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An explicit Numerov-type method for second-order differential equations with oscillating solutions

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Abstract

In this paper a new explicit Numerov-type method is introduced. The construction is based on a modification of a sixth-order explicit Numerov-type method recently developed by Tsitouras [Ch. Tsitouras, Explicit Numerov type methods with reduced number of stages, Comput. Math. Appl. 45 (2003) 37–42]. Two free parameters are added in order to nullify the phase-lag and the amplification. The method is useful only when a good estimate of the frequency of the problem is known in advance. The parameters depend on the product of the estimated frequency and the stepsize. Numerical results obtained for well-known test problems show the efficiency of the new method.
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1. Introduction

In the last decades, there has been a great deal of interest in the research of new methods for the numerical integration of initial value problems (IVP) associated to second-order ordinary differential equations (ODE)

$$y' = f(x, y), \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0, \tag{1.1}$$

in which the first derivative does not appear explicitly. Such problems often arise in different fields of applied sciences such as celestial mechanics, molecular dynamics, quantum mechanics, spatial semi-discretization of wave equations and so on. Quite often the solution of (1.1) exhibits an oscillatory behavior; think, for instance, of the pendulum problem in celestial mechanics or of the Schrödinger equation in quantum mechanics. There are excellent codes available for (1.1), mainly based on Runge–Kutta–Nyström methods or linear multistep methods [2]. For problems having highly oscillatory solutions standard methods with unspecialized use can require a huge number of steps to track the oscillations. One way to obtain a more efficient integration process consists of constructing numerical methods with an increased algebraic order. On the other hand, the construction and implementation of high algebraic order methods is not evident. An alternative way consists of considering methods which take into account the nature of the problem. Two important properties to consider are the *phase-lag* and the *amplification*. These are actually two

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different types of truncation errors. The first is the angle between the analytical solution and the numerical solution while the second is the distance from a standard cyclic solution. We mention the pioneering paper of Brusa and Nigro [3], in which the phase-lag property was introduced as a tool to analyze the behavior of the method for the numerical solution of IVPs with oscillating solutions. We note that a large number of papers have been published proposing methods with minimal phase-lag, see for example [4–7]. The coefficients of these methods are constant values. If a good estimate of the period, or of the dominant frequency, is known in advance, then it is possible to construct numerical methods with zero phase-lag. The coefficients are then depending on the product $v = \omega h$ where ω is the estimated frequency of the problem. This technique is better known as *phase fitting*, a concept introduced by Raptis and Simos [8]. Other examples of phase-fitted methods include two-step methods [9] or Runge–Kutta methods [10–14]. Likewise, we define methods with v-dependent coefficients which are determined in such a way that zero amplification is obtained as *amplification-fitted*. It should be noted that phase fitting and amplification fitting are somehow related to *exponential fitting* [15–20]. The purpose of this paper is to present a Numerov-type method which is based on a combined use of phase fitting and amplification fitting techniques.

The paper is organized as follows. Section 2 is of an introductory nature: we discuss Numerov-type methods and we present the concepts of stability and phase-lag analysis. The construction of the new method is described in Section 3. The stability and phase properties are analyzed in Section 4. In Section 5 some numerical experiments show the relevance of the new method. Finally, in Section 6 some conclusions are drawn.

2. Basic elements of the approach

2.1. Numerov-type methods

In the case of special multistep methods for (1.1), particular Numerov-type algorithms have been proposed by several authors [4–6]. Usually, a certain algebraic order is obtained by the intermediate use of high accuracy interpolatory off-step nodes, which increases the computational cost. Alternatively, Coleman [21] has investigated the order of convergence for Numerov-type methods for (1.1) which can be expressed as

$$Y_i = (1 + c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, \ldots, s, \tag{2.2}$$

