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A New Optimized Symmetric Embedded Predictor-Corrector Method (EPCM) for Initial-Value Problems with Oscillatory Solutions

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Abstract: In this work a new optimized symmetric eight-step embedded predictor-corrector method (EPCM) with minimal phase-lag and algebraic order ten is presented. The method is based on the symmetric multistep method of Quinlan-Tremaine [1], with eight steps and eighth algebraic order and is constructed to solve numerically IVPs with oscillatory solutions. 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 with minimal phase-lag is noticeably most efficient of all the compared methods and for all the problems solved including the two-dimensional Kepler problem and the radial Schrödinger equation.

Keywords: IVPs, phase-lag, oscillatory solution, symmetric, multistep, initial value problems, EPCM, eight-step, predictor-corrector, embedded, Kepler problem, Schrödinger equation.

1 Introduction

Equations of the form

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

are used to mathematical model problems in many areas of quantum chemistry, physical chemistry and chemical physics, astrophysics, astronomy, quantum mechanics, celestial mechanics or electronics.
These ordinary differential equations are of second order in which the derivative y' does not appear explicitly.
Second-order ordinary differential equations have been integrated numerically ever since the 17th century, in the context of physical problems.
The multistep methods can be easily applied to obtain the numerical solution of a m-th order initial value problem.
A publication by Quinlan and Tremaine [1] in 1990 was revived the study of symmetric multistep methods. They have constructed high order symmetric multistep methods based on the work of Lambert and Watson (see [2]).
Many numerical methods have been developed for the numerical solution of the initial value problem (1) (see [17] - [19] and [21]-[25])

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem (1), multistep methods of the form

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

with m steps can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a,b]$ and $h = |x_{i+1} - x_i|$, $i = 0(1)m-1$, where $|a_0| + |b_0| \neq 0$.
If $b_m = 0$ the method is explicit, otherwise it is implicit.
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 (2) is associated with the operator

$$L(x) = \sum_{i=0}^{m} a_i u(x+ih) - h^2 \sum_{i=0}^{m} b_i u''(x+ih) \qquad (3)$$

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where $u \in C^2$.

Definition 1 The multistep method (2) 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

$$L(x) = C_0 u(x) + C_1 u'(x)h + \cdots + C_q u^{(q)}(x)h^q + \ldots, \tag{4}$$

the coefficients C_q are given

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

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

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

The order p is the unique integer for which

$$C_0 = \cdots = C_{p+1} = 0,\ C_{p+2} \neq 0. \tag{5}$$

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

$$C_0 = C_1 = C_2 = 0. \tag{6}$$

In what follows we will assume that the method (2) is consistent.

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

$$y'' = -\omega^2 y \tag{7}$$

a difference equation of the form

$$\sum_{i=1}^{k} A_i(v)(y_{n+i} + y_{n-i}) + A_0(v)y_n = 0 \tag{8}$$

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 (8) is

$$\sum_{i=1}^{k} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \tag{9}$$

From Lambert and Watson (1976) we have the following definitions:

Definition 2 A symmetric $2k$-step method with characteristic equation given by (9) 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. (9) satisfy:

$$s_1 = e^{i\theta(v)},\ s_2 = e^{-i\theta(v)},\ and\ |s_i| \leq 1,\ i = 3(1)2k \tag{10}$$

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

Definition 3 For any method corresponding to the characteristic equation (9) the phase-lag is defined as the leading term in the expansion of

$$t = v - \theta(v) \tag{11}$$

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

Theorem 1[14] *The symmetric $2k$-step method with characteristic equation given by (9) has phase-lag order q and phase-lag constant c given by:*

$$-cv^{q+2} + O(v^{q+4}) = \frac{2\sum_{j=1}^{k} A_j(v)\cos(jv) + A_0(v)}{2\sum_{j=1}^{k} j^2 A_j(v)} \tag{12}$$

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:

$$-cv^{q+2} + O(v^{q+4}) = \frac{T_0}{32A_4(v)+18A_3(v)+8A_2(v)+2A_1(v)} \tag{13}$$

where

$$T_0 = 2A_4(v)\cos(4v) + 2A_3(v)\cos(3v)$$
$$+2A_2(v)\cos(2v) + 2A_1(v)\cos(v) + A_0(v)$$

3 The Embedded Predictor-Corrector pair form (EPCM)

3.1 The general m-step predictor-corrector pair form

From J.D. Lambert (1991) we have that the general m-step predictor-corrector or PC pair is:

$$\left.\begin{aligned} \sum_{i=0}^{m} a_i^*\, y_{n+i} &= h \sum_{i=0}^{m-1} b_i^*\, f_{n+i} \\ \sum_{i=0}^{m} a_i\, y_{n+i} &= h \sum_{i=0}^{m} b_i\, f_{n+i} \end{aligned}\right\} \tag{14}$$

Let the predictor and corrector defined by (14) 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 $p^* + \lambda (< p)$ [4] .
We consider the pair of linear multistep methods:

$$\left.\begin{aligned} \sum_{i=0}^{m} a_i^*\, y_{n+i} &= h^2 \sum_{i=0}^{m-1} b_i^*\, f_{n+i} \\ \sum_{i=0}^{m} a_i\, y_{n+i} &= h^2 \sum_{i=0}^{m} b_i\, f_{n+i} \end{aligned}\right\} \tag{15}$$

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where $|a_0^*|+|b_0^*|\neq 0$, $|a_0|+|b_0|\neq 0$, $b_m^*=0$ and $b_m\neq 0$.
Without loss of generality we assume $a_m^*=1$ and $a_m=1$ we can write:

$$\left.\begin{aligned} & y_{n+m}+\sum_{i=0}^{m-1} a_i^* y_{n+i}=h^2\sum_{i=0}^{m-1} b_i^* f(x_{n+i},y_{n+i}) \\ & y_{n+m}+\sum_{i=0}^{m-1} a_i y_{n+i}=h^2 \\ & \Big(b_m f(x_{n+m},y_{n+m})+\sum_{i=0}^{m-1} b_i f(x_{n+i},y_{n+i})\Big) \end{aligned}\right\} \quad (16)$$

and we have:

$$\left.\begin{aligned} y_{n+m} &= -\sum_{i=0}^{m-1} a_i^* y_{n+i}+ \\ &+h^2\sum_{i=0}^{m-1} b_i^* f(x_{n+i},y_{n+i}) \\ y_{n+m} &= -\sum_{i=0}^{m-1} a_i y_{n+i}+h^2 b_m f(x_{n+m},y_{n+m})+ \\ &+h^2\sum_{i=0}^{m-1} b_i f(x_{n+i},y_{n+i}) \end{aligned}\right\} \quad (17)$$

