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ORIGINAL PAPER

Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions

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Abstract In this paper, we present two optimized eight-step symmetric implicit methods with phase-lag order ten and infinite (phase-fitted). The methods are constructed to solve numerically the radial time-independent Schrödinger equation with the use of the Woods–Saxon potential. They can also be used to integrate related IVPs with oscillating solutions such as orbital problems. We compare the two new methods 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 Schrödinger equation · Orbital problems · Phase-lag · Initial value problems · Oscillating solution · Symmetric · Multistep · Implicit

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1 Introduction

The radial Schrödinger equation can be written as:

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

where $l(l+1)/r^2$ is the *centrifugal potential*, $V(r)$ is the *potential*, E is the *energy* and $W(r) = (l(l+1)/r^2) + V(r)$ is the *effective potential*. It is valid that $\lim_{r\to\infty} V(r) = 0$ and therefore $\lim_{r\to\infty} W(r) = 0$.

We consider $E > 0$ and divide $[0, \infty)$ into subintervals $[a_i, b_i]$ so that $W(r)$ is a constant with value $\bar{W}_i$. After this the problem (1) can be expressed by the approximation:

$$y_i'' = (\bar{W} - E)\, y_i, \tag{2}$$

whose solution is:

$$\begin{aligned} y_i(r) &= A_i \exp\left(\sqrt{\bar{W} - E}\, r\right) + B_i \exp\left(-\sqrt{\bar{W} - E}\, r\right), \\ A_i,\ B_i &\in \mathbb{R}. \end{aligned} \tag{3}$$

Many numerical methods have been developed for the efficient solution of the Schrödinger equation and related problems. For example Raptis and Allison have developed a two-step exponentially fitted method of order four in [5]. More recently Kalogiratou and Simos have constructed a two-step P-stable exponentially fitted method of order four in [6].

Some other notable multistep methods for the numerical solution of oscillating IVPs have been developed by Chawla and Rao [3], who produced a three-stage, two-step P-stable method with minimal phase-lag and order six and by Henrici [4], who produced a four-step symmetric method of order six. Also Anastassi and Simos have developed trigonometrically fitted six-step symmetric methods in [108] and a six-step P-stable trigonometrically fitted method in [110] and Panopoulos, Anastassi and Simos have constructed two optimized eight-step symmetric methods.

Also some research work in numerical methods can be found in [1–137].

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

$$y'' = f(x, y) \tag{4}$$

multistep methods of the form

$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \tag{5}$$

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 (5) is associated with the operator

$$L(x) = \sum_{i=0}^{m} a_i u(x + ih) - h^2 \sum_{i=0}^{m} b_i u''(x + ih) \tag{6}$$

where $u \in C^2$.

Definition 1 The multistep method (5) 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

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

a difference equation of the form

$$\begin{aligned} &A_k(v) y_{n+k} + \cdots + A_1(v) y_{n+1} + A_0(v) y_n \\ &+A_1(v) y_{n-1} + \cdots + A_k(v) y_{n-k} = 0 \end{aligned} \tag{8}$$

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

$$A_k(v) s^k + \cdots + A_1(v) s + A_0(v) + A_1(v) s^{-1} + \cdots + A_k(v) s^{-k} = 0 \tag{9}$$

From Lambert and Watson [8], 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:

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

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

Definition 3 For any method corresponding to the characteristic Eq. 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 phase-lag is q.

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

$$-cv^{q+2} + O(v^{q+4}) = \frac{2A_k(v)\cos(kv) + \cdots + 2A_j(v)\cos(jv) + \cdots + A_0(v)}{2k^2 A_k(v) + \cdots + 2j^2 A_j(v) + \cdots + 2A_1(v)} \tag{12}$$

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:

$$\begin{aligned} &-cv^{q+2} + O(v^{q+4}) \\ &= \frac{2A_4(v)\cos(4v) + 2A_3(v)\cos(3v) + 2A_2(v)\cos(2v) + 2A_1(v)\cos(v) + A_0(v)}{32A_4(v) + 18A_3(v) + 8A_2(v) + 2A_1(v)} \end{aligned} \tag{13}$$