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i), \tag{2.3}$$

where y_{n-1}, y_n and y_{n+1} are approximations of $y(x_n - h)$, $y(x_n)$ and $y(x_n + h)$, respectively. These methods are completely determined by the Butcher table

$$
\begin{array}{c|ccc}
c_1 & a_{11} & \ldots & a_{1s} \\
\vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & \ldots & a_{ss} \\
\hline
 & b_1 & \ldots & b_s
\end{array}
\quad \text{or equivalently by the triplet } (c, A, b).
$$

Many methods, not normally written like this, can be expressed in this form by a little rearrangement. The main result from [21] is that the derivation of the order of a Numerov-type method is reduced to checking certain relationships between the coefficients of the method, just as we do for Runge–Kutta–(Nyström) methods. Implicit methods require the solving of a nonlinear algebraic system at each step. In order to avoid this difficulty one considers explicit methods which can be presented in Butcher notation by the table of coefficients

$$
\begin{array}{c|cccccc}
-1 & 0 & 0 & 0 & \ldots & & 0 \\
0 & 0 & 0 & 0 & \ldots & & 0 \\
c_3 & a_{31} & a_{32} & 0 & \ldots & & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & & \vdots \\
c_s & a_{s1} & a_{s2} & \ldots & a_{s,s-1} & & 0 \\
\hline
 & b_1 & b_2 & \ldots & b_{s-1} & & b_s
\end{array}.
$$

Note that explicit methods only require the evaluation of $f(x_n, y_n)$, $f(x_n + c_3h, Y_3), \ldots, f(x_n + c_sh, Y_s)$ at each step. So they effectively use $s - 1$ stages per step.

2.2. Stability and phase-lag analysis of Numerov-type methods

To investigate the stability properties of methods for solving the IVP (1.1), Lambert and Watson [23] introduced the scalar test equation

$$y' = -\omega^2 y. \tag{2.4}$$

If the Numerov-type method (2.2) and (2.3) is applied to (2.4) we obtain

$$
\begin{aligned}
Y &= (e + c)y_n - cy_{n-1} - v^2 AY, \quad v = \omega h, \\
y_{n+1} &= 2y_n - y_{n-1} - v^2 b^T Y,
\end{aligned}
\tag{2.5}
$$

where $Y = (Y_1, \ldots, Y_s)^T$ and $e = (1, \ldots, 1)^T$, with s elements. Elimination of the vector Y from (2.5) results in the difference equation

$$y_{n+1} - S(v^2)y_n + P(v^2)y_{n-1} = 0, \tag{2.6}$$

where

$$
\begin{aligned}
S(v^2) &= 2 - v^2 b^T (I + v^2 A)^{-1}(e + c), \\
P(v^2) &= 1 - v^2 b^T (I + v^2 A)^{-1} c.
\end{aligned}
$$

For explicit methods S and P are polynomials in v^2. The behavior of the roots of the difference equation (2.6) depends on the characteristic equation

$$\xi^2 - S(v^2)\xi + P(v^2) = 0. \tag{2.7}$$

The following definition is originally formulated by van der Houwen and Sommeijer [7] for Runge–Kutta–Nyström methods. Here, it is slightly adapted to be more pertinent for our approach.

Definition 1. For the Numerov-type method (2.2) and (2.3) the quantities

$$\phi(v) = v - \arccos\left(\frac{S(v^2)}{2\sqrt{P(v^2)}}\right), \qquad d(v) = 1 - \sqrt{P(v^2)}$$

are called the phase-lag (or dispersion) and the amplification (or dissipation), respectively. The method is said to have phase-lag order q and dissipation order u if

$$\phi(v) = c_\phi v^{q+1} + \mathcal{O}(v^{q+3}), \qquad d(v) = c_d v^{u+1} + \mathcal{O}(v^{u+3}).$$

The constants c_ϕ and c_d are called the phase-lag and dissipation constants, respectively. Methods with $d(v) = 0$ are called zero-dissipative.