From this pair, a general predictor-corrector (PC) pair form, for the numerical integration of special second-order initial-value problems (1) is formally defined as follows:

$$\left.\begin{aligned} y^*_{n+m} &= -\sum_{i=0}^{m-1} a_i^* y_{n+i}+ \\ &+h^2\sum_{i=0}^{m-1} b_i^* f(x_{n+i},y_{n+i}) \\ y_{n+m} &= -\sum_{i=0}^{m-1} a_i y_{n+i}+h^2 b_m f(x_{n+m},y^*_{n+m})+ \\ &+h^2\sum_{i=0}^{m-1} b_i f(x_{n+i},y_{n+i}) \end{aligned}\right\} \quad (18)$$

where $|a_0^*|+|b_0^*|\neq 0$, $|a_0|+|b_0|\neq 0$ and $b_m\neq 0$.
If the method is symmetric then $a_i^*=a_{m-i}^*$, $b_i^*=b_{m-i}^*$, $a_i=a_{m-i}$ and $b_i=b_{m-i}$, $i=0(1)\lfloor\frac{m}{2}\rfloor$.
From (18) for $m=8$, we get the form of the symmetric predictor-corrector eight-step method:

$$\left.\begin{aligned} & y_4^*=-\Big(y_{-4}+a_3^*(y_3+y_{-3})+a_2^*(y_2+y_{-2})+ \\ & +a_1^*(y_1+y_{-1})+a_0^* y_0\Big) \\ & \quad +h^2\Big(b_3^*(f_3+f_{-3})+b_2^*(f_2+f_{-2})+ \\ & +b_1^*(f_1+f_{-1})+b_0^* f_0\Big) \\ & y_4=-\Big(y_{-4}+a_3(y_3+y_{-3})+a_2(y_2+y_{-2})+ \\ & +a_1(y_1+y_{-1})+a_0 y_0\Big) \\ & \quad +h^2\Big(b_4(f_4+f_{-4})+b_3(f_3+f_{-3})+ \\ & +b_2(f_2+f_{-2})+b_1(f_1+f_{-1})+b_0 f_0\Big) \end{aligned}\right\} \quad (19)$$

where $y_i=y(x+ih)$, $f_i=f(x+ih,y(x+ih))$, $i=-4(1)3$, $f_4=f(x+4h,y_4^*)$ and h is the step length.
The characteristic equation (9) becomes

$$\sum_{i=1}^{4} A_i(v)(s^i+s^{-i})+A_0(v)=0 \quad (20)$$

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

3.2 The m-step embedded predictor-corrector (EPCM) pair form

From (18) for $a_i=a_i^*$, $i=0(1)m-1$, we get:

$$\left.\begin{aligned} y^*_{n+m} &= -\sum_{i=0}^{m-1} a_i^* y_{n+i}+h^2\sum_{i=0}^{m-1} b_i^* f(x_{n+i},y_{n+i}) \\ y_{n+m} &= -\sum_{i=0}^{m-1} a_i^* y_{n+i}+h^2 b_m f(x_{n+m},y^*_{n+m})+ \\ &\quad +h^2\sum_{i=0}^{m-1} b_i f(x_{n+i},y_{n+i}) \end{aligned}\right\} \quad (21)$$

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

For the coefficients b_i^* and b_i of the above general m-step predictor-corrector pair form (21), we can write:
$b_i=b_i+0=b_i-b_i^*+b_i^*=(b_i-b_i^*)+b_i^*$,
if we call $\beta_i=b_i-b_i^*$, $i=0(1)m-1$, then we get:

$$b_i=\beta_i+b_i^*, \quad (22)$$

so we have:

$$\begin{aligned} & h^2\sum_{i=0}^{m-1} b_i f(x_{n+i},y_{n+i})= \\ &=h^2\sum_{i=0}^{m-1}(\beta_i+b_i^*)f(x_{n+i},y_{n+i})= \\ & h^2\sum_{i=0}^{m-1}\beta_i f(x_{n+i},y_{n+i})+ \\ & +h^2\sum_{i=0}^{m-1} b_i^* f(x_{n+i},y_{n+i}) \end{aligned} \quad (23)$$

and we can write:

$$\left.\begin{aligned} y^*_{n+m} &= -\sum_{i=0}^{m-1} a_i^* y_{n+i}+h^2\sum_{i=0}^{m-1} b_i^* f(x_{n+i},y_{n+i}) \\ y_{n+m} &= -\sum_{i=0}^{m-1} a_i^* y_{n+i}+h^2 b_m f(x_{n+m},y^*_{n+m}) \\ &+h^2\sum_{i=0}^{m-1}\beta_i f(x_{n+i},y_{n+i})+ \\ &+h^2\sum_{i=0}^{m-1} b_i^* f(x_{n+i},y_{n+i}) \end{aligned}\right\} \quad (24)$$