3 Construction of the new optimized multistep methods

We consider the eight-step symmetric implicit methods of the form:

$$\begin{aligned} y_4 = &-y_{-4} - a_3(y_3 + y_{-3}) - a_2(y_2 + y_{-2}) - a_1(y_1 + y_{-1}) \\ &+h^2\left(b_4(f_4 + f_{-4}) + b_3(f_3 + f_{-3}) + b_2(f_2 + f_{-2})\right. \\ &\left.+b_1(f_1 + f_{-1}) + b_0 f_0\right) \end{aligned} \tag{14}$$

where $a_3 = -2, \quad a_2 = 2, \quad a_1 = -1, \quad y_i = y(x+ih)$ and $f_i = f(x+ih, y(x+ih))$

3.1 First optimized method with infinite order of phase-lag (phase-fitted)

We want the first method to have infinite order of phase-lag, that is the phase-lag will be nullified using b_4 coefficient.

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:

$$\begin{aligned} &b_0 = 70\, b_4 - \frac{12629}{3024}, \quad b_1 = -56\, b_4 + \frac{20483}{4032}, \\ &b_2 = 28\, b_4 - \frac{3937}{2016}, \quad b_3 = -8\, b_4 + \frac{17671}{12096} \end{aligned} \tag{15}$$

and the phase-lag becomes:

$$
\begin{aligned}
PL &= \frac{1}{1260}\,\frac{A}{B}, \qquad \text{where} \\
A &= 24192\,(\cos(v))^4 + 24192\,(\cos(v))^4\,v^2 b_4 + 17671\,(\cos(v))^3\,v^2 \\
&\quad -96768\,(\cos(v))^3\,v^2 b_4 - 24192\,(\cos(v))^3 + 14152\,(\cos(v))^2\,v^2 b_4 \\
&\quad -12096\,(\cos(v))^2 - 11811\,(\cos(v))^2\,v^2 + 2109\,\cos(v)\,v^2 \\
&\quad +15120\,\cos(v) - 96768\,\cos(v)\,v^2 b_4 - 409\,v^2 + 24192\,v^2 b_4 - 3024 \quad \text{and} \\
B &= 12 + 25\,v^2
\end{aligned} \tag{16}
$$

so by satisfying $PL = 0$, we derive

$$
\begin{aligned}
b_4 &= -\frac{1}{24192}\,\frac{C}{D}, \qquad \text{where} \\
C &= 24192\,(\cos(v))^4 + \left(17671\,v^2 - 24192\right)(\cos(v))^3 \\
&\quad - \left(12096 + 11811 v^2\right)(\cos(v))^2 \\
&\quad + \left(15120 + 2109\,v^2\right)\cos(v) - 409\,v^2 - 3024 \\
D &= v^2\left(\cos(v)^4 - 4\cos(v)^3 + 6\cos(v)^2 - 4\cos(v) + 1\right)
\end{aligned} \tag{17}
$$

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

3.2 Second optimized method with tenth order of phase-lag

For this method, we use all b_i coefficients for achieving maximum algebraic order or maximum phase-lag order. After achieving maximum algebraic order, that is 10, the coefficients become:

$$
b_0 = \frac{17273}{72576},\ b_1 = \frac{280997}{181440},\ b_2 = -\frac{33961}{181440},\ b_3 = \frac{173531}{181440},\ b_4 = \frac{45767}{725760} \tag{18}
$$

If we repeat the procedure of the previous section and expand phase-lag using the Taylor series, we can nullify the leading term (that is the coefficient of h^{10}). However, we obtain the same method as (18). The same method will be produced if we attempt any combination of algebraic order and phase-lag order. This happens due to the symmetry of the specific a_i.

4 Numerical results

4.1 The problems

The efficiency of the two newly constructed methods will be measured through the integration of five initial value problems with oscillating solution.