The magnitude of the phase-lag and the amplification is an important feature for solving (1.1) with periodic or oscillating solutions.

It should be desirable that the numerical solution mimics the periodic behavior of the numerical solution of (2.4). The amplitude of the numerical solution is preserved when the roots of (2.7) lie on the unit circle. This property is equivalent to the fact that the coefficients of (2.7) satisfy the conditions

$$P(v^2) = 1 \quad \text{and} \quad |S(v^2)| < 2, \quad v \in (0, v_{\text{per}}^2),$$

and the interval $(0, v_{\text{per}}^2)$ is called the *interval of periodicity*, see Lambert and Watson [23]. Let us note that $P(v^2) = 1$ is obviously a necessary condition for the existence of a non-empty periodicity interval. When the method possesses a dissipation, the numerical solution remains bounded when the coefficients of (2.7) satisfy the conditions

$$P(v^2) < 1 \quad \text{and} \quad |S(v^2)| < 1 + P(v^2), \quad v \in (0, v_{\text{stab}}^2),$$

and the interval $(0, \nu^2_{\text{stab}})$ is called the *interval of absolute stability*, see Chawla and Sharma [24]. For a long time it was often believed that the property of zero-dissipation is of primary interest when solving periodic IVPs. For example, in celestial mechanics it is desirable that the numerical orbits do not spiral inwards or outwards. On the contrary, rather recently Simos and Williams [6] have shown that a high phase-lag order is a more important property than zero-dissipation. Since then, many authors have explored the idea of constructing dissipative methods, see for example [1,22]. Surely, the construction of these methods is not restricted by the requirement to be zero-dissipative. There are more free parameters involved which can be tuned on the current problem.

3. Derivation of the new method

In this section we present an explicit Numerov-type method which is both phase-fitted and amplification-fitted. It is obvious that such a method is capable to integrate exactly the test equation (2.4). For the construction we consider the following dissipative method of Tsitouras [1]

$$
\begin{array}{c|ccccc}
-1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
\dfrac{1}{2} & \dfrac{1}{16} & \dfrac{5}{16} & 0 & 0 & 0 \\
-\dfrac{1}{2} & -\dfrac{7}{144} & -\dfrac{5}{48} & \dfrac{1}{36} & 0 & 0 \\
1 & -\dfrac{2}{9} & \dfrac{1}{3} & \dfrac{2}{9} & \dfrac{2}{3} & 0 \\
\hline
 & \dfrac{1}{60} & \dfrac{13}{30} & \dfrac{4}{15} & \dfrac{4}{15} & \dfrac{1}{60}
\end{array}
\tag{3.8}
$$

in which we modify the final stage (2.3) with the parameters γ_1 and γ_2:

$$
y_{n+1} = 2\gamma_1 y_n - \gamma_2 y_{n-1} + h^2 \sum_{i=1}^{4} b_i f(x_n + c_i h, Y_i).
\tag{3.9}
$$

Applying the modified two-step method (3.8) and (3.9) to (2.4), the following expressions for S and P are obtained:

$$
S(\nu^2) = 2\gamma_1 - \nu^2 + \frac{1}{12}\nu^4 - \frac{1}{360}\nu^6 + \frac{1}{10368}\nu^8,
$$

$$
P(\nu^2) = \gamma_2 - \frac{1}{51840}\nu^8.
$$

Requiring that the phase-lag and the amplification are both equal to zero one easily obtains

$$
\gamma_1 = \cos(\nu) + \frac{1}{2}\nu^2 - \frac{1}{24}\nu^4 + \frac{1}{720}\nu^6 - \frac{1}{20\,736}\nu^6, \qquad \gamma_2 = 1 + \frac{1}{51\,840}\nu^8.
\tag{3.10}
$$

When $\nu \to 0$ the method reduces to the classical method [1].

