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EXPLICIT EIGHTH ORDER TWO-STEP METHODS WITH NINE STAGES FOR INTEGRATING OSCILLATORY PROBLEMS

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We present a new explicit hybrid two step method for the solution of second order initial value problem. It costs only nine function evaluations per step and attains eighth algebraic order so it is the cheapest in the literature. Its coefficients are chosen to reduce amplification and phase errors. Thus the method is well suited for facing problems with oscillatory solutions. After implementing a MATLAB program, we proceed with numerical tests that justify our effort.

Keywords: Initial Value Problem; Second Order; Numerov; Order conditions; Phase-Lag.

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1. Introduction.

We consider the initial value problem of second order

$$y'' = f(t, y), \quad y(t_0) = y^{[0]}, \quad y'(t_0) = y'^{[0]}, \quad (1)$$

where $f : \mathfrak{R}^N \rightarrow \mathfrak{R}^N$ and $y^{[0]}, y'^{[0]} \in \mathfrak{R}^N$. Observe that y' is not involved in (1).

In this paper we investigate the class of the above problems with oscillatory solutions. Our result are methods which can be applied to many problems in celestial mechanics, quantum mechanical scattering theory, in theoretical physics and chemistry in electronics and many fields of engineering.

Implicit hybrid Numerov-type methods were introduced by Hairer¹, Cash² and Chawla³ basically for satisfying P-stability (see Lambert and Watson⁴ or Simos and Tsitouras⁵), a useful property for dealing periodic problems. Later Chawla⁶ and Chawla and Rao^{7,8} used explicit modifications of these methods especially for reducing phase errors, Brusa and Nigro⁹.

After a decade where only sixth order methods were produced, Simos¹⁰ was enforced to add many additional stages for achieving an eighth order method with

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Table 1. The stages and the formula of the method we consider.

$Y^{[1]}$	$=$	$y^{[k-1]}$
f_{k+c_1}	$=$	$f(t_k - h, Y^{[1]})$
$Y^{[2]}$	$=$	$y^{[k]}$
f_{k+c_2}	$=$	$f(t_k, Y^{[2]})$
$Y^{[3]}$	$=$	$(1 + c_3)y^{[k]} - c_3y^{[k-1]} + h^2(d_{11}f_{k+c_1} + d_{12}f_{k+c_2})$
f_{k+c_3}	$=$	$f(t_k + c_3h, Y^{[3]})$
$Y^{[4]}$	$=$	$(1 + c_4)y^{[k]} - c_4y^{[k-1]} + h^2(d_{21}f_{k+c_1} + d_{22}f_{k+c_2} + a_{21}f_{k+c_3})$
f_{k+c_4}	$=$	$f(t_k + c_4h, Y^{[4]})$
...		...
$Y^{[s]}$	$=$	$(1 + c_s)y^{[k]} - c_sy^{[k-1]} + h^2 \left(\begin{array}{l} d_{s1}f_{k+c_1} + d_{s2}f_{k+c_2} + a_{s1}f_{k+c_3} \\ + a_{s2}f_{k+c_4} + \dots + a_{s,s-1}f_{k+c_{s-1}} \end{array} \right)$
f_{k+c_s}	$=$	$f(t_k + c_sh, Y^{[s]})$
$y^{[k+1]}$	$=$	$2y^{[k]} - y^{[k-1]} + h^2 \left(\begin{array}{l} w_1f_{k+c_1} + w_2f_{k+c_2} + b_1f_{k+c_3} + b_2f_{k+c_4} + \dots \\ + b_{s-3}f_{k+c_{s-1}} + b_{s-2}f_{k+c_s} \end{array} \right)$

some extra characteristics. Later Tsitouras and Simos¹¹, presented an explicit ten-stages method of eighth algebraic order and of phase-lag order 14, which was 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, Simos¹² derived an 8–th algebraic order method of phase-lag order 16 using 13 stages, something that affected 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.

Tsitouras^{13,14}, considered another approach, similar to the one used for the construction of Runge-Kutta-Nyström(RKN) methods avoiding that purposeless derivation of intermediate points. Instead of spending much effort increasing the accuracy 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 instead of the six stages needed according to classical implementation⁸.

At the same time Papakostas and Tsitouras¹⁵, presented high phase-lag order Runge-Kutta and Runge-Kutta-Nyström methods with non zero amplification error. Finally the results given by Simos and his colleagues^{16,17,18} concerning Schrödinger equation, encouraged us to deal with the derivation of non zero dissipative two-

step sixth order methods of high phase-lag order using the new implementation, Papageorgiou et. al¹⁹. Later these type of methods were studied theoretically by Coleman²⁰ and Chan et. al.²¹ through B2-series and P-series respectively. Some other methods presented recently can be found in Psihogios and Simos^{22,23} and Calvo et. al²⁴.