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or

$$\left.\begin{array}{l} y^*_{n+m} = -\sum\limits_{i=0}^{m-1} a^*_i y_{n+i} + h^2 \sum\limits_{i=0}^{m-1} b^*_i f(x_{n+i}, y_{n+i}) \\ y_{n+m} = -\sum\limits_{i=0}^{m-1} a^*_i y_{n+i} + h^2 \sum\limits_{i=0}^{m-1} b^*_i f(x_{n+i}, y_{n+i}) \\ +h^2 b_m f(x_{n+m}, y^*_{n+m}) + h^2 \sum\limits_{i=0}^{m-1} \beta_i f(x_{n+i}, y_{n+i}) \end{array}\right\} \quad (25)$$

where $|a^*_0| + |b^*_0| \neq 0$, $|a^*_0| + |\beta_0| \neq 0$ and $b_m \neq 0$.
From m-step predictor-corrector pair (15) we have that $b^*_m = 0$ and $b_m \neq 0$,
so if we call $\beta_m = b_m - b^*_m$, then we get:

$$\beta_m = b_m - b^*_m = b_m - 0 = b_m \neq 0 \quad (26)$$

Finally for:

$$\beta_i = b_i - b^*_i, i = 0(1)m \quad (27)$$

the m-step predictor-corrector pair form (25) becomes:

$$\left.\begin{array}{l} y^*_{n+m} = -\sum\limits_{i=0}^{m-1} a^*_i y_{n+i} + h^2 \sum\limits_{i=0}^{m-1} b^*_i f(x_{n+i}, y_{n+i}) \\ y_{n+m} = y^*_{n+m} + h^2 \sum\limits_{i=0}^{m} \beta_i f(x_{n+i}, y_{n+i}) \end{array}\right\} \quad (28)$$

where $|a^*_0| + |b^*_0| \neq 0$, $|a^*_0| + |\beta_0| \neq 0$.

We call the above method Embedded Predictor-Corrector Method (EPCM), in the sense that the predictor method is fully contained in the corrector method (see [8]).

If the method is symmetric then $a^*_i = a^*_{m-i}$, $b^*_i = b^*_{m-i}$ and $\beta_i = \beta_{m-i}$, $i = 0(1)\lfloor \frac{m}{2} \rfloor$.

4 Construction of the new embedded predictor-corrector (EPCM) method

From the form (2) and without loss of generality we assume $a_m = 1$ and we can write:

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

finally we get:

$$y_{n+m} = -\sum_{i=0}^{m-1} a_i y_{n+i} + h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \quad (29)$$

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

4.1 The explicit (predictor) method - with phase-lag order infinite

From the form (29) with $m = 8$ and $b_8 = 0$ we get the form of the eight-step symmetric explicit methods:

$$\begin{array}{l} y_4 = -\Big(y_{-4} + a_3 (y_3 + y_{-3}) + a_2 (y_2 + y_{-2}) + \\ +a_1 (y_1 + y_{-1}) + a_0 y_0\Big) + \\ +h^2 \Big(b_3 (f_3 + f_{-3}) + b_2 (f_2 + f_{-2}) + \\ +b_1 (f_1 + f_{-1}) + b_0 f_0\Big). \end{array} \quad (30)$$

where $y_i = y(x + ih)$, $f_i = f(x + ih, y(x + ih))$, and h is the step length.
The characteristic equation (9) becomes

$$\sum_{i=1}^{4} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \quad (31)$$

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

From (30) with

$$\begin{array}{llll} a_3 = -2, & a_2 = 2, & a_1 = -1, & a_0 = 0, \\ b_3 = \frac{17671}{12096}, & b_2 = -\frac{23622}{12096}, & & \\ b_1 = \frac{61449}{12096}, & b_0 = -\frac{50516}{12096}, & & \end{array} \quad (32)$$

we obtain the multistep symmetric method of Quinlan-Tremaine [1], with eight steps, eighth algebraic order, eighth order of phase-lag and interval of periodicity $(0, v_0^2)$, where $v_0^2 = 0.52$.
From (30) and by keeping the same a_i coefficients (32) and by nullifying the phase-lag, we get:

$$\begin{array}{llll} a^*_3 = -2, & a^*_2 = 2, & a^*_1 = -1, & a^*_0 = 0, \\ b^*_0 = -20\, b^*_3 + \frac{601}{24}, & & b^*_1 = 15\, b^*_3 - \frac{101}{6}, & \\ b^*_2 = -6\, b^*_3 + \frac{109}{16}, & & b^*_3 = \frac{A}{B} & \end{array}$$

where

$$\begin{array}{l} A = -192\, (\cos(v))^4 + 192\, (\cos(v))^3 + \\ + \left(96 - 327\, v^2\right) (\cos(v))^2 \\ \quad + \left(-120 + 404\, v^2\right) \cos(v) - 137\, v^2 + 24 \\ B = 96\, v^2 (\cos(v) - 1)^3 \end{array} \quad (33)$$

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:

$$\begin{array}{l} b^*_3 = \frac{17671}{12096} - \frac{45767}{725760}\, v^2 + \frac{164627}{47900160}\, v^4 - \frac{520367}{15850598400}\, v^6 + \\ + \frac{76873}{89669099520}\, v^8 - \frac{9190171}{32011868528640000}\, v^{10} - \\ \quad - \frac{6662921}{340606281144729600}\, v^{12} - \frac{2866814089}{2043637686868377600000}\, v^{14} - \\ \quad - \frac{10228341391}{1692132004727016652800 0}\, v^{16} - \\ \quad - \frac{1074205110763}{483949753351926762700800000}\, v^{18} - \\ \quad - \frac{1485941749021}{20325889640780924033433600000}\, v^{20} + \ldots, \end{array}$$

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where $v = \omega\, h$, ω is the frequency and h is the step length. The local truncation error of the above method is given by:

$$L.T.E. = \frac{45767}{725760}\, h^{10} \left(y_n^{(10)} + y_n^{(8)} \omega^2 \right) + O(h^{12}) \quad (34)$$

The above optimized explicit symmetric multistep method (33) has eight steps, eight algebraic order, infinite order of phase-lag (phase-fitted) (see [6]) and an interval of periodicity $(0, v_0^2)$, where $v_0^2 = 0.643168$.