It is worth noticing that we have modified two-step methods in various ways, but in many cases the solution for the γ-parameters is rather complicated. On the other hand, the modification (3.9) ensures a very simple solution. Another advantage compared to many other existing ν-dependent methods is that there are no critical ν-values where the method is undefined. A criticism should be that the γ-values (3.10) grow enormously (in absolute value) with larger ν-values. Nevertheless, large ν-values will never appear in practical applications for the following reasons: the ω-values are always restricted since explicit methods are only concerned with the solution of non-stiff problems. Furthermore, any reasonable accuracy requires a stepsize h such that ν is small enough.

The principal truncation error (plte) of the new method is

$$
\text{plte} = \text{plte}^{\text{Class}} + \frac{h^8 \omega^8 y}{15\,120},
$$

where plte$^{\text{Class}}$ represents the plte of the classical method and is given in [1] (p. 39). As expected, the plte will disappear when solving the scalar test equation (2.4).

4. Stability and phase-lag analysis

The theory of Lambert and Watson [23] was reconsidered by Coleman and Ixaru [25] for zero-dissipative methods whose coefficients depend on one parameter which is proportional with the stepsize. We follow the main concepts of that paper. Consider a dissipative Numerov-type method depending on $\theta = kh$ where k is an estimation of the true frequency of the problem. An application of such a method to the test equation (2.4) leads to

$$y_{n+1} - S(v^2; \theta)y_n + P(v^2; \theta)y_{n-1} = 0.$$

For explicit methods $S(v^2; \theta)$ and $P(v^2; \theta)$ are polynomials in v^2 with coefficients which depend on the parameter θ which specifies the method of concern,

$$S(v^2; \theta) = \sum_{j=0}^{s-1} s_j(\theta)v^{2j}, \qquad P(v^2; \theta) = \sum_{j=0}^{s-1} p_j(\theta)v^{2j}.$$

For the new method we have that

$$S(v^2; \theta) = 2\cos(\theta) - (v^2 - \theta^2) + \frac{1}{12}(v^4 - \theta^4) - \frac{1}{360}(v^6 - \theta^6) + \frac{1}{10\,368}(v^8 - \theta^8),$$

$$P(v^2; \theta) = 1 - \frac{1}{51\,840}(v^8 - \theta^8). \tag{4.11}$$

The stability properties are now determined by $S(v^2; \theta)$ and $P(v^2; \theta)$ which has the important consequence that the interval of absolute stability becomes a two-dimensional region. Indeed, for methods with frequency-dependent parameters we should never discuss the stability of a single method, but a family of methods, depending on the parameter θ. We can now give the following definition.

Definition 2. For a dissipative Numerov-type method with $S(v^2; \theta)$ and $P(v^2; \theta)$ the region of absolute stability is a region in the $v - \theta$ plane ($v, \theta > 0$), throughout which

$$P(v^2; \theta) < 1 \quad \text{and} \quad |S(v^2; \theta)| < P(v^2; \theta) + 1.$$

Any closed curve defined by

$$P(v^2; \theta) = 1 \quad \text{or} \quad |S(v^2; \theta)| = P(v^2; \theta) + 1$$

is a stability boundary.

The region of absolute stability of the new method is drawn in Fig. 1. Equations of stability boundaries can be written without difficulty for the exponentially-fitted versions of the Numerov method, see [25]. For the new method we have partly succeeded to describe the region of absolute stability in an analytical way. From (4.11) it is clear that the diagonal line $\theta = v$ (i.e. the fitted k equals the test ω) is a stability boundary. By construction we have that

$$S(v^2; v) = 2\cos(v) \quad \text{and} \quad P(v^2; v) = 1.$$

Therefore, when the main frequency is known the interval of periodicity is $(0, \infty)$ except the points $(n\pi)^2$ for integers n. Furthermore, expression (4.11) reveals that the region of absolute stability is included in the half-plane $\theta < v$. Similar stability results are obtained for Runge–Kutta methods in [26].