The methods we consider here are of the form given in Table 1, where $h = t_{k+1} - t_k = t_k - t_{k-1} = \dots = t_1 - t_0$. The vectors $y^{[k+1]}$, $y^{[k]}$ and $y^{[k-1]}$ approximate $y(t_k + h)$, $y(t_k)$ and $y(t_k - h)$ respectively while $Y^{[1]} \in \mathfrak{R}^N$, $Y^{[2]} \in \mathfrak{R}^N, \dots$ form f 's, which are the stages of the method. These stages do not approximate any internal points. They are used in a tricky way to achieve a high order final formula.

Following tradition we make use of known information at mesh, setting:

$$Y^{[1]} = y^{[k-1]}, Y^{[2]} = y^{[k]}.$$

Since $f(t_{k-1}, Y^{[1]})$ has been evaluated in the previous step, only $f(t_k, Y^{[2]})$ is an actual stage in the current step.

2. Algebraic order of the new method.

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. Thus this is the main factor of increasing the efficiency of our effort. Using the notation of Nyström methods the new one can be formulated in a table like the Butcher^{25,26} tableau,

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

In vector notation, for an autonomous system $y'' = f(y)$, an s -stage Numerov type method takes the form

$$\begin{aligned} y^{[k+1]} &= 2y^{[k]} - y^{[k-1]} + h^2 \cdot (b \otimes I_s) \cdot f(Y) \\ Y &= (e + c) \otimes y^{[k]} - c \otimes y^{[k-1]} + h^2 \cdot (A \otimes I_s) \cdot f(Y) \end{aligned} \quad (2)$$

with $I_s \in \mathfrak{R}^{s \times s}$ the identity matrix, $A \in \mathfrak{R}^{s \times s}, b^T \in \mathfrak{R}^s, c \in \mathfrak{R}^s$ the coefficient matrices of the method and

$$e = [1 \ 1 \ \dots \ 1]^T \in \mathfrak{R}^s.$$

For this case the independent variable t can be considered as an extra component of y , setting

$$y''_{N+1} = 0, y^{[0]}_{N+1} = t_0, y^{[0]}_{N+1} = 1.$$

As an example lets take a look at Numerov made explicit by Chawla⁶. This two stage method is given by

$$\begin{aligned} Y^{[1]} &= y^{[k-1]}, Y^{[2]} = y^{[k]}, Y^{[3]} = 2y^{[k]} - y^{[k]} + h^2 f(t_k, Y^{[2]}), \\ y^{[k+1]} - 2y^{[k]} + y^{[k-1]} &= \frac{1}{12} \cdot (f(t_{k+1}, Y^{[3]}) + 10f(t_k, Y^{[2]}) + f(t_{k-1}, Y^{[1]})). \end{aligned} \quad (3)$$

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By the above analysis we have the following matrices characterizing (3):

$$A = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

$$b = \left[\frac{1}{12} \quad \frac{5}{6} \quad \frac{1}{12} \right],$$

and

$$c = [-1 \ 0 \ 1]^T.$$

The first two rows of A have no entries since no f 's are involved in the evaluation of $Y^{[1]}$ and $Y^{[2]}$. The third row of A is $[0 \ 1 \ 0]$ because

$$Y^{[3]} = \dots + h^2(0 \cdot f(t_{k-1}, Y^{[1]}) + 1 \cdot f(t_k, Y^{[2]}) + 0 \cdot f(t_{k+1}, Y^{[3]})).$$

Methods like (3) are called explicit because we compute the stages in sequence. In the Nyström notation used here this is reflected by a strictly lower triangular coefficient matrix A . On the other hand, if $a_{ij} \neq 0$ for some $i \leq j$ the method is called implicit. This leads to the solutions of non-linear algebraic systems increasing the computational effort.

For the explicit methods we introduce in this paper we take $s = 10$ and the corresponding matrices become:

$$A = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ d_{11} & d_{12} & 0 & \cdots & 0 \\ d_{21} & d_{22} & a_{21} & 0 & \cdots & 0 \\ \vdots & & & \ddots & \vdots \\ d_{81} & d_{82} & a_{81} & \cdots & a_{87} & 0 \end{bmatrix},$$

$$b = [w_1 \ w_2 \ b_1 \ b_2 \ \cdots \ b_8],$$

and

$$c = [-1 \ 0 \ c_1 \ c_2 \ \cdots \ c_8]^T.$$

The new method needs only nine function evaluations per step since $f(Y^{[1]})$ has been already evaluated in the previous step.

