Explicit Numerov type methods for second order IVPs with oscillating solutions.

G. Papageorgiou, Ch. Tsitouras and I. Th. Famelis *†

Department of Applied Mathematics and Physical Sciences,
National Technical University of Athens, Zografou Campus
15780, Athens, GREECE

Abstract

New explicit hybrid Numerov type methods are presented in this paper. These efficient methods are constructed using a new approach

* E-mails: {papag,tsitoura,ifamelis}@math.gsd.ntua.gr

†Corresponding Author: Ioannis Th. Famelis, Department of Applied Mathematics and Physical Sciences, National Technical University of Athens, Zografou Campus 15780, Athens, GREECE, Tel. +301 7721701, E-mail: ifamelis@math.gsd.ntua.gr

where we do not need the use of the intermediate high accuracy interpolatory nodes, since only the Taylor expansion of the internal points is needed. The methods share sixth algebraic order at a cost of five stages per step while their phase lag order is 14 and partly satisfy the dissipation order conditions. It has be seen that the property of phase-lag is more important than the non empty interval in constructing numerical methods for the solution of Schrodinger equation and related problems [1, 16, 18]. Numerical results over some well known problems in physics and mechanics indicate the superiority of the new methods.

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1 Introduction.

The initial value problem of second order

$$y'' = f(y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \tag{1}$$

especially when the solution is oscillating, is of continued interest in many fields of celestial mechanics, quantum mechanics, scattering theory, theoretical physics and chemistry, and electronics (see [11, 12]). When solving (1) numerically we have to pay attention in the algebraic order of the method used, since this is the main factor of achieving higher accuracy with lower computational cost, i.e. this is the main factor of increasing the efficiency of our effort.

If we also feel that the solution of (1) is of periodic nature it is essential to consider some special property, such as phase-lag (or dispersion), amplification (or dissipation), interval of periodicity, exponential fitting, adaptive properties, Chebyshev polynomials fitting etc. Methods with the above properties can be divided into two categories

(i) Methods with constant coefficients (phase-lag, interval of periodicity)

(ii) Methods with coefficients dependent on the frequency of the problem (exponential fitting, adaptive properties, fitting to Chebyshev polynomials etc)

If the frequency is known with high accuracy then methods of type (ii) are preferred. But most of the times we are not in case of having a good approximation of the frequency of the problem. Another unpleasant situation

arrives when the problem has many frequencies.

So it is important to consider methods of type (i) sharing the properties of small phase-lag and amplification. These are actually two types of truncation errors. The first is the angle between the true and the approximated solution, while the second is the distance from a standard cyclic solution.

One of the most widely used method for solving (1) is the Numerov method which is fourth algebraic and sixth phase-lag order. This method is implicit and its implementation involve computations of Jacobians and solutions of non-linear systems of equations, [4]. So many authors proposed explicit modifications of Numerov method trying simultaneously to increase the phase-lag order. The algebraic orders achieved were at most only six, [5, 6, 14]. Simos was enforced to add many additional stages for achieving an eighth order method with some extra characteristics [15]. Recently Tsitouras and Simos [23], presented an explicit ten-stages method of eighth algebraic order and of phase-lag order 14, which is the best method of this type appeared in the literature until then. That method was of zero dissipation, something common when implementing two step hybrid methods for problems with periodic solutions. Similarly, Simos [17] derived an 8th algebraic order method of phase-lag order 16 using 13 stages, something that may affect

the overall efficiency of the method. These methods require the evaluation of interpolatory off-step nodes. This technique increases the computational cost since the interpolation points share high accuracy too, something that is useless. So six stages are needed per step for a sixth order method while an eighth order method uses ten stages per step.

In [19], that purposeless derivation of intermediate points was the motivation for considering another approach, similar to the one used for the construction of Runge-Kutta-Nyström(RKN) methods. Instead of spending much effort increasing the order of internal nodes we simply involve them in a scheme, where only the final result of the approximation in every step has to achieve the demanded order. Using this technique one can manage to derive sixth order method at a cost of four stages (see [19]) instead of the six stages needed according to classical implementation, [6].