The phase-lag and the amplification of θ-dependent Numerov-type methods will be denoted as

$$\phi(v; \theta) = v - \arccos\left(\frac{S(v^2; \theta)}{2\sqrt{P(v^2; \theta)}}\right), \qquad d(v; \theta) = 1 - \sqrt{P(v^2; \theta)}. \tag{4.12}$$

However, in practice the pair v, θ used in this approach should be replaced by the pair $v, r = \theta/v$. Coleman and Duxbury [27] have pointed out that the latter choice is better suited for the analysis of the properties of the functions
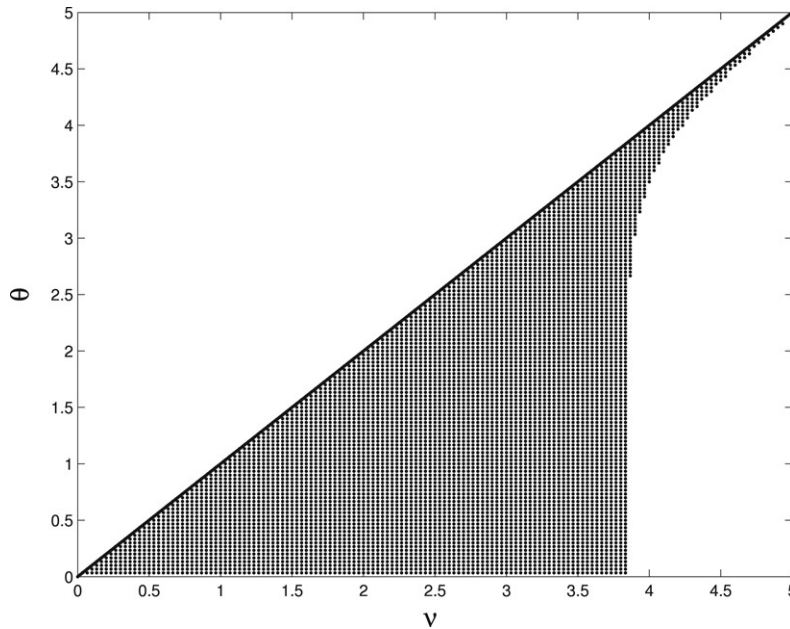
Fig. 1. ν–θ plot for the new method.

$S(\nu^2; \theta)$ and $P(\nu^2; \theta)$ in the ν–θ plane because such an analysis becomes more transparent if rays $\theta = r\nu$ with fixed values of r are followed. So we have the following definition.

Definition 3. The phase-lag order is q if (see also [15,26,27])

$$\phi(\nu; r\nu) = c_\phi(r)\nu^{q+1} + \mathcal{O}(\nu^{q+3}),$$

and the dissipation order is u if

$$d(\nu; r\nu) = c_d(r)\nu^{u+1} + \mathcal{O}(\nu^{u+3}),$$

where $r = \theta/\nu$.

Using (4.11) and (4.12) one easily verifies that the phase-lag and the amplification of the new method are given by

$$\phi(\nu^2; r\nu) = \frac{1 - r^8}{30\,240}\nu^7 + \mathcal{O}(\nu^9), \tag{4.13}$$

$$d(\nu^2; r\nu) = \frac{1 - r^8}{103\,680}\nu^8 + \mathcal{O}(\nu^{10}), \tag{4.14}$$

and therefore the phase-lag order is six and the dissipation order is seven. Expressions (4.13) and (4.14) indicate that the phase-lag order and the dissipation order are equal to those of the corresponding classical method [1]. We consider the particular case $r = 1$ which represents the situation when the fitted k equals the test ω. According to Sections 2 and 3 and Definition 3 the method is phase-fitted if $\phi(\nu^2; \nu) = 0$. Therefore, when the main frequency is exactly known the phase-lag order of a phase-fitted method is equal to infinity. Similarly, the method is amplification-fitted if $d(\nu^2; \nu) = 0$. The method is then zero-dissipative. In many real applications the main frequency is not exactly known. When a good estimate is available we have that $r \approx 1$. The magnitude of the phase-lag (4.13) and the amplification (4.14) is then much smaller than that of the corresponding classical method.