4.1.1 Orbital problem by Franco and Palacios

The "almost" periodic orbital problem studied by [10] can be described by

$$y'' + y = \epsilon\, e^{i\,\psi\,x}, \quad y(0) = 1, \quad y'(0) = i, \quad y \in \mathcal{C}, \tag{19}$$

or equivalently by

$$\begin{aligned} u'' + u &= \epsilon\ \cos(\psi\,x), \quad u(0) = 1, \quad u'(0) = 0,\\ v'' + v &= \epsilon\ \sin(\psi\,x), \quad v(0) = 0, \quad v'(0) = 1, \end{aligned} \tag{20}$$

where $\epsilon = 0.001$ and $\psi = 0.01$.

The theoretical solution of the problem (19) is given below:

$$\begin{aligned} y(x) &= u(x) + i\, v(x), \quad u, v \in \mathcal{R}\\ u(x) &= \frac{1 - \epsilon - \psi^2}{1 - \psi^2}\ \cos(x) + \frac{\epsilon}{1 - \psi^2}\ \cos(\psi\,x)\\ v(x) &= \frac{1 - \epsilon\psi - \psi^2}{1 - \psi^2}\ \sin(x) + \frac{\epsilon}{1 - \psi^2}\ \sin(\psi\,x) \end{aligned} \tag{21}$$

The system of Eqs. 20 has been solved for $x \in [0, 1000\,\pi]$. The estimated frequency is $w = 1$.

4.1.2 Inhomogeneous equation

$y'' = -100\,y + 99\,\sin(t)$, with $y(0) = 1, y'(0) = 11$, $t \in [0, 1000\,\pi]$.
Theoretical solution: $y(t) = \sin(t) + \sin(10\,t) + \cos(10\,t)$.
Estimated frequency: $w = 10$.

4.1.3 Two-body problem

$y'' = -y/(y^2 + z^2)^{\frac{3}{2}}$; $z'' = -z(y^2 + z^2)^{\frac{3}{2}}$; 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 $w = 1/(y^2 + z^2)^{\frac{3}{4}}$ as frequency of the problem.

4.1.4 Duffing equation

$y'' = -y - y^3 + 0.002\cos(1.01\,t)$, with $y(0) = 0.200426728067$, $y'(0) = 0$, $t \in [0, 1000\,\pi]$.

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: $w = 1$.

4.1.5 The inverse resonance problem

We will integrate problem (1) (where $r = x$) with $l = 0$ at the interval [0, 15] using the well known Woods–Saxon potential

$$V(x) = \frac{u_0}{1+q} + \frac{u_1\,q}{(1+q)^2}, \quad q = \exp\left(\frac{x - x_0}{a}\right), \quad \text{where} \tag{22}$$
$$u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a}$$

and with boundary condition $y(0) = 0$.

The potential $V(x)$ decays more quickly than $l(l+1)/x^2$, so for large x (asymptotic region) the Schrödinger equation (1) becomes

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \tag{23}$$

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

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[\sin(k\,x - \pi\,l/2) + \tan(\delta_l)\ \cos(k\,x - \pi\,l/2)], \end{aligned} \tag{24}$$

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

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{25}$$

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 three different values for the energy: (i) 989.701916 and (ii) 341.495874 and (iii) 163.215341. As for the frequency ω we will use the suggestion of Ixaru and Rizea [7]:

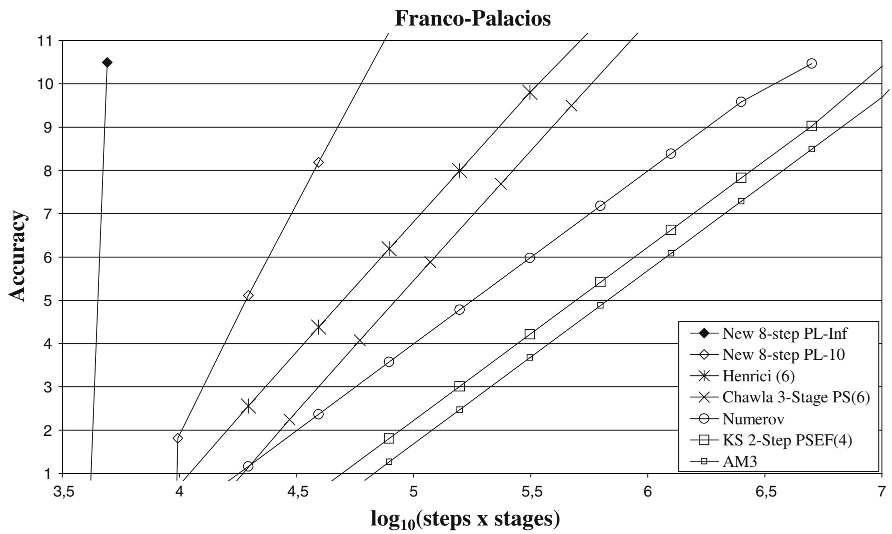

Fig. 1 Efficiency for the orbital problem by Franco and Palacios

$$\omega = \begin{cases} \sqrt{E-50} & x \in [0,\ 6.5] \\ \sqrt{E} & x \in [6.5,\ 15] \end{cases} \tag{26}$$

4.2 The methods

We have used several multistep methods for the integration of the Schrödinger equation. These are:

- The new method with infinite order of phase-lag shown in (17)
- The new method with eighth order of phase-lag shown in (18)
- The P-stable method of Henrici with minimal phase-lag and order six [4]
- The three-stage method of Chawla and Rao of order six [3]
- The Classical method of Numerov
- The P-stable exponentially fitted method of Kalogiratou and Simos of order four [6]
- The three-step method of Adams–Moulton

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 $\log_{10}$(steps $\times$ stages). In Fig. 1, we see the results for the Franco-Palacios almost periodic problem, in Fig. 2 the results for the inhomogeneous equation in Fig. 3 the results for the two-body problem and in Fig. 4 the results for the Duffing equation. In Figs. 5, 6 and 7, we see the results for the Schrödinger