4.2 The implicit method (corrector)

From (29) for $m = 8$, we get the form of the symmetric implicit eight-step method:

$$y_4 = -y_{-4} - a_3(y_3 + y_{-3}) - a_2(y_2 + y_{-2}) - -a_1(y_1 + y_{-1}) + h^2 \Big(b_4(f_4^* + f_{-4}) + b_3(f_3 + f_{-3}) +b_2(f_2 + f_{-2}) + b_1(f_1 + f_{-1}) + b_0 f_0 \Big).$$

where $y_i = y(x + ih)$, $f_i = f(x + ih, y(x + ih))$, $f_4^* = f(x + 4h, y_4^*)$ and h is the step length.
The characteristic equation (9) becomes

$$\sum_{i=1}^{4} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \quad (35)$$

where

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

From (35) and by keeping the same a_i coefficients (32) ($a_4 = 1$, $a_3 = -2$, $a_2 = 2$, $a_1 = -1$, $a_0 = 0$) we satisfy as many algebraic equations as possible, but we keep b_4 free. After achieving 10th algebraic order, the coefficients now depend on b_4:

$$b_0 = 70\, b_4 - \tfrac{12629}{3024}, \qquad b_1 = -56\, b_4 + \tfrac{20483}{4032}, \qquad b_2 = 28\, b_4 - \tfrac{3937}{2016}, \qquad b_3 = -8\, b_4 + \tfrac{17671}{12096} \quad (36)$$

and the phase-lag becomes:

$$\begin{aligned} &PL = \tfrac{C}{D}, \qquad \text{where} \\ &C = 24192\,(\cos(v))^4 + 24192\,(\cos(v))^4\, v^2 b_4 + \\ &+17671\,(\cos(v))^3\, v^2 - 96768\,(\cos(v))^3\, v^2 b_4 - \\ &-24192\,(\cos(v))^3 + 14152\,(\cos(v))^2\, v^2 b_4 - \\ &-12096\,(\cos(v))^2 - 11811\,(\cos(v))^2\, v^2 + \\ &+2109\,\cos(v)\, v^2 + 15120\,\cos(v) - \\ &-96768\,\cos(v)\, v^2 b_4 - 409\, v^2 + 24192\, v^2 b_4 - \\ &-3024 \quad \text{and} \\ &D = 1260\,\left(12 + 25\, v^2\right). \end{aligned} \quad (37)$$

We expand the phase-lag using the Taylor series and nullify the leading term (that is the coefficient of h^{10}). After that we obtain the implicit symmetric multistep method:

$$a_4 = 1, \quad a_3 = -2, \quad a_2 = 2, \quad a_1 = -1, \quad a_0 = 0 \quad b_0 = \frac{17273}{72576}, \quad b_1 = \frac{280997}{181440}, \quad b_2 = -\frac{33961}{181440}, \quad b_3 = \frac{173531}{181440}, \quad b_4 = \frac{45767}{725760} \quad (38)$$

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

$$L.T.E. = -\frac{58061}{31933440}\, h^{12} y_n^{(12)} + O(h^{14}) \quad (39)$$

The above optimized implicit symmetric multistep method (38), has eight steps, tenth algebraic order, tenth order of phase-lag (see [7]) and interval of periodicity $(0, v_0^2)$, where $v_0^2 = 2.39021991$.

4.3 The new EPCM method with minimal phase-lag

If the coefficients b_i^*, $i = 0(1)m$ in pair of linear multistep methods (15), depend on v, ($b_i^* = b_i^*(v)$), then from (27) we get $\beta_i = b_i - b_i^* = b_i - b_i^*(v) = \beta_i(v)$, $i = 0(1)m$. So the embedded predictor-corrector pair form (EPCM) (28) becomes:

$$\left. \begin{aligned} y_{n+m}^* &= -\sum_{i=0}^{m-1} a_i^* y_{n+i} + h^2 \sum_{i=0}^{m-1} b_i^*(v) f(x_{n+i}, y_{n+i}) \\ y_{n+m} &= y_{n+m}^* + h^2 \sum_{i=0}^{m} \beta_i(v) f(x_{n+i}, y_{n+i}) \end{aligned} \right\} \quad (40)$$

where

$$|a_0^*| + |b_0^*(v)| \neq 0, |a_0^*| + |\beta_0(v)| \neq 0, \qquad \beta_i(v) = b_i - b_i^*(v),\ i = 0(1)m, b_m^*(v) = 0. \quad (41)$$

In the above pair form the coefficients $b_i^*(v)$ and $\beta_i(v)$, depend on v (where $i = 0(1)m$, $v = \omega\, h$, ω is the frequency and h is the step length).
If the method is symmetric then $a_i^* = a_{m-i}^*$, $b_i^*(v) = b_{m-i}^*(v)$ and $\beta_i(v) = \beta_{m-i}(v)$, $i = 0(1)\lfloor \frac{m}{2} \rfloor$.
From (40) for $m = 8$, we get the form of the symmetric embedded predictor-corrector method (EPCM) with eight-steps:

$$\left. \begin{aligned} y_4^* &= -\Big(y_{-4} + a_3^*\,(y_3 + y_{-3}) + a_2^*\,(y_2 + y_{-2}) + \\ &\quad + a_1^*\,(y_1 + y_{-1}) + a_0^* y_0 \Big) \\ &\quad + h^2 \Big(b_3^*(v)\,(f_3 + f_{-3}) + b_2^*(v)\,(f_2 + f_{-2}) + \\ &\quad + b_1^*(v)\,(f_1 + f_{-1}) + b_0^*(v) f_0 \Big) \\ y_4 &= y_4^* + h^2 \Big(\beta_4(v)\,(f_4 + f_{-4}) + \beta_3(v)\,(f_3 + f_{-3}) + \\ &\quad + \beta_2(v)\,(f_2 + f_{-2}) + \beta_1(v)\,(f_1 + f_{-1}) + \beta_0(v) f_0 \Big) \end{aligned} \right\} \quad (42)$$

where $y_i = y(x + ih)$, $f_i = f(x + ih, y(x + ih))$, $i = -4(1)3$, $f_4 = f(x + 4h, y_4^*)$ and h is the step length.
The characteristic equation (9) becomes

$$\sum_{i=1}^{4} A_i(v)(s^i + s^{-i}) + A_0(v) = 0 \quad (43)$$

where
$A_i(v) = a_i^* + v^2(\beta_i(v) - a_i^* \beta_4(v)) - v^4 b_i^*(v) \beta_4(v), i =$