5. Numerical illustrations

In order to evaluate the effectiveness of the new method we consider several model problems. The new method has been compared with existing two-step explicit hybrid codes. We have selected both dissipative and zero-dissipative methods of algebraic order six. The algorithms have been denoted by:
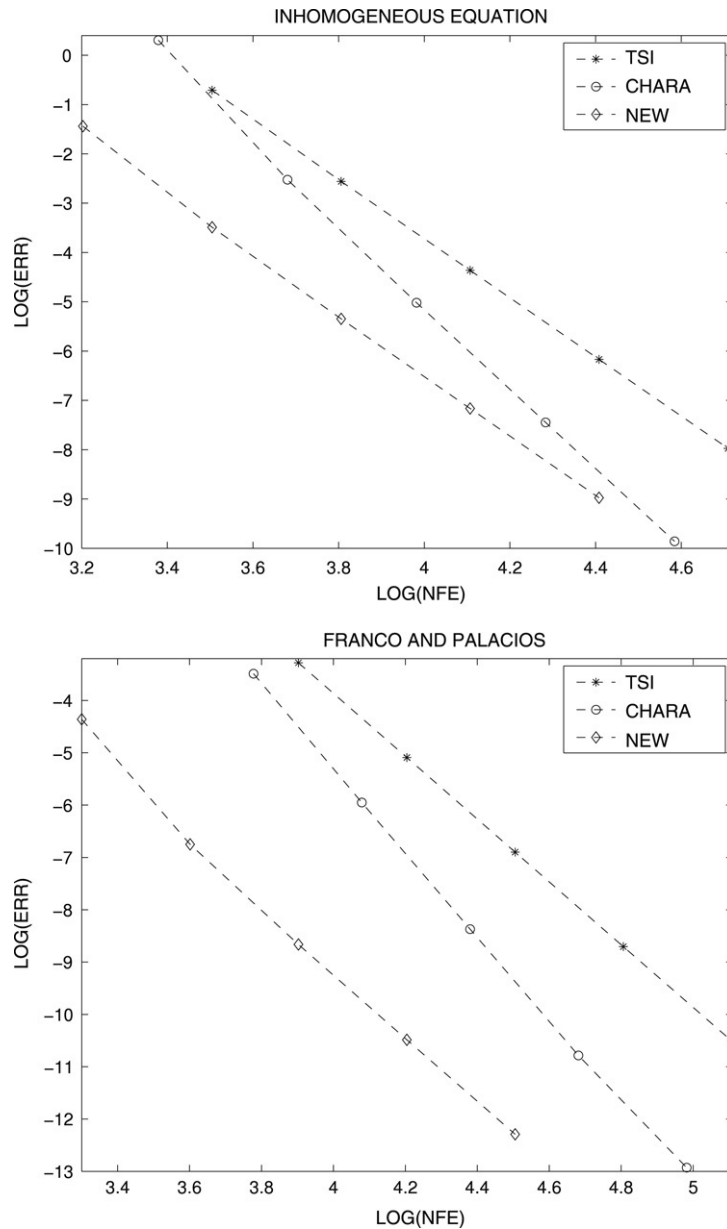
Fig. 2. Efficiency curves for Problems 1 and 2.

- TSI: method with phase-lag order six and dissipation order seven derived by Tsitouras [1].
- CHARA: zero-dissipative method with phase-lag order eight derived by Chawla and Rao [5].
- NEW: the new method defined by (3.8)–(3.10).

The criterion used in the numerical comparisons is the usual test based on computing the maximum global error over the whole integration interval. In Figs. 2 and 3 we have depicted the efficiency curves for the tested codes. These figures show the decimal logarithm of the maximum global error (ERR) versus the computational effort measured by the number of function evaluations (NFE).