At the same time Papakostas and Tsitouras [13], presented high phase-lag order Runge-Kutta and Runge-Kutta-Nyström methods with non zero amplification error. Even in [20], it was notified that the zero amplification error is not so promising. Finally the results given in [1, 16, 18] conserning Schrödinger equation, encouraged us to deal with the derivation of non zero dissipative two-step sixth order methods of high phase-lag order. In order

to fulfill the dispersion and the dissipation conditions we added a fifth stage which increased the degrees of freedom during the construction of the new scheme. These extra parameters were used for increasing phase-lag order and partly satisfy the amplification order conditions.

2 Basic theory.

To study the stability properties of methods posed for solving (1), it is constructive to consider the scalar test problem

$$y' = -\omega^2 y, \quad \omega \in \Re \; . \tag{2}$$

When applying an explicit two step hybrid method to the problem (2) we obtain a difference equation of the form

$$y_{n+1} + S\left(v^2\right) y_n + C\left(v^2\right) y_{n-1} = 0, \tag{3}$$

where $y_n \approx y\left(nh\right)$ the computed approximations at $n = 1, 2, \ldots$, $v = \omega h$, h the step size used, and $S\left(v^2\right), C\left(v^2\right)$ polynomials in v^2. All the methods until now, make the assumption $C\left(v^2\right) \equiv 1$. This was not obligatory but mostly a pleasant (as believed) outcome of oversimplifications due to the symmetries

of the methods proposed. The characteristic equation associated with (3) is

$$\lambda^2 + S\left(v^2\right)\lambda + C\left(v^2\right) = 0. \tag{4}$$

Following Lambert and Watson [10], we say that the numerical method (3) has interval of periodicity $(0, v_0^2)$ if $C\left(v^2\right) \equiv 1$ and $\mid S\left(v^2\right) \mid < 2$ for all $v^2 \in (0, v_0^2)$. Consequently the method is called P-stable if $v_0 = \infty$. In our new proposal here $C\left(v^2\right) \neq 1$ so it is of interest to consider the *amplification* (or dissipation) order q as the number satisfying

$$1 - C\left(v^2\right) = O\left(v^q\right).$$

Since the solution of (2) is $y(x) = e^{i\omega x}$ we may write

$$e^{2iv} + S\left(v^2\right) \cdot e^{iv} + C\left(v^2\right) = O,$$

satisfying (4). So the phase-lag order of the method is p if

$$\cos 2v + S\left(v^2\right)\cos v + C\left(v^2\right) = O\left(v^p\right).$$

3 The new method

According to the implementation of [6], let $h > 0$ and $t_n = t_0 + nh, \quad n = 0, 1, 2, ...$; We may construct a sixth order method for the approximation of

y_{n+1}using values from two steps. i.e. $[t_{n-1}, t_n]$ and $[t_n, t_{n+1}]$. The available values are $y_{n-1},\ y''_{n-1} = f_{n-1}$ and y_n while we get $y''_n = f_n = f(y_n)$ at a cost of one function evaluation.

We also need three more values of second derivatives within the interval $[t_{n-1}, t_{n+1}]$ in order to form the required interpolant. These extra values ought to be of fourth algebraic order. If it was possible to derive them without cost then we could construct a sixth order method at a cost of four stages. Unfortunately we can not achieve this task since $y_{n-1},\ y''_{n-1},\ y_n$ and y''_n are not enough information to give us interpolatory approximations of intermediate values of the desired accuracy. So the total cost increases to six stages.