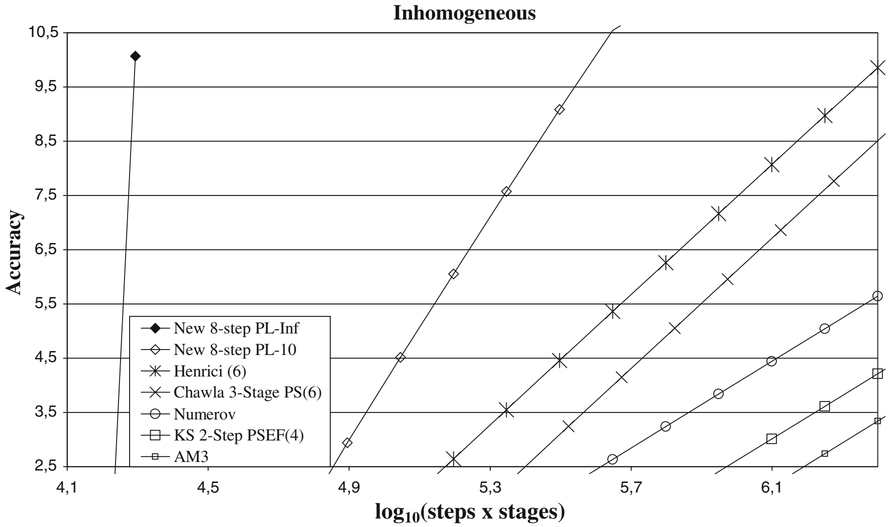

Fig. 2 Efficiency for the inhomogeneous equation

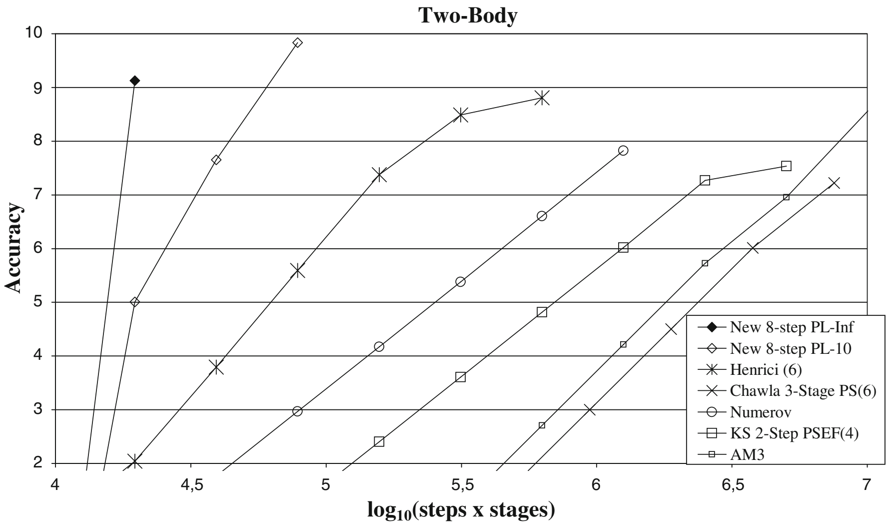

Fig. 3 Efficiency for the two-body problem

equation for energies $E = 163.215341$, $E = 341.495874$ and $E = 989.701916$, respectively.

Among all the methods used, the new optimized method with infinite order of phase-lag was the most efficient, with the exception of the Duffing equation, had almost identical results with the new method with phase-lag order 10.

The difference from the other methods was about 1.2 decimal digits better for the Schrödinger equation for energy $E = 989.701916$ and about 0.7 d.d. for

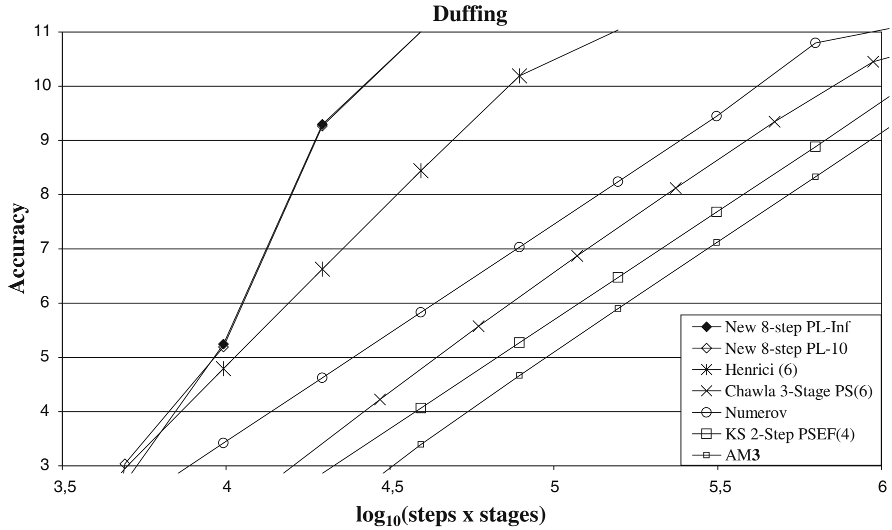

Fig. 4 Efficiency for the Duffing equation

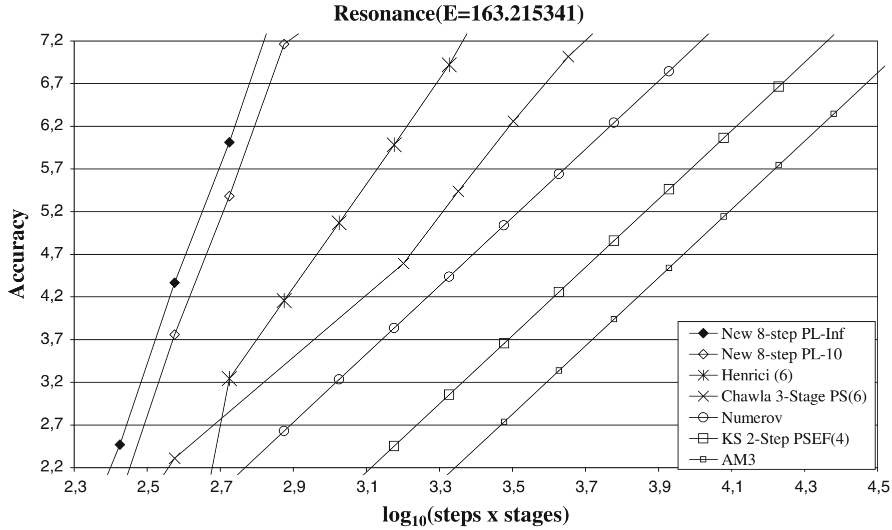

Fig. 5 Efficiency for the Schrödinger equation using $E = 163.215341$

$E = 163.215341$ and $E = 341.495874$. For the other three problems the difference was enormous, where there was an almost vertical increase in the accuracy compared to the other methods. There were no case where the efficiency dropped below the efficiency of the others.

