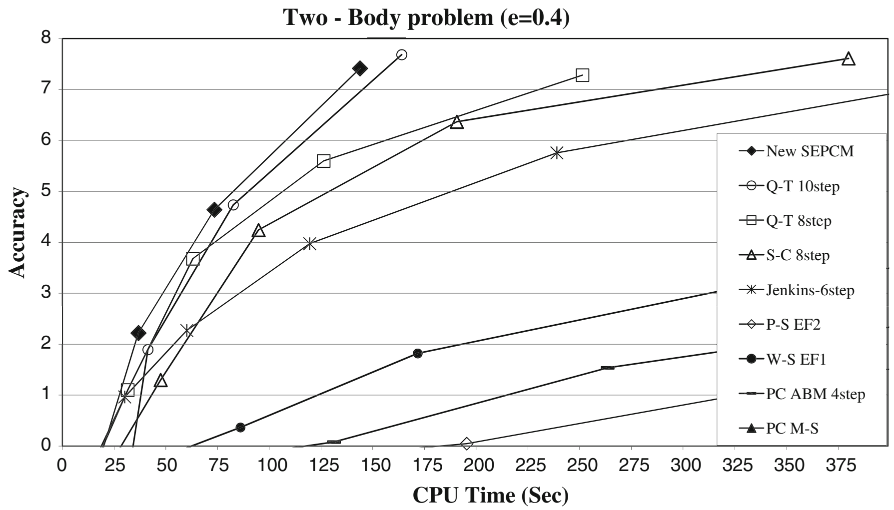

Fig. 6 Efficiency for the two-body problem using eccentricity e = 0.4

Among all the methods used, the new optimized symmetric eight-step semi-embedded predictor–corrector method with 10th algebraic order and minimal phase-lag was the most efficient.

The difference from the multistep symmetric method of Quinlan–Tremaine [78] with ten steps and tenth algebraic order was at least 0.5 decimal digits better for all the problems. The difference from the multistep symmetric method of Quinlan–Tremaine [78] with eight steps and eighth algebraic order was at least 1 decimal digit better and higher from the other compared methods for all the problems.

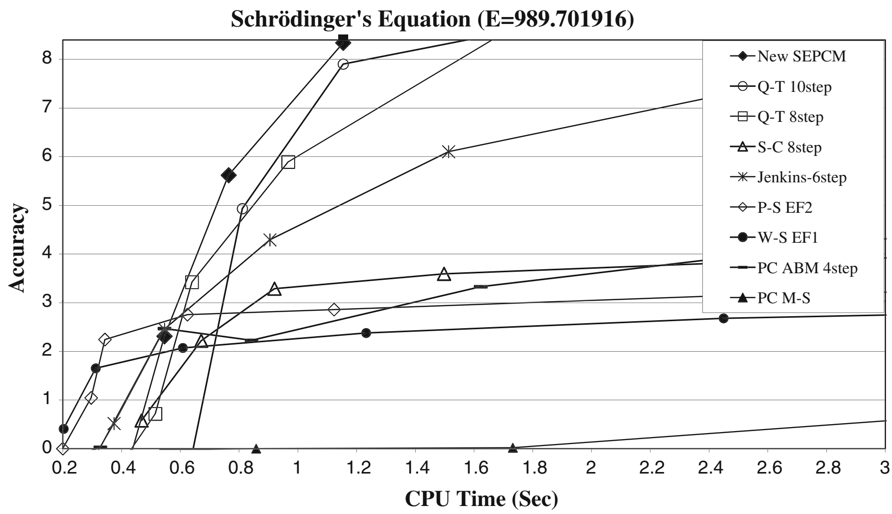

Fig. 7 Efficiency for the resonance problem using E = 989.701916

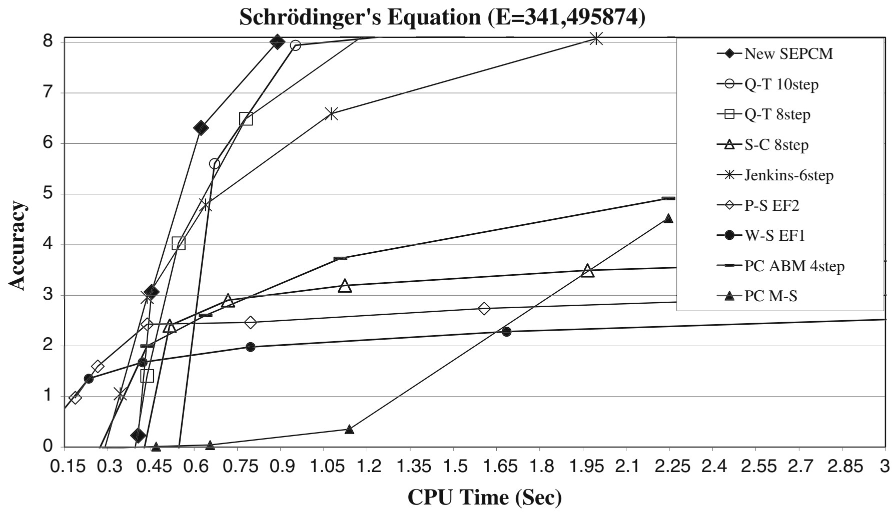

Fig. 8 Efficiency for the resonance problem using E = 341.495874

The interval of periodicity of the new optimized symmetric eight-step semi-embedded predictor–corrector method with 10th algebraic order and minimal phase-lag is about two times larger than the multistep symmetric method of Quinlan–Tremaine with eight steps and eighth algebraic order.

The new optimized symmetric eight-step semi-embedded predictor–corrector method with 10th algebraic order and minimal phase-lag can achieve the required accuracy with a stepsize two times bigger than the multistep symmetric method of Quinlan–Tremaine with eight steps and eighth algebraic order, for all the problems solved.

5 Conclusions

We have constructed a new predictor–corrector (PC) pair form (SEPCM) (39) for the numerical integration of second-order initial-value problems (1). From the form (39) we have developed a new optimized symmetric eight-step semi-embedded predictor–corrector method with 10th algebraic order and minimal phase-lag (43).

The new predictor–corrector pair form (SEPCM) (39) has the advantage that reduces the computational expense if the additions on the factor $A_n = \sum_{i=0}^{m-1} a_i y_{n+i}$, are done twice.

We have applied the new optimized symmetric eight-step semi-embedded predictor–corrector method with 10th algebraic order and minimal phase-lag (43) along with a group of recently developed methods from the literature to the Schrödinger equation and related orbital problems and other methods from the general literature. We concluded that the new optimized symmetric eight-step semi-embedded predictor–corrector method with 10th algebraic order and minimal phase-lag (43) are highly efficient compared to other optimized methods which also reveals the importance of phase-lag when solving ordinary differential equations with oscillatory solutions such as orbital problems.

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