Our method shares 62 parameters. As can be seen above there are 44 coefficients for A (namely $d_{11}, d_{12}, d_{21}, d_{22}, a_{21}, \dots$), 10 coefficients for vector b and 8 entries for vector c . The numbers of equations of condition for various orders coincides the corresponding number for Runge-Kutta-Nystrom²⁷ methods and they are listed in Table 2. For achieving 8-th order, $1+1+2+3+6+10+20+36 = 79$ equations have to be satisfied. In Appendix-A we list the equations up to 8-th order in various Tables.

Table 2. Number of order conditions.

order	1	2	3	4	5	6	7	8	9	10	11	12	13	14
conditions	1	1	2	3	6	10	20	36	72	137	275	541	1098	2208

The parameters are less than equations and we meet a similar problem in the construction of Runge-Kutta (RK) methods. Traditionally we make simplifying assumptions that reduce the number of conditions but commit a smaller number of coefficients. Tsitouras²⁸ addressed this problem for implicit methods of the same type and derived an eighth order P-stable method at a cost of six stages. Analogously to the manipulation we used there and other papers^{29,30,31}, we make the following simplifying assumptions:

$$w_1 = b_1 = b_2 = 0 \tag{4}$$

and

$$\begin{aligned} (Ae)_{(3-10)} &= \frac{1}{2} (c^2 + c)_{(3-10)} \\ (Ac)_{(3-10)} &= \frac{1}{6} (c^3 - c)_{(3-10)} \\ (Ac^2)_{(3-10)} &= \frac{1}{12} (c^4 + c)_{(3-10)} \\ (Ac^3)_{(5-10)} &= \frac{1}{20} (c^5 - c)_{(5-10)} \end{aligned} \tag{5}$$

with

$$c^i = [(-1)^i \ 0 \ c_1^i \ c_2^i \ \dots \ c_8^i]^T,$$

and for $k_1 < k_2$

$$(v)_{(k_1-k_2)} = [v_{k_1} \ v_{k_1+1} \ \dots \ v_{k_2}]^T.$$

The requirement (4) is obligatory in contrary to assumptions made in Ref. 28, since the available a_{ij} 's for explicit methods are not enough to satisfy equations (5) for all indexes. The remaining order conditions are given in Table 3. In this table operation "*" may understood as component-wise multiplication:

$$[u_1 \ u_2 \ \dots \ u_n]^T * [v_1 \ v_2 \ \dots \ v_n]^T = [u_1 v_1 \ u_2 v_2 \ \dots \ u_n v_n]^T.$$

This operation has the less priority. Parentheses, powers and dot products are always evaluated before "*".

Table 3. Equations of condition up to eighth order, under assumptions (4) - (5).

$b \cdot e = 1,$	$b \cdot c = 0$	$b \cdot c^2 = \frac{1}{6},$
$b \cdot c^3 = 0,$	$b \cdot c^4 = \frac{1}{15},$	$b \cdot c^5 = 0,$
$b \cdot c^6 = \frac{1}{28},$	$b \cdot A \cdot c^4 = \frac{1}{840},$	$b \cdot c^7 = 0$
$b \cdot (c * A \cdot c^4) = \frac{1}{180},$	$b \cdot A \cdot c^5 = 0$	

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So only forty four equations are required assuming eleven order conditions and satisfaction of $3 + 8 + 8 + 8 + 6 = 33$ assumptions (4) - (5). This leaves eighteen coefficients as free parameters. In order to shorten the problem we force $c_8 = 1$, $c_7 = -1$, $c_6 = \frac{1}{4}$, $c_5 = -\frac{1}{4}$, $c_3 = -c_4$. Then we may express all the coefficients with respect to 13 free parameters, namely $a_{63}, a_{64}, a_{73}, a_{74}, a_{75}, a_{76}, a_{83}, a_{84}, a_{85}, a_{86}, a_{87}, b_7$ and c_2 .

3. Periodic problems.

Following Lambert and Watson⁴ and in order to study the periodic properties of methods posed for solving (1), it is constructive to consider the scalar test problem

$$y' = -\omega^2 y, \quad \omega \in \Re. \quad (6)$$

When applying an explicit two step hybrid method of the form (2) to the problem (6) we obtain a difference equation of the form

$$y^{[k+1]} + S(v^2)y^{[k]} + P(v^2)y^{[k-1]} = 0, \quad (7)$$

where $y^{[k]} \approx y(nh)$ the computed approximations at $n = 1, 2, \dots$, $v = \omega h$, and $S(v^2), P(v^2)$ polynomials in v^2 .

The interval of periodicity $(0, v_0)$ includes all $0 < v < v_0$ with $P(v^2) \equiv 1$ and $0 < |S(v^2)| < 2$. A method with $v_0 = \infty$ is P-stable.

Zero dissipation property is fulfilled by requiring

$$P(v^2) = 1 + v^2 b (I_s + v^2 A)^{-1} \equiv 1,$$

and helps a numerical method that solves (6) to stay in its cyclic orbit.

