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Explicit Two-Step Methods for Second-Order Linear IVPs

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Abstract—We present a new type of method for the integration of systems of linear inhomogeneous initial value problems with constant coefficients. Our methods are of hybrid explicit Numerov type. The methods are constructed without the intermediate use of high accuracy interpolatory nodes, since only the Taylor expansion at the internal points is needed. Then we derive the order conditions taking advantage of the special structure of the problem considered. We present a method with algebraic order seven at a cost of only four stages per step. Numerical results over some linear problems, especially arising from the semidiscretization of the wave equation, indicate the superiority of the new method. © 2002 Elsevier Science Ltd. All rights reserved.

Keywords—Initial value problem, Numerical solution, Hybrid Numerov methods, Wave equation, Semidiscretization of PDEs.

1. INTRODUCTION

The initial value problem of second order

$$\frac{\vartheta^2 y}{\vartheta t^2} = Ly + g(t), \qquad y(t_0) = y_0, \qquad y'(t_0) = y_0', \tag{1}$$

where $L \in \Re^{n\times n}$ and $g : \Re \to \Re^n$ usually arises when, for example, the method of lines is applied to linear wave equations.

This problem is a special case of the general class of second-order initial value problems

$$y'' = f(t, y), \qquad y(t_0) = y_0, \qquad y'(t_0) = y_0', \tag{2}$$

where $f : \Re \times \Re^n \to \Re^n$.

When solving (2) numerically, we have to pay attention to the algebraic order of the method used. This is the main factor in achieving higher accuracy with lower computational cost; i.e., this is the main factor of increasing the efficiency of our effort. Various types of methods for the numerical approximation of the solution of (2) are considered in [1]. One of the most widely used methods for solving (2) is the Numerov method which has algebraic order four. This method is

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implicit, which means that its implementation involves computations of Jacobians for the solution of nonlinear systems of equations [2]. Many authors proposed explicit modifications of the Numerov method. The highest algebraic order achieved was six [3–5]. Recently, Tsitouras presented an explicit method of algebraic order eight suitable for problems with oscillating solutions [6].

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

The purposeless derivation of accurate solutions at intermediate points was our motivation for considering another approach, similar to the one used for the construction of Runge-Kutta-Nyström (RKN) methods [7]. Instead of spending much effort increasing the order of internal nodes, we simply involve them in a scheme, where only the final result has to achieve the demanded order. So we managed to derive a sixth-order method at a cost of four stages instead of the six stages needed according to the classical implementation [4]. Here we intend to make use of the special structure of problem (1) and increase the order of the resulting methods.

There have been several attempts to develop efficient methods for integrating linear systems of first-order ODEs [8,9]. Recently, Zingg and Chisholm [10] presented Runge-Kutta methods of orders four, five, and six for first-order linear initial value problems. It is natural to extend that work for Nyström methods. Unfortunately, this is not as effective as it seems it might be at first. Classical Nyström methods share coefficients satisfying two sets of order conditions [1, p. 267]. One set comes when matching Taylor series expansion from the propagation of y, and the other set from the propagation of y'. When using a not so restrictive assumption [1, p. 268], we finally solve only one of the sets of equations. This technique cannot be applied to the reduced set of order conditions for linear problems. The assumption mentioned before is valid along with some of the conditions that do not belong to the reduced set then.

2. THE NEW METHOD

Following the implementation of [4], let $h > 0$ and $t_n = t_0 + nh$, $n = 0, 1, 2, \dots$. 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 a fourth result using $y''_n = f_n = f(t_n, y_n)$ at a cost of one function evaluation.

We also need four more values of second derivatives within the interval $[t_{n-1}, t_{n+1}]$ with accuracy $O(h^6)$. Then we are able to form the required interpolant of order $O(h^8)$. It is desirable to derive them without cost, and construct a sixth-order method at a cost of five stages. This cannot be achieved since the values y_{n-1}, y''_{n-1}, y_n, and y''_n are not enough information to give us interpolatory approximations of the accuracy needed. So the total cost increases to at least six stages.

Interpolatory nodes carry a lot of information that is useless even for conventional methods [7]. Implementing the new method, we only need y''_n and three extra function evaluations f_a, f_b, and f_c. The new method has the form

$$
\begin{aligned}
f_n &= f\left(t_n, y_n\right), \\
y_a &= c_1 y_{n-1} + \left(1 - c_1\right) y_n + h^2\left(d_{11} f_{n-1} + d_{12} f_n\right), \\
f_a &= f\left(t_n - c_1 h, y_a\right), \\
y_b &= c_2 y_{n-1} + \left(1 - c_2\right) y_n + h^2\left(d_{21} f_{n-1} + d_{22} f_n + g_{21} f_a\right), \\
f_b &= f\left(t_n - c_2 h, y_b\right), \\
y_c &= c_3 y_{n-1} + \left(1 - c_3\right) y_n + h^2\left(d_{31} f_{n-1} + d_{32} f_n + g_{31} f_a + g_{32} f_b\right), \\
f_c &= f\left(t_n - c_3 h, y_c\right), \\
y_{n+1} &= -y_{n-1} + 2 y_n + h^2\left(w_1 f_{n-1} + w_2 f_n + b_1 f_a + b_2 f_b + b_3 f_c\right).
\end{aligned}
$$