$0(1)4, a^*_4 = 1, b^*_4(v) = 0$.
We derive the coefficients $\beta_i(v) = b_i - b^*_i(v), i = 0(1)4$, from (33) and (38) as follow:

$$\begin{aligned} &\beta_0(v) = 20 b^*_3(v) - \tfrac{1800151}{72576},\ \beta_1(v) = \tfrac{3335237}{181440} \\ &-15\, b^*_3(v),\ \beta_2(v) = 6\, b^*_3(v) - \tfrac{1270021}{181440}, \\ &\beta_3(v) = \tfrac{173531}{181440} - b^*_3(v),\ \beta_4(v) = \tfrac{45767}{725760} \end{aligned} \tag{44}$$

From (42), (33) and (44) a new eight-step symmetric embedded predictor-corrector method (EPCM) obtained:

$$\left.\begin{aligned} y^*_4 =& -y_{-4} + 2(y_3 + y_{-3}) - \\ & -2(y_2 + y_{-2}) + (y_1 + y_{-1}) + \\ & + h^2 \Big(b^*_3(v)(f_3 + f_{-3}) + \\ & + (\tfrac{109}{16} - 6\, b^*_3(v))(f_2 + f_{-2}) + \\ & + (15\, b^*_3(v) - \tfrac{101}{6})(f_1 + f_{-1}) + \\ & + (\tfrac{601}{24} - 20\, b^*_3(v)) f_0 \Big) \\ y_4 =& y^*_4 + h^2 \Big(\tfrac{45767}{725760}(f^*_4 + f_{-4}) + \\ & + (\tfrac{173531}{181440} - b^*_3(v))(f_3 + f_{-3}) + \\ & + (6\, b^*_3(v) - \tfrac{1270021}{181440})(f_2 + f_{-2}) + \\ & + (\tfrac{3335237}{181440} - 15\, b^*_3(v))(f_1 + f_{-1}) + \\ & + (20 b^*_3(v) - \tfrac{1800151}{72576}) f_0 \Big) \end{aligned}\right\} \tag{45}$$

where $y_i = y(x + ih)$, $f_i = f(x + ih, y(x + ih))$, $f^*_4 = f(x + 4h, y^*_4)$, $b^*_3(v) = \frac{A}{B}$,

$$\begin{aligned} A =& -192\, (\cos(v))^4 + 192\, (\cos(v))^3 + \\ & + \left(96 - 327\, v^2\right)(\cos(v))^2 + \\ & + \left(-120 + 404\, v^2\right)\cos(v) - 137\, v^2 + 24 \\ B =& 96\, v^2\, (\cos(v) - 1)^3 \end{aligned}$$

$v = \omega\, h$, 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:

$$\begin{aligned} b^*_3(v) =& \tfrac{17671}{12096} - \tfrac{45767}{725760}\, v^2 + \tfrac{164627}{47900160}\, v^4 - \\ & - \tfrac{520367}{15850598400}\, v^6 + \tfrac{76873}{89669099520}\, v^8 - \\ & - \tfrac{9190171}{3201186852864000}\, v^{10} - \tfrac{6662921}{34060628114472960}\, v^{12} - \\ & - \tfrac{2866814089}{2043637686868837760000}\, v^{14} - \\ & - \tfrac{10228341391}{169213200472701665280000}\, v^{16} - \\ & - \tfrac{1074205110763}{48394975335192676270080000}\, v^{18} - \\ & - \tfrac{1485941749021}{20325889640780924033433600000}\, v^{20} + \ldots, \end{aligned}$$

where $v = \omega\, h$, ω is the frequency and h is the step length.
In order to find the Local Truncation Error(LTE), we express $y_{\pm i}$, $i = 1(1)4$ and $f_{\pm j}$, $j = 0(1)4$ via Taylor series and we substitute in (33). Based on this procedure we obtain the following expansion for the LTE:

$$\begin{aligned} L.T.E. =& \left(\frac{12506213339}{5794003353600}\, y_n^{(12)} + \right. \\ & \left. + \frac{2094618289}{526727577600}\, y_n^{(10)} \omega^2 \right) h^{12} + O(h^{14}) \end{aligned} \tag{46}$$

The above method (EPCM) (45) has eight steps, tenth algebraic order, tenth order of phase-lag and an interval of periodicity $(0, v_0^2)$ where $v_0^2 = 1.3073505$.

5 Numerical results

5.1 The problems

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

5.1.1 Duffing's Equation

$$\begin{aligned} & y'' = -y - y^3 + 0.002 \cos(1.01\, t), \\ & y(0) = 0.200426728067,\ y'(0) = 0, \\ & \text{with } t \in [0, 1000\,\pi]. \end{aligned} \tag{47}$$

Theoretical solution:
$y(t) = 0.200179477536 \cos(1.01\, t) + 2.46946143 \cdot 10^{-4} \cos(3.03\, t) + 3.04014 \cdot 10^{-7} \cos(5.05\, t) + 3.74 \cdot 10^{-10} \cos(7.07\, t) + \ldots$.
Estimated frequency: $w = 1$.

5.1.2 Nonlinear Equation

$$y'' = -100\, y + \sin(y),\ y(0) = 0,\ y'(0) = 1\ t \in [0, 20\,\pi]. \tag{48}$$

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

5.1.3 Orbital Problem by Stiefel and Bettis

The "almost" periodic orbital problem studied by [5] can be described by

$$y'' + y = 0.001\, e^{i\,x},\ y(0) = 1,\ y'(0) = 0.9995\, i,\ y \in \mathcal{C}, \tag{49}$$

or equivalently by

$$\begin{aligned} & u'' + u = 0.001\, \cos(x), \quad u(0) = 1, \quad u'(0) = 0, \\ & v'' + v = 0.001\, \sin(x), \quad v(0) = 0, \quad v'(0) = 0.9995. \end{aligned} \tag{50}$$

The theoretical solution of the problem (49) 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 (50) has been solved for $x \in [0, 1000\,\pi]$.
Estimated frequency: $w = 1$.