The dissipation order q of a method is the number satisfying $1 - P(v^2) = O(v^q)$. Notice that

$$P(v^2) = 1 + \sum_{j=0}^{\infty} v^{2j+1} b \cdot A^j \cdot c = 1 + v z_1 + v^3 z_3 + \dots$$

A method of algebraic order $2 \cdot i$ satisfies the terms in the series above for $j = 0, 1, \dots, i - 1$. This means that for an eighth order method it is desirable to solve

$$z_9 = b \cdot A^4 \cdot c = 0, \quad z_{11} = b \cdot A^5 \cdot c = 0, \dots \text{ etc.},$$

in order to get higher dissipation order. For a zero-dissipative method only $z_9 = z_{11} = z_{13} = z_{15} = z_{17} = 0$ is required, since for the lower triangular matrix A , all other z 's vanish,

$$z_{2i+1} = b \cdot A^i \cdot c = 0, \text{ for } i > 8.$$

The phase-lag of the method is the angle difference between numerical and theoretical cyclic solution of (6). Since the solution of (6) is

$$y(x) = e^{i\omega x},$$

we may write equation (7) as

$$e^{2iv} + S(v^2) \cdot e^{iv} + P(v^2) = O(v^p), \quad (8)$$

with the number p the phase-lag order of the method. Since

$$S(v^2) = 2 - v^2b \cdot (I + v^2A)^{-1} \cdot (e - c)$$

we observe that expression (8) is a series of the form

$$\begin{aligned} \sum_{i=2}^{\infty} v^{2i} \left(\sum_{j=1}^{i-1} \frac{1}{2(i-j)!} b \cdot A^{j-1} \cdot (e + c) + b \cdot A^{i-1} \cdot e - 2 \sum_{j=1}^i \frac{1}{(2j)! \cdot (2(i-j))!} \right) = \\ = v^2l_2 + v^4l_4 + v^6l_6 + O(v^8). \end{aligned}$$

This series is satisfied for v^{2j} , $j = 1, 2, \dots, i$, when $2 \cdot i$ is the algebraic order of the method. Thus it is interesting to eliminate as many as possible higher order coefficients of it. We proceed solving the 44 equations for algebraic order using MATHEMATICA³² and managed to get lengthy expressions for all the coefficients with respect to the 13 free ones. These expressions can't be presented here but can be requested from the author by e-mail. Then we wrote a MATLAB³³ function requiring simultaneously:

$$z_9 = 0, z_{11} = 0, l_{10} = 0, l_{12} = 0, l_{14} = 0, l_{16} = 0, \text{ and } l_{18} = 0. \quad (9)$$

We evaluated the 13 parameters satisfying (9) and concluded to a method with phase error of $O(v^{20})$, while the amplification error is $O(v^{13})$. We conjecture that no zero dissipation method with this low phase lag exist in the class of methods we considered. In consequence the new method is dissipative and does not possess an interval of periodicity. Sacrificing high phase lag order for achieving zero dissipation property alone was not proved a good choice.

The coefficients of the new method are given in the Appendix-B as a part of a MATLAB program.

4. Numerical Tests.

To illustrate the efficiency of our new method we compared it with

- PL22 : The eighth order method given in Tsitouras³⁴,
- PL14 : The sixth order method given in Papageorgiou et al¹⁹,
- NEW : The new method implemented in Appendix-B.

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

Four problems are chosen for our comparisons that are well known from the relevant literature.

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

method	order	stages	phase-lag	amplification
PL22	8	10	22	9
PL14	6	5	14	9
NEW	8	9	20	13

4.1. Bessel equation

First we considered the following problem

$$y'' = \left(-100 + \frac{1}{4t^2}\right)y, \quad y(1) = J_0(10), \quad y'(1) = -0.5576953439142885,$$

whose theoretical solution is

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

We solved the above equation in order to find the 100th root of the solution which occurs when $t = 32.59406213134967$.

4.2. Inhomogeneous equation

Our second test problem was an inhomogeneous problem:

$$y'' = -100y(t) + 99 \sin(t), \quad y(0) = 1, \quad y'(0) = 11$$

with analytical solution

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

We integrated that problem in the interval $t \in [0, 10\pi]$ as in Simos et. al.³⁵ or Simos and Tsitouras¹¹.

4.3. Duffing equation

Then we considered the following problem

$$y'' = -y - y^3 + \frac{1}{500} \cdot \cos(1.01t),$$

$$y(0) = 0.200426728067, \quad y'(0) = 0,$$

with theoretical solution given by Van Dooren³⁶ as

$$y(x) = .200179477536 \cos(1.01t) + 2.46946143 \cdot 10^{-4} \cos(3.03t)$$

$$+ 3.04014 \cdot 10^{-7} \cos(5.05t) + 3.74 \cdot 10^{-10} \cos(7.07t).$$

We solved the above equation in the region $t \in [0, \frac{20.5}{1.01}\pi]$ because $y(\frac{20.5}{1.01}\pi) = 0$.