As regards the other methods, the one of Henrici was the most efficient, with next the method of Chawla, the method of Numerov and finally the methods of Kalogiratou–Simos and Adams–Moulton.

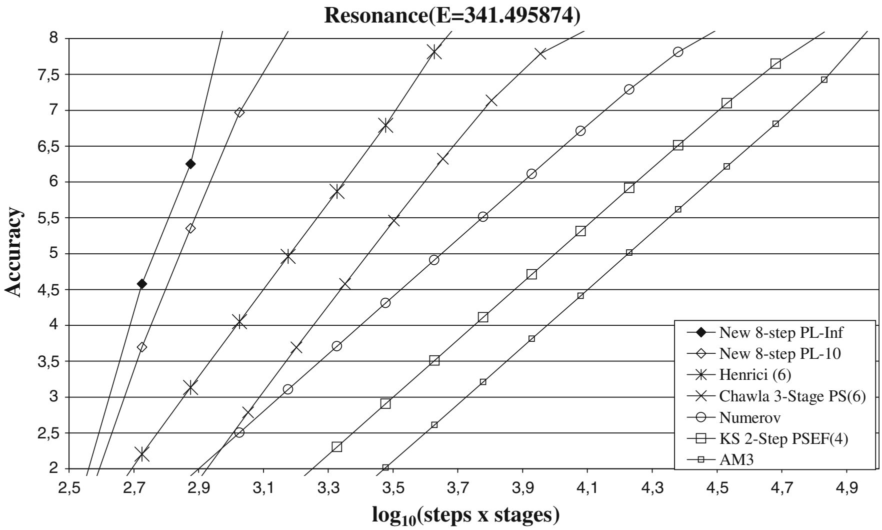

Fig. 6 Efficiency for the Schrödinger equation using $E = 341.495874$

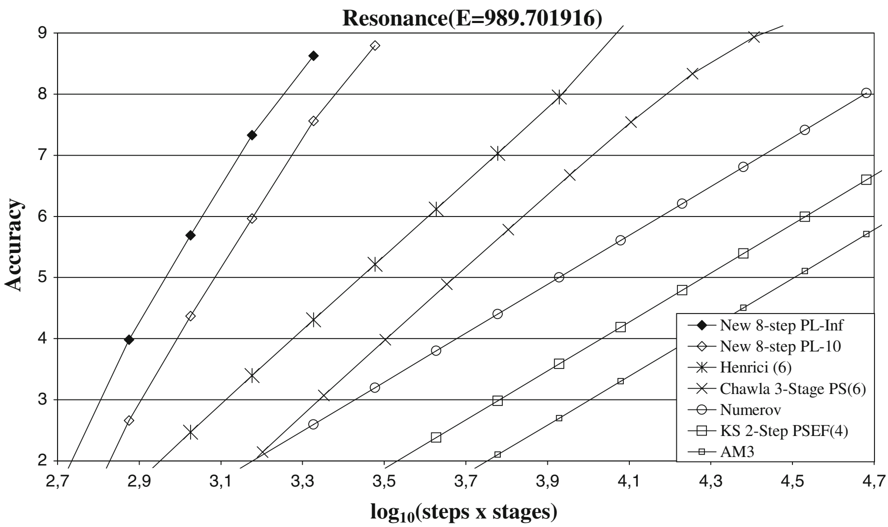

Fig. 7 Efficiency for the Schrödinger equation using $E = 989.701916$

5 Conclusions

We have constructed two optimized eight-step symmetric implicit methods. The first one has phase-lag of order infinite (phase-fitted). The second one has phase-lag of order 10. We have applied the new methods along with a group of recently developed methods from the literature to the Schrödinger equation and related problems. We concluded that the new methods 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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