Interpolatory nodes carry a lot of information that is useless even for conventional methods [19]. Implementing the new method we only need y''_n and three extra function evaluations in order to achieve the desired order. We add another stage, so to achieve high phase lag order. So we finally have four extra function evaluations f_a, f_b, f_c and f_d. This is still less than the cost of six stages. The new method has the form:

$$f_n = f(x_n, y_n)$$

$$
\begin{aligned}
f_a &= f(x_n - c_1 h, (1-c_1)y_n + c_1 y_{n-1} + h^2(d_{11} f_{n-1} + d_{12} f_n)) \\
f_b &= f(x_n - c_2 h, (1-c_2)y_n + c_2 y_{n-1} + h^2(d_{21} f_{n-1} + d_{22} f_n + a_{21} f_a)) \\
f_c &= f(x_n - c_3 h, (1-c_3)y_n + c_3 y_{n-1} + h^2(d_{31} f_{n-1} + d_{32} f_n + a_{31} f_a + a_{32} f_b)) \\
f_d &= f(x_n - c_4 h, (1-c_4)y_n + c_4 y_{n-1} + h^2(d_{41} f_{n-1} + d_{42} f_n + a_{41} f_a + a_{42} f_b + a_{43} f_c)) \\
y_{n+1} &= 2y_n - y_{n-1} + h^2(w_1 f_{n-1} + w_2 f_n + b_1 f_a + b_2 f_b + b_3 f_c + b_4 f_d). \qquad (5)
\end{aligned}
$$

Using the notation of Nyström methods we consider the following matrices.

$$
A = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
d_{11} & d_{12} & 0 & 0 & 0 & 0 \\
d_{21} & d_{22} & a_{21} & 0 & 0 & 0 \\
d_{31} & d_{32} & a_{31} & a_{32} & 0 & 0 \\
d_{41} & d_{42} & a_{41} & a_{42} & a_{43} & 0
\end{bmatrix},
$$

$$
b = \begin{bmatrix} w_1 & w_2 & b_1 & b_2 & b_3 & b_4 \end{bmatrix},
$$

and

$$
c = \begin{bmatrix} 1 & 0 & c_1 & c_2 & c_3 & c_4 \end{bmatrix}^T
$$

Now the method can be formulated in a table like the Butcher Tableau:

$$\begin{array}{c|c} c & A \\ \hline & b \end{array}$$

(see [2, 3]).

Then we take the Taylor series expansions of the exact value $y(t_n+h)$ and the $f_a, f_b, f_c, f_d, y_{n+1}$. For a sixth order method we match the corresponding expansions up to h^7, and we arrive at an expression of the following form :

$$h^2\left(q_{21}F_{21}\right)+h^3\left(q_{31}F_{31}\right)+...+h^7\left(q_{71}F_{71}+...+q_{7,10}F_{7,10}\right)+O\left(h^8\right), \quad (6)$$

where q_{ij} are expressions of the coefficients of the method while F_{ij} are elementary differentials with respect to y', f and $f^{(k)}=\frac{\partial^k f}{\partial t^k}$, $k=1,2,...,6$ (see [7]). The order conditions for a sixth order method are in total 23 [8]. The enumeration of order conditions follows from the Nyström methods theory (see [7, 8]).

Reduction of the order conditions is achieved using the simplifying assumption:

$$Ae=\frac{1}{2}\left(c^2-c\right), \quad (7)$$

with $e=\left[\begin{array}{cccccc}1 & 1 & 1 & 1 & 1 & 1\end{array}\right]^T$ and $c^i=\left[\begin{array}{cccccc}1 & 0 & c_1^i & c_2^i & c_3^i & c_4^i\end{array}\right]$. Equation (7) reduces all q's with corresponding elementary differentials containing f.