4.4. Wave equation

Finally we chose the Wave equation³⁷

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

with initial (and boundary) conditions

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

We implemented the case

$$b = 100, g = 9.81, d = 10 \left(2 + \cos \frac{2\pi x}{b} \right), \lambda = \frac{g |u|}{2500d}$$

following Houwen and Sommeijer³⁷. 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.

We computed the end point global error e_{ij} achieved by i -th method for j -th problem and then recorded the values $-\log(e_{ij})$ in Tables 5, 6, 7 and 8. All problems were tested for the same computational cost for all methods.

Table 5. Accurate digits for Besell equation

Method	Function Evaluations					
	4000	5000	6000	7000	8000	9000
PL22	9.3	9.5	9.9	10.3	10.7	11.1
PL14	9.0	9.6	10.1	10.5	10.8	11.1
NEW	9.1	10.0	10.7	11.4	11.9	12.4

Table 6. Accurate digits for Inhomogeneous equation

Method	Function Evaluations					
	3000	3600	4200	4800	5400	6000
PL22	7.7	8.9	9.7	9.9	10.2	10.5
PL14	8.8	9.4	9.9	10.4	10.9	11.3
NEW	8.8	9.8	10.7	11.4	12.2	12.8

We observe in average an improvement of 1.3 digits over the 8-th order method which is considerable for methods of the same algebraic order. Other explicit eighth order methods that are special tuned for oscillatory problems can be found in

Table 7. Accurate digits for Duffing equation

Method	Function Evaluations					
	2000	3000	4000	5000	6000	7000
PL22	4.5	6.9	8.3	9.3	10.1	10.9
PL14	4.3	7.1	8.3	9.0	9.6	10.1
NEW	5.7	8.2	9.6	10.5	10.9	11.1

Table 8. Accurate digits for the wave equation

Method	Function Evaluations					
	1080	1620	2160	2700	3240	3780
PL22	6.4	7.9	9.1	10.1	10.8	11.5
PL14	7.4	9.1	10.4	11.3	12.1	13.0
NEW	6.6	9.4	11.3	12.4	13.6	14.4

the literature^{11,12,15}, but it was proved that the 22-th phase-lag order method of Tsitouras³⁴ has already outperformed them.

The improvement over the sixth order method is little less than 1.0 digit. The results of this five stage-method were extraordinary in Papageorgiou et al¹⁹ and it was hard to overthrow them. It seems that the stage reduction and raising the amplification order of our new method was of crucial importance for gaining efficiency. Running the methods for larger intervals doesn't change the overall icon.

5. Conclusion

A new 8–th order method with nine stages is constructed using a recently introduced approach. Equations of condition for the attainable algebraic order and compact forms for the expression of phase-lag and amplification are given. The numerical results confirm our theoretical considerations for superior performance over problems with oscillatory solutions. In a future work it is very possible to manage dropping one stage yet, thus decreasing their number to 8. But it is of question if pleasant properties such as phase-lag could be kept in small magnitude.

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Table 9. Truncation error coefficients of 1–st to 6–th order.

order	equations
1	$b \cdot e - 1$
2	$b \cdot c$
3	$b \cdot A \cdot e - \frac{1}{12}, \quad \frac{b \cdot c^2}{2} - \frac{1}{12}$
4	$b \cdot A \cdot c, \quad b \cdot (c * A \cdot e) - \frac{1}{12}, \quad \frac{b \cdot c^3}{6}$
5	$b \cdot A^2 \cdot e - \frac{1}{360}, \quad \frac{1}{2} b \cdot A \cdot c^2 - \frac{1}{360}, \quad b \cdot (c * A \cdot c) + \frac{1}{60}$ $\frac{1}{2} b \cdot (A \cdot e)^2 - \frac{7}{240}, \quad \frac{1}{2} b \cdot (c^2 * A \cdot e) - \frac{1}{60}, \quad \frac{b \cdot c^4}{24} - \frac{1}{360}$
6	$b \cdot A^2 \cdot c, \quad b \cdot A \cdot (c * A \cdot e) - \frac{1}{360}, \quad \frac{1}{6} b \cdot A \cdot c^3,$ $b \cdot (c * A^2 \cdot e) + \frac{1}{720}, \quad \frac{1}{2} b \cdot (c * A \cdot c^2) - \frac{1}{144}, \quad b \cdot (A \cdot c * A \cdot e) + \frac{1}{120},$ $\frac{1}{2} b \cdot (c^2 * A \cdot c), \quad \frac{1}{2} b \cdot (c * (A \cdot e)^2) - \frac{1}{60}, \quad \frac{1}{6} b \cdot (c^3 * A \cdot e) - \frac{1}{180},$ $\frac{b \cdot c^5}{120}$