We have used the following four model problems.

Problem 1. An inhomogeneous equation studied by van der Houwen and Sommeijer [7]

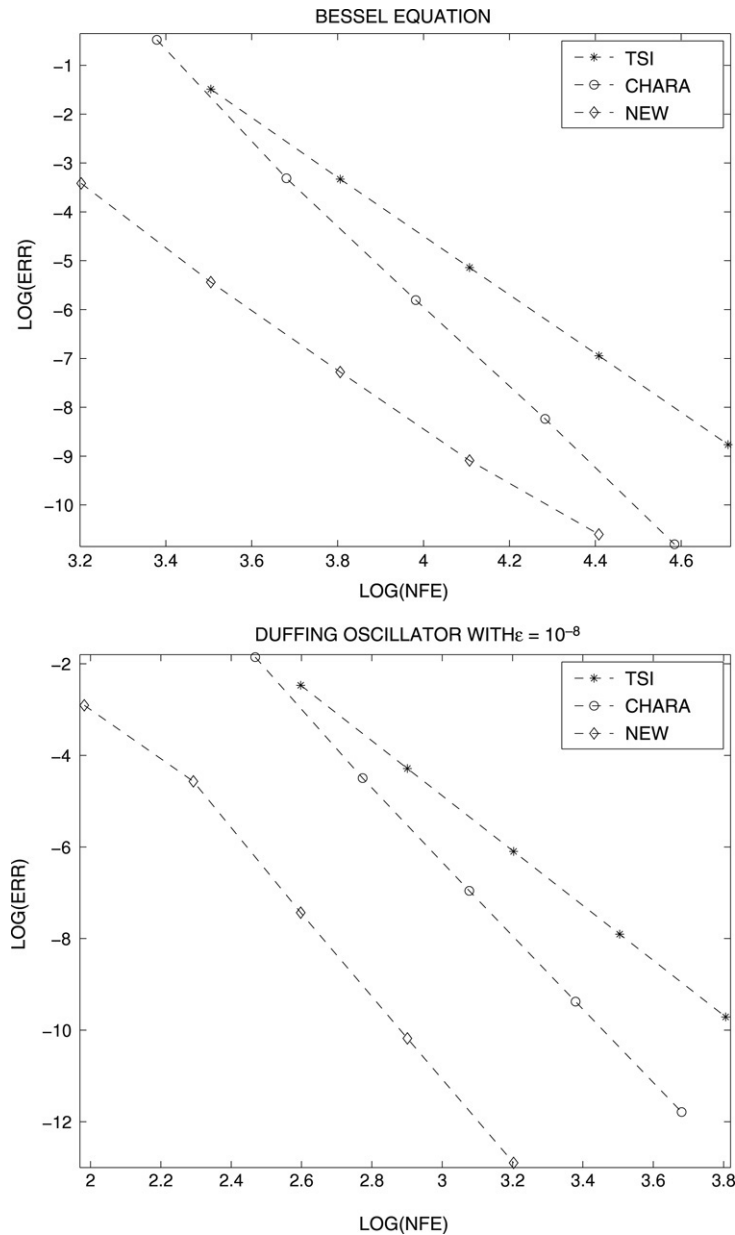$$y'' = -100y + 99\sin(x), \qquad y(0) = 1, \qquad y'(0) = 11.$$

Fig. 3. Efficiency curves for Problems 3 and 4.

The exact solution is given by:

$$y(x) = \cos(10x) + \sin(10x) + \sin(x).$$

It consists of a rapidly and slowly oscillating function; the slowly varying function is due to the inhomogeneous term. The optimized methods will take care of the rapidly oscillating component and the algebraic order will take care of the slowly varying component. The equation has been solved in the interval [0, 100]. The fitted frequency is $\omega = 10$. The numerical results stated in Fig. 2 have been computed with stepsizes $h = 2^{-j}$, $j = 3, \ldots, 7$ for TSI and $j = 2, \ldots, 6$ for the CHARA and NEW codes.