E.g.:

$$q_{42} = bAe + bc - 1/12$$

with $F_{42} = f'f$ is simplified by

$$q_{41} = \frac{1}{2}bc^2 - \frac{1}{12}$$

with $F_{41} = f''y'^{\,2}$, since

$$q_{42} = bAe+bc-\frac{1}{12} = b\frac{1}{2}\left(c^2 - c\right)-bc-1/12 = \frac{1}{2}bc^2-2bc-\frac{1}{12} = \frac{1}{2}bc^2-\frac{1}{12} = q_{41}$$

(Notice that $q_{31} = bc$ ought to be zero satisfying lower order condition). So, finally the equations that should be satisfied so that a method has algebraic order six are presented in Table 1 (see [21]).

Our methods have 20 parameters in view of (7). So, using a symbolic manipulation package we can solve the 13 equations of algebraic order and have 7 free parameters to solve for the dissipation and the dispersion order conditions. We observe that

$$1 - C\left(v^2\right) = -v^7 b \cdot A^3 \cdot c + v^9 b \cdot A^4 \cdot c.$$

On the other hand phase lag is an infinite series of the form

$$l_8 v^8 + l_{10} v^{10} + l_{12} v^{12} + O\left(v^{14}\right).$$

In Table 2 we present the simplified form of l_8, l_{10}, l_{12} when simplifying assumptions and the algebraic order conditions of Table 1 hold.

In [23], Tsitouras and Simos following tradition asked for 1-$C\left(v^2\right) \equiv 0$. They were lucky enough to achieve a special solution at a cost of one parameter. But then they could satisfy only $l_8 = l_{10} = l_{12} = 0$, getting a forced $l_{14} \neq 0$.

This holds in our case too. So here we can not get zero dissipation and a higher phase-lag order together. What we can achieve is to fulfill $l_8 = l_{10} = l_{12} = 0$ so $p = 14$ and $b \cdot A^3 \cdot c = 0$ so $q = 9$. That means that we manage to construct a method with order 6 and phase lag order 14 with a cost of five stages. A specific choice is given in Table 3.

4 Numerical results

To illustrate our new sixth order method we compared it with the following methods:

Method 1: The sixth order RKN method of Tsitouras & Papacostas [13],

Method 2: The six stages two-step method of Chawla & Rao [6],

Method 3: The 8th order method of Simos in [15],

Method 4: The 8th order method of Tsitouras & Simos [23],

Method 5: The general purpose sixth order method of Tsitouras [19],

Method 6: The method of Simos [17] of order 8 with 13 stages.

Method 7: The New Method.

The main characteristics of the methods can be found in Table 4.

The three problems chosen for our comparisons are well known in the relevant literature.

4.1 Bessel equation

First we considered the following problem

$$y'' = \left(-100 + \frac{1}{4x^2}\right) y,\ y(1) = J_0(10x),\ y'(1) = -0.5576953439142885,$$

whose theoretical solution is

$$y(x) = \sqrt{x} J_0(10x).$$

We solved the above equation in order to find the 100th root of the solution which is equal to 32.59406213134967 (see [23]).

4.2 Inhomogeneous equation

Our second test problem was an inhomogeneous problem

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

with analytical solution

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

We integrated that problem in the interval $x \in [0, 10\pi]$ as in [17, 23].

4.3 Wave equation, [9]

Finally we chose the Wave equation

$$\frac{\partial^2 u}{\partial t^2} = gd\,(x)\,\frac{\partial^2 u}{\partial x^2} + \frac{1}{4}\lambda^2\,(x,u)\,u,\ x \in [0,b]\,,\ t \geq 0,$$

with initial (and boundary) conditions

$$\frac{\partial u}{\partial x}\,(t,0) \quad = \quad \frac{\partial u}{\partial x}\,(t,b) = 0$$

$$
\begin{aligned}
u\,(0,x) &= \sin\frac{\pi x}{b}, \frac{\partial u}{\partial t} \\
(0,x) &= -\frac{\pi}{b}\sqrt{gd}\cos\frac{\pi x}{b}.
\end{aligned} \tag{8}
$$

We implemented the case $b = 100$, $g = 9.81$, $d = 10\left(2 + \cos\frac{2\pi x}{b}\right), \lambda = \frac{g|u|}{2500d}$ as in [9]. By using the method of lines with $\Delta x = 10$, this problem was converted into a system of ODEs with eleven equations. The ninth component u_9 of the system approximates $u(t,x)$ at $x = 8\Delta x = 80$. A very accurate integration calculated the 10th zero of u_9 is 63.35062926689779. So we integrated the methods to this point and recorded the values of the 9th component.