Appendix A. Order conditions and Truncation error coefficients

The truncation error derives by the subtraction of (2) from its theoretical correspondence. It is a series of the form

$$h^2 T_{11} F_{11} + h^3 T_{21} F_{21} + h^4 \cdot (T_{31} F_{31} + T_{32} F_{32}) + h^5 \cdot (T_{41} F_{41} + T_{42} F_{42} + T_{43} F_{43}) + \dots$$

where T_{ij} 's are the truncation error terms depending exclusively to the coefficients of the method A, b, c . F_{ij} 's are elementary differentials with respect to y' , f and $f^{(k)} = \frac{\partial^k f}{\partial t^k}$, $k = 1, 2, \dots$ ³⁸ and depend to each problem. So for a fourth order method

$$T_{11} = T_{21} = T_{31} = T_{32} = T_{41} = T_{42} = T_{43} = 0,$$

has to be satisfied. Observe that a p -th order method has truncation error of $O(h^{p+2})$ and not $O(h^{p+1})$. This happens because we have accuracy reduction from the non-existence of y' in the formulas (2), see Ref. 39 p. 464.

A serious understanding of the derivation of order conditions needs investigation through B2-series of Coleman²⁰. Here we list the first 23 truncation error expressions for orders one through six, in Table 9. The next 20 terms for 7–th order and the 36 ones for 8–th algebraic order are given in Tables 10 and 11 respectively. These terms can be thought belonging to various sets along with their order. Thus the set $T^{(1)} = \{T_{11}\}$, while

$$T^{(2)} = \{T_{21}\}, T^{(3)} = \{T_{31}, T_{32}\}, \dots$$

It must be noticed that the presentation in these Tables is rather simplified assuming that lower order coefficients are already known. For example the first of the sixth order terms is not

$$T_{61} = b \cdot A^2 \cdot c$$

Table 10. Truncation error coefficients of 7–th order, forming set $T^{(7)}$.

$b \cdot A^3 \cdot e - \frac{1}{20160}$,	$\frac{1}{2}b \cdot A^2 \cdot c^2 - \frac{1}{20160}$,	$b \cdot A \cdot (c * A \cdot c) + \frac{11}{15120}$,
$\frac{1}{2}b \cdot A \cdot (A \cdot e)^2 - \frac{17}{20160}$,	$\frac{1}{2}b \cdot A \cdot (c^2 * A \cdot e) - \frac{1}{3360}$,	$\frac{1}{24}b \cdot A \cdot c^4 - \frac{1}{20160}$,
$b \cdot (c * A^2 \cdot c) - \frac{17}{10080}$,	$b \cdot (c * A \cdot (c * A \cdot e)) - \frac{37}{10080}$,	$\frac{1}{6}b \cdot (c * A \cdot c^3) + \frac{11}{10080}$,
$b \cdot (A \cdot e * A \cdot A \cdot e) - \frac{1}{20160}$,	$\frac{1}{2}b \cdot (A \cdot c^2 * A \cdot e) - \frac{17}{4032}$,	$\frac{1}{2}b \cdot (c^2 * A^2 \cdot e) - \frac{1}{1344}$,
$\frac{1}{4}b \cdot (c^2 * A \cdot c^2) - \frac{1}{1344}$,	$\frac{1}{2}b \cdot (A \cdot c)^2 - \frac{29}{30240}$,	$b \cdot (c * A \cdot c * A \cdot e) + \frac{13}{5040}$,
$\frac{1}{6}b \cdot (c^3 * A \cdot c) + \frac{13}{15120}$,	$\frac{1}{6}b \cdot (A \cdot e)^3 - \frac{11}{2240}$,	$\frac{1}{4}b \cdot (c^2 * (A \cdot e)^2) - \frac{43}{6720}$,
$\frac{1}{24}b \cdot (c^4 * A \cdot e) - \frac{1}{1344}$,	$\frac{b \cdot c^6}{720} - \frac{1}{20160}$	

Table 11. Truncation error coefficients of 8–th order, forming set $T^{(8)}$.