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5.1.4 Two-dimensional Kepler problem (Two-Body Problem)

$$y'' = -\frac{y}{(y^2+z^2)^{\frac{3}{2}}},\ z'' = -\frac{z}{(y^2+z^2)^{\frac{3}{2}}}, \quad (51)$$

with $y(0) = 1-e,\ y'(0) = 0,\ z(0) = 0,\ z'(0) = \sqrt{\frac{1+e}{1-e}},\ t \in [0, 1000\,\pi]$, where e is the eccentricity.
The theoretical solution of this problem is given below:
$y(t) = \cos(u) - e$
$z(t) = \sqrt{1-e^2}\sin(u)$.
where u can be found by solving the equation $u - e\ sin(u) - t = 0$.
We used the estimation $w = \frac{1}{(y^2+z^2)^{\frac{3}{4}}}$ as frequency of the problem.

5.1.5 Schrödinger's equation - Resonance problem

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

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

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 (52) can be expressed by the approximation $y_i'' = (\bar{W} - E)\, y_i$, whose solution is:

$$y_i(x) = A_i \exp\left(\sqrt{\bar{W} - E}\, x\right) + \\ +B_i \exp\left(-\sqrt{\bar{W} - E}\, x\right),\ A_i,\ B_i\ \in \mathcal{R}. \quad (53)$$

We will integrate problem (52) with $l = 0$ at the interval $[0, 15]$ using the well known Woods-Saxon potential:

$$V(x) = \frac{u_0}{1+q} + \frac{u_1\, q}{(1+q)^2},\ q = \exp\left(\frac{x - x_0}{a}\right), \quad (54)$$
$$\text{where } u_0 = -50,\quad a = 0.6,\quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a}$$

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 (52) becomes

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \quad (55)$$

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

$$y(x) \approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ \approx D[sin(k\,x - \pi\,l/2) + \tan(\delta_l)\ \cos(k\,x - \pi\,l/2)], \quad (56)$$

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

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \quad (57)$$

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 values: $E = 341.495874$ and $E = 989.701916$.
As for the frequency ω we will use the suggestion of Ixaru and Rizea (see [26] and [27]):

$$\omega = \begin{cases} \sqrt{E+50}, & x \in [0,\ 6.5] \\ \sqrt{E}, & x \in [6.5,\ 15] \end{cases} \quad (58)$$

5.2 The methods

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

– The new optimized eight-step symmetric embedded predictor-corrector method (EPCM) with tenth algebraic order and minimal phase-lag (45) (New EPCM 8-step)
– The symmetric 10-step method of Quinlan-Tremaine of algebraic order ten [1] (Q-T 10step)
– The optimized symmetric 8-step method (33) of algebraic order eight and infinite order of phase-lag (phase-fitted) [6] (Q-T 8step PF)
– The symmetric 8-step method of Quinlan-Tremaine of algebraic order eight [1] (Q-T 8step)
– The 8-step predictor-corrector method Störmer-Cowell [2] of algebraic order eight: "S-C 8step"
– The 10-stage exponentially-fitted method of Simos and Aguiar of algebraic order nine [11] (Simos- Aguiar)
– The symmetric 6-step method of Jenkins of algebraic order six [9] (Jenkins-6step)
– The 2-step, 3-stage exponentially-fitted predictor-corrector method of Simos and Williams of algebraic order six [10] (Si-Wi EF1)
– The 3-step, 3-stage exponentially-fitted predictor-corrector method of Psihoyios and Simos of algebraic order five [12] (Psi-Si EF2)
– The 4-step predictor-corrector method Milne-Simpson of algebraic order four (M-S PC 4)
– The 4-step predictor-corrector method Adams-Bashforth - Moulton of algebraic order four (ABM PC 4).

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5.3 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 eight-step symmetric embedded predictor-corrector method (EPCM) (45) and the multistep symmetric method of Quinlan-Tremaine [1] with eight steps for all the problems solved.

In Figure 1 we see the results for the Duffing's equation, in Figure 2 the results for the Nonlinear equation, in Figure 3 the results for the Stiefel-Bettis almost periodic problem, in Figures 4 and 5 the results for the two-dimensional Kepler problem for eccentricities e=0.05 and e=0.8 and in Figures 6 and 7 we see the results for the resonance problem for energies $E = 989.701916$ and $E = 341.495874$..

Among all the methods used, the new optimized eight-step symmetric embedded predictor-corrector method (EPCM) with tenth algebraic order and minimal phase-lag is the most efficient.

The interval of periodicity of the new optimized eight-step symmetric embedded predictor-corrector method (EPCM) with tenth algebraic order is about 2.5 times larger than the multistep symmetric method of Quinlan-Tremaine with eight steps and eighth algebraic order and about two times larger than the optimized symmetric 8-step method (33) with eight steps and eighth algebraic order.

The new optimized eight-step symmetric embedded predictor-corrector method (EPCM) with tenth algebraic order and minimal phase-lag can achieve the required accuracy with a step-size, four times larger than the multistep symmetric method of Quinlan-Tremaine with eight steps and eighth algebraic order for the Stiefel-Bettis almost periodic problem, three times larger than the multistep symmetric method of Quinlan-Tremaine with eight steps and eighth algebraic order for the resonance problem and two times larger than the multistep symmetric method of Quinlan-Tremaine with eight steps and eighth algebraic order for the other problems solved.

An interesting remark is that the new optimized eight-step symmetric embedded predictor-corrector method (EPCM) with tenth algebraic order and minimal phase-lag, is more efficient than the multistep symmetric method of Quinlan-Tremaine, with ten steps and tenth algebraic order.

6 Conclusions

We have developed a new optimized eight-step symmetric embedded predictor-corrector method (EPCM) (45) from the form (40).

The new method (EPCM) (45) has eight steps, tenth algebraic order, tenth order of phase-lag and it can be used to solve numerically initial-value problems with oscillatory solutions, for which we know or we can estimate the frequency.

The form (40) has the advantage that reduces the computational expense if the additions on the factor $\sum_{i=0}^{m-1} a_i y_{n+i}$, are done twice.

We have applied the new optimized eight-step symmetric embedded predictor-corrector method (EPCM) with tenth algebraic order (45) along with a group of several methods from the literature to five oscillatory problems.

We concluded that that the new optimized eight-step symmetric embedded predictor-corrector method (EPCM) with tenth algebraic order and minimal phase-lag (45) is noticeably more efficient compared to other methods.