The two step methods were run at constant step size and the observed end-point error e was recorded at a fixed number of stages. Then we passed in Tables 5,6 and 7 the value $-\log e$, i.e. the accurate digits of the solution. The $*$ in the tables means that in that case the method has given unacceptable results. That means that the accurate digits of the solution were a negative number. The eighth order Runge-Kutta-Nyström method given in [13], were used to propagate the first step.

The Runge-Kutta-Nyström pair were run at variable step size mode, ac-

cording to the guidelines and step-size control algorithm introduced in [22]. Then using linear interpolation on the function evaluations and the corresponding accurate digits observed for each tolerance, we recorded the error that might have been generated at the stages used by two-step methods.

Interpreting the results it is obvious that the new method generally performs better than the other methods which are of the same or even higher algebraic order. We note as well that the advantage is clear even the nonlinear realistic model of wave equation. It is worth mentioning that the sixteenth phase-lag order methods have too many stages and may only become competitive when applied at quadruple precision.

5 Conclusion

A new method is constructed using a new approach. Using this new promising technique we manage to construct very efficient methods with low order and a small number of stages. This method is performing very well in double precision. So increasing the number of stages we intend to produce methods with even higher algebraic and phase lag order which will have excellent behavior for every requested accuracy. We note that the methods of the type

we derived here are nonsymmetric (dissipative). Our results in agreement with those given in [1, 16, 18] indicate that the crucial property for a method for the solution of oscillatory problems is the phase-lag.

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Table 1: The equations needed for algebraic order six.

$$b \cdot e = 1$$

$$b \cdot c = 0$$

$$b \cdot c^2 = \tfrac{1}{6}$$

$$b \cdot c^3 = 0$$

$$b \cdot A \cdot c = 0$$

$$b \cdot c^4 = \tfrac{1}{15}$$

$$b \cdot A \cdot c^2 = \tfrac{1}{180}$$

$$b \cdot c \cdot A \cdot c = -\tfrac{1}{60}$$

$$b \cdot c^5 = 0$$

$$b \cdot c^2 \cdot A \cdot c = 0$$

$$b \cdot c \cdot A \cdot c^2 = -\tfrac{1}{72}$$

$$b \cdot A \cdot c^3 = 0$$

$$b \cdot A^2 \cdot c = 0$$

Table 2: The equations needed for phase lag order twelve.

$$l_8 = b \cdot A^3 \cdot e + \tfrac{1}{2} b \cdot A^2 \cdot e - \tfrac{29}{20160}$$

$$l_{10} = b \cdot A^4 \cdot e + \tfrac{1}{2} b \cdot A^3 \cdot e - \tfrac{1}{2} b \cdot A^3 \cdot c + \tfrac{1}{24} b \cdot A^2 \cdot e - \tfrac{2}{14175}$$

$$l_{12} = b \cdot A^5 \cdot e + \tfrac{1}{2} b \cdot A^4 \cdot e - \tfrac{1}{2} b \cdot A^4 \cdot c + \tfrac{1}{24} b \cdot A^3 \cdot e - \tfrac{1}{24} b \cdot A^3 \cdot c$$

$$+ \tfrac{1}{720} b \cdot A^2 \cdot e - \tfrac{743}{119750400}$$

Table 3: The coefficients of the new method.