$b \cdot A^3 \cdot c$,	$b \cdot A^2 \cdot (c * A \cdot e) - \frac{1}{20160}$,	$\frac{1}{6}b \cdot A^2 \cdot c^3$,
$b \cdot A \cdot (c * A^2 \cdot e) + \frac{1}{7560}$,	$\frac{1}{2}b \cdot A \cdot (c * A \cdot c^2) - \frac{1}{4320}$,	$b \cdot A \cdot (A \cdot c * A \cdot e) + \frac{11}{30240}$,
$\frac{1}{2}b \cdot A \cdot (c^2 * A \cdot c)$,	$\frac{1}{2}b \cdot A \cdot (c * (A \cdot e)^2) - \frac{1}{3360}$,	$\frac{1}{6}b \cdot A \cdot (c^3 * A \cdot e) - \frac{1}{10080}$,
$\frac{1}{120}b \cdot A \cdot c^5$,	$b \cdot (c * A^3 \cdot e) - \frac{23}{60480}$,	$\frac{1}{2}b \cdot (c * A^2 \cdot c^2) + \frac{1}{2160}$,
$b \cdot (c * A \cdot (c * A \cdot c)) + \frac{1}{720}$,	$\frac{1}{2}b \cdot (c * A \cdot (A \cdot e)^2) - \frac{1}{1260}$,	$\frac{1}{2}b \cdot (c * A \cdot (c^2 * A \cdot e)) + \frac{1}{4032}$,
$\frac{1}{24}b \cdot (c * A \cdot c^4) - \frac{1}{4320}$,	$b \cdot (A \cdot e * A^2 \cdot c) - \frac{17}{20160}$,	$b \cdot (A \cdot e * A \cdot (c * A \cdot e)) - \frac{13}{5040}$,
$\frac{1}{6}b \cdot (A \cdot c^3 * A \cdot e) + \frac{11}{20160}$,	$\frac{1}{2}b \cdot (c^2 * A^2 \cdot c)$,	$\frac{1}{2}b \cdot (c^2 * A \cdot (c * A \cdot e)) - \frac{1}{1344}$,
$\frac{1}{12}b \cdot (c^2 * A \cdot c^3)$,	$b \cdot (A \cdot c * A^2 \cdot e) - \frac{1}{3780}$,	$\frac{1}{2}b \cdot (A \cdot c * A \cdot c^2) + \frac{1}{1440}$,
$b \cdot (c * A \cdot e * A^2 \cdot e) - \frac{17}{20160}$,	$\frac{1}{2}b \cdot (c * A \cdot c^2 * A \cdot e) - \frac{43}{20160}$,	$\frac{1}{6}b \cdot (c^3 * A^2 \cdot e) - \frac{1}{30240}$,
$\frac{1}{12}b \cdot (c^3 * A \cdot c^2) - \frac{1}{2160}$,	$\frac{1}{2}b \cdot (c * (A \cdot c)^2)$,	$\frac{1}{2}b \cdot (A \cdot c * (A \cdot e)^2) + \frac{13}{10080}$,
$\frac{1}{2}b \cdot (c^2 * A \cdot c * A \cdot e) + \frac{13}{10080}$,	$\frac{1}{24}b \cdot (c^4 * A \cdot c)$,	$\frac{1}{6}b \cdot (c * (A \cdot e)^3) - \frac{73}{20160}$,
$\frac{1}{12}b \cdot (c^3 * (A \cdot e)^2) - \frac{1}{672}$,	$\frac{1}{120}b \cdot (c^5 * A \cdot e) - \frac{1}{6720}$,	$\frac{b \cdot c^7}{5040}$

but actually

$$T_{61} = \frac{1}{120} b \cdot c + \frac{1}{6} b \cdot A \cdot c + b \cdot A^2 \cdot c.$$

Taking in account that

$$T_{21} = b \cdot c = 0, \text{ and } T_{41} = b \cdot A \cdot c = 0$$

from lower order terms we conclude to that listed in Table 9. In case of studying a third order method this would not correspond to its real truncation error since $b \cdot A \cdot c = 0$ is not fulfilled by such a method. Tsitouras⁴⁰ presented a small list of 13 order conditions for the special case of linear problems. It is natural that many coefficients, such as T_{53} from the tables given here, couldn't appear in that list²¹!

After using (4) and the row from (5), all equations containing expression $A^i \cdot e$, $i > 0$, coincide with others and vanish. For example it is easily seen that only one of the elements from $T^{(3)}$ is needed since

$$T_{31} = b \cdot A \cdot e - \frac{1}{12} = b \cdot \frac{1}{2} \cdot (c^2 + c) - \frac{1}{12} = \frac{1}{2} b \cdot c^2 + \frac{1}{2} b \cdot c - \frac{1}{12} = \frac{1}{2} b \cdot c^2 - \frac{1}{12} = T_{32}$$

In a similar way after using the second row of (5), we may discard all equations containing $A^i \cdot c^2$, $i > 0$. Continuing this way we conclude to equations of Table 3. In that table there exist only two equations of seventh order. Namely the equations of the fourth line, $b \cdot c^6 = \frac{1}{28}$ and $b \cdot A \cdot c^4 = \frac{1}{840}$. The three equations on the fifth and sixth lines of the same table are of eighth order.