Table 1 Comparison for CPU time, Step Length and Maximum Error

Test Problem	Method	Accuracy (digits)	CPU Time	Step Length	Maximum Error
Duffing Equation	Q-T 8step	10,85886874	18,2989173	0,05	1,38398E-11
	New EPCM 8-step	10,98660532	11,0916711	0,1	1,03132E-11
Nonlinear Equation	Q-T 8step	11,63199947	3,9468253	0,003867188	2,33346E-12
	New EPCM 8-step	12,30138202	2,4804159	0,007734375	4,99595E-13
Stiefel-Bettis	Q-T 8step	11,53466705	57,1119661	0,015	2,91966E-12
	New EPCM 8-step	12,02231899	16,7857076	0,06	9,49907E-13
Two-dimensional Kepler Problem e=0.05	Q-T 8step	9,260886526	52,0419336	0,02	5,4842E-10
	New EPCM 8-step	9,03466034	30,7009968	0,04	9,23293E-10
Two-dimensional Kepler Problem e=0.8	Q-T 8step	5,978655841	710,3661536	0,0015	1,05037E-06
	New EPCM 8-step	6,614648263	402,9193828	0,003	2,42858E-07
Schrödinger Equation E=341,495874	Q-T 8step	8,377298275	1,2948083	0,004	4,19471E-09
	New EPCM 8-step	8,423390297	0,7644049	0,011313708	3,77233E-09
Schrödinger Equation E=989.701916	Q-T 8step	10,7507576	2,1996141	0,002	1,77518E-11
	New EPCM 8-step	11,07739125	1,1544074	0,005656854	8,36775E-12

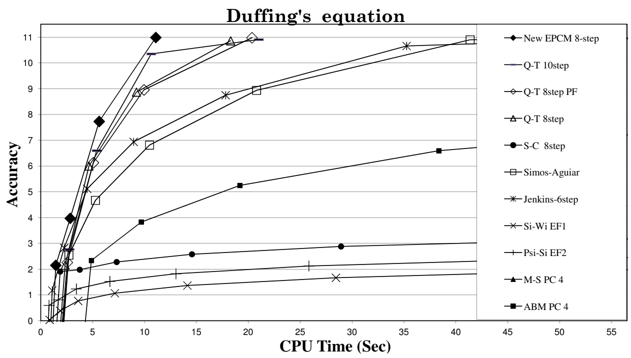

Fig. 1 Efficiency for the Duffing equation

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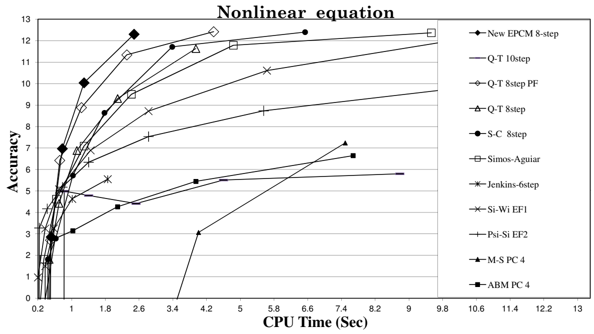

Fig. 2 Efficiency for the Nonlinear equation

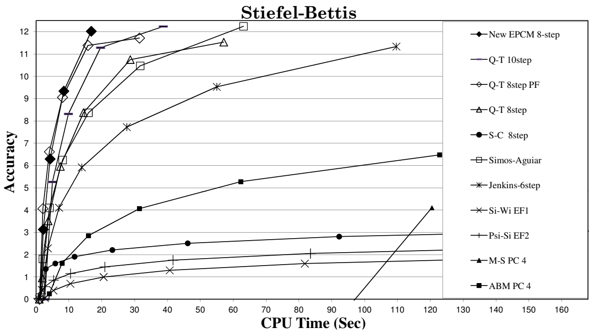

Fig. 3 Efficiency for the Orbital Problem by Stiefel and Bettis

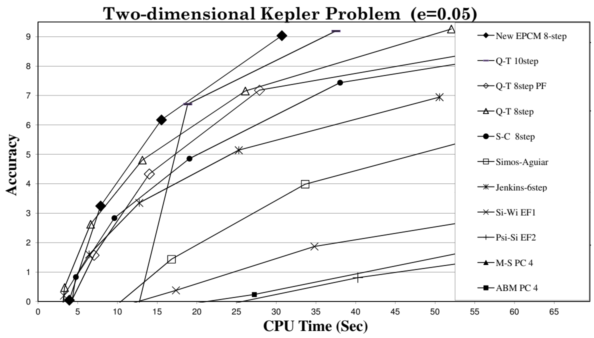

Fig. 4 Efficiency for the Two-body problem using eccentricity e =0.05

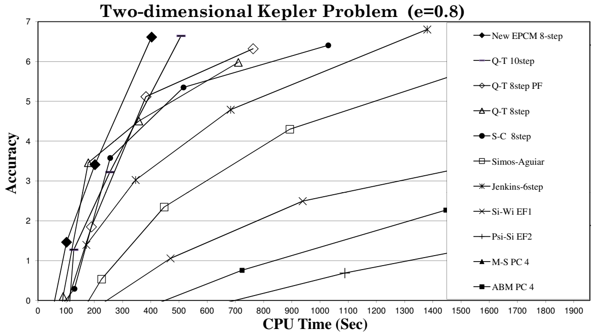

Fig. 5 Efficiency for the Two-body problem using eccentricity e =0.8

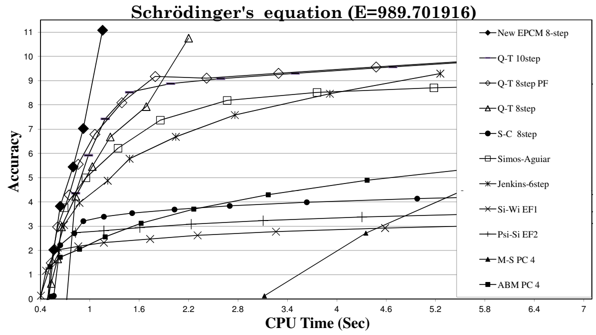

Fig. 6 Efficiency for the Resonance problem using E = 989.701916

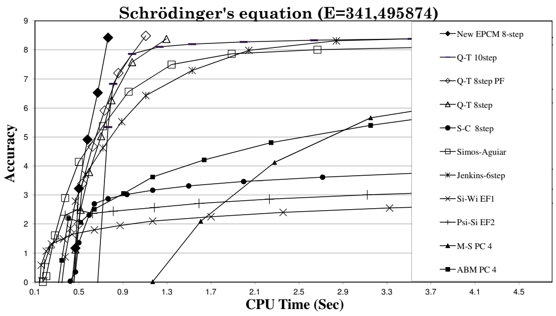

Fig. 7 Efficiency for the Resonance problem using E = 341.495874

References

[1] D. G. Quinlan and S. Tremaine, Symmetric Multistep Methods for the Numerical Integration of Planetary Orbits, The Astronomical Journal, **100**, 1694-1700 (1990).