$d_{11} = -0.01198958741218540$ $d_{12} = 0.8033023565368236$

$d_{21} = -0.1354926086240548$ $d_{22} = 3.570963452815986$

$a_{21} = 0.1056425232832385$ $d_{31} = 0.005343514535940652$

$d_{32} = -0.1244946227062173$ $a_{31} = -0.03293580148977421$

$a_{32} = 0.008375035141675025$ $d_{41} = -0.05260980968085666$

$d_{42} = 0.1793101099560068$ $a_{41} = 0.03279785282508096$

$a_{42} = -0.007712984194627411$ $a_{43} = 0.0006109986184401625$

$c_1 = 1.853745004884331$ $c_2 = -2.207808474569488$

$c_3 = 0.2575963849069488$ $c_4 = -0.2448438326576166$

$w_1 = -0.01095654182197717$ $w_2 = -1.535330518304029$

$b_1 = 0.003328481791861325$ $b_2 = 0.001185580954875260$

$b_3 = 1.253365756591692$ $b_4 = 1.288407240787577$

Table 4: The main characteristics of the methods under comparison.

method	order	stages	phase-lag	amplification
1	6	5	10	8
2	6	6	10	∞
3	8	13	16	∞
4	8	10	14	∞
5	6	4	8	7
6	8	13	16	∞
7	6	5	14	9

Table 5: Accurate digits for the inhomogeneous equation

	Function Evaluations									
	900	1500	2100	2700	3300	3900	4500	5100	5700	6300
Method 1	1.5	3.0	4.1	4.4	4.9	5.3	5.6	6.0	6.2	6.5
Method 2	1.1	3.2	4.4	5.3	6.	6.6	7.1	7.5	7.9	8.2
Method 3	*	0.2	1.7	3.4	4.7	5.7	6.6	7.4	8.1	8.7
Method 4	*	1.3	3.2	4.6	5.7	6.6	7.3	8.0	8.6	9.1
Method 5	0.9	2.3	3.2	3.9	4.5	4.9	5.3	5.6	5.9	6.2
Method 6	*	0.3	3.1	5.4	7.2	8.6	9.6	10.3	10.8	11.1
Method 7	3.5	6.4	7.7	8.4	9.1	9.7	10.2	10.7	11.	11.5

Table 6: Accurate digits for the Bessel equation

	Function Evaluations									
	900	1500	2100	2700	3300	3900	4500	5100	5700	6300
Method 1	2.3	3.5	5.1	5.6	6.0	6.3	6.6	6.9	7.1	7.3
Method 2	1.7	3.7	5.0	5.9	6.6	7.2	7.7	8.1	8.5	8.8
Method 3	*	0.6	2.3	4.0	5.2	6.3	7.1	7.8	8.4	8.9
Method 4	*	1.8	3.8	5.1	6.3	7.1	7.9	8.5	9.1	9.6
Method 5	1.7	3.0	3.9	4.6	5.1	5.5	5.9	6.2	6.5	6.8
Method 6	1.1	4.3	5.7	6.6	7.4	8.0	8.5	9.0	9.4	9.7
Method 7	3.8	6.1	7.3	8.0	8.5	9.0	9.3	9.7	9.9	10.3

Table 7: Accurate digits for the wave equation

	Function Evaluations									
	360	720	1080	1440	1800	2160	2520	2880	3240	3600
Method 1	2.9	4.0	5.1	6.4	7.8	8.1	8.2	8.2	8.3	8.5
Method 2	2.3	3.4	5.0	6.1	6.9	7.5	8.1	8.6	9.0	9.3
Method 3	*	*	2.0	2.9	4.5	5.7	6.7	7.5	8.2	8.9
Method 4	*	*	3.0	4.7	5.9	6.9	7.8	8.5	9.1	9.7
Method 5	2.5	3.4	4.4	5.2	5.7	6.2	6.6	6.9	7.3	7.5
Method 6	*	3.0	5.7	8.3	9.6	10.3	10.8	11.3	11.7	12.0
Method 7	2.2	5.6	7.4	8.6	9.6	10.4	11.0	11.6	12.1	12.9