Another interesting issue is to keep the magnitude of the Euclidean norm of the principal truncation error small. So for a sixth order method it is important to have the value

$$\|T^{(7)}\|_2 = \sqrt{T_{7,1}^2 + T_{7,2}^2 + \dots + T_{7,20}^2},$$

as small as possible. Similar we want for eighth order methods a minimized value for

$$\|T^{(9)}\|_2 = \sqrt{T_{9,1}^2 + T_{9,2}^2 + \dots + T_{9,72}^2}.$$

For our new method we evaluated $\|T_{\text{NEW}}^{(9)}\|_2 = 1.79 \times 10^{-3}$, while for its competitor we have $\|T_{\text{PL22}}^{(9)}\|_2 = 8.51 \times 10^{-3}$, almost five times larger.

Appendix B. MATLAB Program

We implement a MATLAB program using the coefficients of our new method. As input we have:

INPUT	
variable	usage
fcn	the function
x0	left point
xe	end point
y0	initial vector
y1	$y(x_0+h)$
n	number of steps

In the output we get the vector $x = [x_0, x_0 + h, x_0 + 2h, \dots, x_0 + nh]^T$ and the matrix $y \in \mathbb{R}^{N \times n}$ with the corresponding values of $y(x)$. The program was written in minimal length gaining space. Documentation, checks and other programming techniques were omitted so the final listing gives accent to the actual method.

```
function [x,y]=numer_order8_stages9(fcn,x0,xe,y0,y1,n);
%
% 9 stages, 8th order, explicit method, for solving y'' = f(x,y)

% The coefficients
```

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```

c=[-1 0 -1.618033988749895 -0.08935969452190693 ...
-0.7180027509073757 0.7180027509073757 -0.25 0.25 -1 1]';

b=[0.02267478608411768 0 0 0 0.1091598371161353 0.1091598371161353...
0.3880338950775969 0.3880338950775969 -0.01986851827784987 0.002806267806267806];

a=[0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0;
0.4363389981249825,0.06366100187501753,0,0,0,0,0,0,0,0;
-0.02663944838475621,-0.02138085097354293,0.007333029599869930,0,0,0,0,0,0,0;
-0.05259994463359025,0.1179873479656171,0.006223764486158627, ...
-0.1728485681165938,0,0,0,0,0,0;
-0.1594931414841811,1.756644381705087,0.002177668974400012, ...
-1.462560200318788,0.4799966417324492,0,0,0,0,0,0;
-0.01315251843525407,0.08148753879227717,0.002255441346558031, ...
-0.1407999204529257,-0.02359301393743279,0.00005247268677732879,0,0,0,0;
0.1182251406950030,-0.2071467658425108,-0.009902612273876664, ...
0.2377506314405291,-0.1720715921748083,0.008456715906120000, ...
0.1809384822495436,0,0,0;
0.6545342597532786,4.968502507588174,-0.05384950599580273, ...
-4.016696408666935,-1.055358930155700,0.2067362330539400, ...
1.043495190976432,-1.747363346553386,0,0;
-0.2731258141928670,-19.26209659195308,0.2868033393908071, ...
21.50877058850632,-1.286133152186278,0.7520725477949123, ...
-1.229894203564763,0.6765130737370460,-0.1729097875320912,0];

s=10; % stages
h=(xe-x0)/n; % step length
m=length(y0); % dimension of system
x=[x0 x0+h zeros(1,n-1)]'; % output of x
y=zeros(m,n+1); % output of y
y(:,1)=y0; y(:,2)=y1; F=zeros(m,s); f1=feval(fcn,x0,y0);

for k=2:n,

    f0=f1;
    F(:,1)=f0;
    f1=feval(fcn,x(k),y(:,k)); % The first stage
    F(:,2)=f1;
    for o=3:s, % Another 8 stages
        F(:,o)=feval(fcn,x(k)+c(o)*h,(1+c(o))*y(:,k)-c(o)*y(:,k-1)+h*h*F*a(o,:))';
    end;

    y(:,k+1)=2*y(:,k)-y(:,k-1)+h*h*F*b';
    x(k+1)=x(k)+h;

end;

```

In order to run the Bessel equation for 1000 steps (using 9000 stages) we may write in the command window of MATLAB:

```

>> fcn=inline('-(100+1/4/x^2).*y','x','y');
>> isteps=1000;
>> y0=besselj(0,10);
>> x0=1;
>> xend=32.59406213134967;
>> h=(xend-x0)/isteps;
>> y1=sqrt(x0+h)*besselj(0,10*(x0+h));
>> [x,y]=numer_order8_stages9(fcn,x0,xend,y0,y1,isteps);
>> -log10(abs(y(end)))
ans =
    12.4250

```

Rounding this we conclude to the last number 12.4 in the third line of the corresponding Table-5.

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