Problem 2. An "almost" periodic orbit problem studied by Franco and Palacios [28]

$$z'' = -z + \epsilon e^{i\psi x}, \qquad z(0) = 1, \qquad z'(0) = i,$$

where $\epsilon = 0.001$ and $\psi = 0.01$. The analytical solution $z(x) = u(x) + iv(x)$ is given by:

$$u(x) = \frac{1 - \epsilon - \psi^2}{1 - \psi^2} \cos(x) + \frac{\epsilon}{1 - \psi^2} \cos(\psi x),$$

$$v(x) = \frac{1 - \epsilon\psi - \psi^2}{1 - \psi^2} \sin(x) + \frac{\epsilon}{1 - \psi^2} \sin(\psi x).$$

The solution represents a motion of a perturbation of a circular orbit in the complex plane. The problem may be solved either as a single equation in complex arithmetic or as a pair of coupled equations. The equation has been solved in the interval [0, 1000]. The fitted frequency is $\omega = 1$. The numerical results stated in Fig. 2 have been computed with stepsizes $h = 2^{-j}$, $j = 1, \ldots, 5$ for TSI, $j = 0, \ldots, 4$ for CHARA and $j = -1, \ldots, 3$ for NEW.

Problem 3. An equation related to Bessel's equation.

This is a classical test equation widely used by several authors such as van der Houwen and Sommeijer [7], Coleman and Duxbury [27] and so on. This is of the form

$$y'' = -\left(100 + \frac{1}{4x^2}\right) y.$$

The exact solution is given by $y(x) = \sqrt{x} J_0(10x)$, where J_0 is the Bessel function of the first kind of order zero. The initial values are $y(1) = J_0(10)$ and $y'(1) = \frac{1}{2} J_0(10) - 10 J_1(10)$, where J_1 is the Bessel function of order 1. The equation has been solved in the interval [1, 100]. The fitted frequency is $\omega = 10$. The numerical results stated in Fig. 3 have been computed with the same stepsizes as considered in Problem 1.

Problem 4. Duffing oscillator

$$y' + y = \epsilon y^3, \qquad y(0) = 1, \qquad y'(0) = 0. \tag{5.15}$$

The equation has been solved in the interval [0, 100] with the perturbation parameter $\epsilon = 10^{-8}$. The fitted frequency is $\omega = 1$. The error has been calculated using a reference solution obtained by means of the perturbation techniques developed by Farto et al. [29]. The numerical results stated in Fig. 3 have been computed with stepsizes $h = 2^{-j}$, $j = 0, \ldots, 4$ for TSI, $j = -1, \ldots, 3$ for CHARA and $j = -2, \ldots, 2$ for NEW.

6. Conclusions

In this paper we have modified the sixth-order method of Tsitouras [1]. Two free parameters are added in such a way that the phase-lag and the amplification vanish. As a consequence, the exact solution of the scalar test equation (2.4) is reproduced. The method has coefficients simpler and less expensive to evaluate compared to many other existing ν-dependent methods. In addition, the coefficients have no critical ν-values where the method is undefined. A detailed analysis reveals that the new method shares some important properties with its classical companion such as the algebraic order, phase-lag order and dissipation order. The stability properties, on the contrary, are very different to the classical method and they depend on the fitted frequency and the stepsize. From the numerical experiments carried out it is remarkable to see that the CHARA code behaves as an eight-order method on the test problems considered. This can be understood as follows: in [30] it was explained that for zero-dissipative methods the phase-lag order is equal to the order of the solution of the test equation (2.4). The test problems considered are very similar to the test equation. Although the new method reaches only order six on Problems 1 and 3, it can be seen from Figs. 2 and 3 that it is the most efficient one.

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