[2] L. D. Lambert and I. A. Watson, Symmetric multistep methods for periodic initial value problems, J. Inst. Math. Appl., **18**, 189-202 (1976).

[3] J. M. Franco, M. Palacios, J. Comput. Appl. Math., **30**, (1990).

[4] J. D. Lambert, Numerical Methods for Ordinary Differential Systems, The Initial Value Problem, John Wiley and Sons, 104-107 (1991).

[5] E. Stiefel, D. G. Bettis, Stabilization of Cowell's method, Numer. Math., **13**, 154-175 (1969).

[6] G. A. Panopoulos, Z. A. Anastassi and T. E. Simos: Two New Optimized Eight-Step Symmetric Methods for the Efficient Solution of the Schrödinger Equation and Related Problems, MATCH Commun. Math. Comput. Chem., **60**, 773-785 (2008).

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[7] G. A. Panopoulos, Z. A. Anastassi and T. E. Simos, Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions, *Journal of Mathematical Chemistry* **46**, 604-620 (2009).
[8] G. A. Panopoulos and T. E. Simos, A New Phase-Fitted Eight-Step Symmetric Embedded Predictor-Corrector Method (EPCM) for Orbital Problems and Related IVPs with Oscillating Solutions. Computer Physics Communications, submitted (2013).
[9] http://www.burtleburtle.net/bob/math/multistep.html
[10] T. E. Simos and P. S. Williams, Bessel and Neumann fitted methods for the numerical solution of the radial Schrödinger equation, Computers and Chemistry, **21**, 175-179 (1977).
[11] T. E. Simos and Jesus Vigo-Aguiar, A dissipative exponentially-fitted method for the numerical solution of the Schrödinger equation and related problems, Computer Physics Communications, **152**, 274-294 (2003).
[12] T. E. Simos and G. Psihoyios, Special issue - Selected Papers of the International Conference on Computational Methods in Sciences and Engieneering (ICCMSE 2003) Kastoria, Greece, 12-16 September 2003 - Preface, J COMPUT APLL MATH, **175**, IX-IX (2005).
[13] T. Lyche, Chebyshevian multistep methods for Ordinary Differential Eqations, Num. Math., **19**, 65-75 (1972).
[14] T. E. Simos, Chemical Modelling - Applications and Theory, Specialist Periodical Reports, The Royal Society of Chemistry, Cambridge, **1**, (2000)
[15] J. D. Lambert and I. A. Watson, Symmetric multistep methods for periodic initial values problems, J. Inst. Math. Appl., **18**, 189-202 (1976).
[16] Simos TE, Explicit 2-Step Methods with Minimal Phase-Lag for the Numerical-Integration of Special 2nd-Order Initial-Value Problems and Their Application to the One-Dimensional Schrödinger-Equation, Journal of Computational and Applied Mathematics, **39**, 89-94 (1992).
[17] Bo Zhang and Zhicai Juan, Modeling User Equilibrium and the Day-to-day Traffic Evolution based on Cumulative Prospect Theory, Information Science Letters, **1**, 9-12 (2013).
[18] D. Kundu, A. Sarhan and Rameshwar D. Gupta, On Sarhan-Balakrishnan Bivariate Distribution, Journal of Statistics Applications & Probability, **1**, 163-170 (2012).
[19] T. E. Simos, On the Explicit Four-Step Methods with Vanished Phase-Lag and its First Derivative, Applied Mathematics & Information Sciences, (in press).
[20] Simos TE, A High-Order Predictor-Corrector Method for Periodic IVPs, Applied Mathematics Letters, **6**, 9-12 (1993).
[21] G. A. Panopoulos, Z. A. Anastassi, T. E. Simos, A new symmetric eight-step predictor-corrector method for the numerical solution of the radial Schrdinger equation and related orbital problems, International Journal of Modern Physics, **22**, 133-153 (2011).
[22] G. A. Panopoulos, Z. A. Anastassi, T. E. Simos, A symmetric eight-step predictor-corrector method for the numerical solution of the radial Schrdinger equation and related IVPs with oscillating solutions. Computer Physics Communications **182**, 1626-1637 (2011).
[23] M. R. Girgis, T. M. Mahmoud, H. F. Abd El-Hameed and Z. M. El-Saghier, Routing and Capacity Assignment Problem in Computer Networks Using Genetic Algorithm, Information Science Letters, **1**, 13-25 (2013).
[24] G. A. Panopoulos, Z. A. Anastassi and T. E. Simos, A new Eight-Step Symmetric Embedded Predictor-Corrector Method (EPCM) for Orbital problems and Related IVP's with Oscillatory Solutions, The Astronomical Journal, **145**, (2013).
[25] G. A. Panopoulos, T. E. Simos, A new optimized symmetric 8-step semi-embedded predictorcorrector method for the numerical solution of the radial Schrdinger equation and related orbital problems, Journal of Mathematical Chemistry, published online, (May 2013).
[26] L. Gr. Ixaru and M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation, Comput. Phys. Commun., **38**, 329-337 (1985).
[27] L. Gr. Ixaru and M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies, Computer Physics Communications, **19**, 23-27 (1980).

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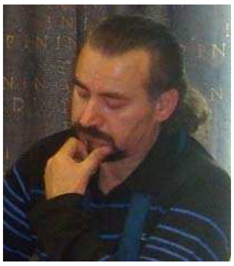

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