Using the notation of Nyström methods, we consider the following matrices:

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ d_{11} & d_{12} & 0 & 0 & 0 \\ d_{21} & d_{22} & g_{21} & 0 & 0 \\ d_{31} & d_{32} & g_{31} & g_{32} & 0 \end{bmatrix},$$

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

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

Now the method can be formulated in a table like the following Butcher tableau [11,12]:

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

Then we consider the Taylor series expansions of f_a, f_b, f_c, y_{n+1}, and $y(t_n + h)$. For a seventh-order method, we match the corresponding expansions up to h^8, and we arrive at an expression of the form [13]

$$h^2 (q_{2,1}F_{2,1}) + h^3 (q_{3,1}F_{3,1}) + \cdots + h^8 (q_{8,1}F_{8,1} + \cdots + q_{8,21}F_{8,21}) + O(h^9), \tag{3}$$

where q_{ij} are expressions of the coefficients of the method while F_{ij} are elementary differentials with respect to y', f, $f' = \frac{\partial f}{\partial y}$ and $f^{(k)} = \frac{\partial^k f}{\partial y^k}$, $k = 2, \ldots, 6$. The order conditions for a seventh-order method are in total 44. The enumeration of order conditions follows from the theory of Nyström methods [1,13].

If we had to solve a scalar ODE of the type (2), then some of the elementary differentials appearing in (3) may coincide. For example, $f'' f^{(3)} y'^{\,4} = f^{(3)} f'' y'^{\,4}$ for scalar equations. This is not true for systems of ODEs since $f^{(3)}$, f'', y' are matrices or even tensors. We cannot take advantage of such a coincidence when dealing with scalar inhomogeneous linear equations, as all the differentials that might reduce, vanish. Our gain is that we may proceed with our calculations based on this simplified problem.

Observing the series of the form (3) coming from scalar linear problems, we found that only a subset of the 44 order conditions needs to be solved. Further reduction of the order conditions is achieved using the simplifying assumption

$$Ae = \frac{1}{2}\left(c^2 - c\right), \tag{4}$$

with $e = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \end{bmatrix}^\top$ and $c^i = \begin{bmatrix} 1 & 0 & c_1^i & c_2^i & c_3^i \end{bmatrix}$. Equation (4) reduces all qs with corresponding elementary differentials containing f. For example, $q_{42} = bAe + bc - 1/12$ with $F_{42} = f'f$ is simplified by $q_{41} = (1/2)bc^2 - 1/12$ with $F_{41} = f''y'^{\,2}$, since $q_{42} = bAe + bc - 1/12 = b(1/2)(c^2 - c) - bc - 1/12 = (1/2)bc^2 - 2bc - 1/12 = (1/2)bc^2 - 1/12 = q_{41}$. (Notice that $q_{31} = bc$ ought to be zero satisfying a lower order condition.) Finally, we may find the remaining order conditions for the case we study here in Table 1.

After assumption (4), only 14 coefficients remain free to satisfy the 13 order conditions $q_{21} = q_{31} = \cdots = q_{83} = 0$. We solved these equations using optimization toolbox of Matlab [14], requiring 12–13 digits of accuracy. Then we refined the various solutions we got using standard routines of Mathematica [15], at 17–18 digits of accuracy. A specific choice with minimal truncation error is given in Table 2.

The truncation error of the new method is

$$\text{LTE} = h^9 \begin{pmatrix} 1.34 \cdot 10^{-4} f'^3 y' + 8.42 \cdot 10^{-6} f'^2 f''' y'^3 \\ +1.89 \cdot 10^{-6} f' f^{(5)} y'^5 + 3.95 \cdot 10^{-7} f^{(6)} y'^6 \end{pmatrix} + O\left(h^{10}\right).$$

Table 1. The equations of condition for inhomogeneous linear systems with constant coefficients.

$$q_{21} = b \cdot e - 1$$
$$q_{31} = b \cdot c$$
$$q_{41} = \frac{1}{2} b \cdot c^2 - \frac{1}{12}$$
$$q_{51} = \frac{1}{6} b \cdot c^3$$
$$q_{52} = b \cdot A \cdot c + \frac{1}{6} b \cdot c$$
$$q_{61} = \frac{1}{24} b \cdot c^4 - \frac{1}{360}$$
$$q_{62} = \frac{1}{2} b \cdot A \cdot c^2 + \frac{1}{24} b \cdot c - \frac{1}{360}$$
$$q_{71} = \frac{1}{120} b \cdot c^5$$
$$q_{72} = \frac{1}{6} b \cdot A \cdot c^3 + \frac{1}{120} b \cdot c$$
$$q_{73} = \frac{1}{6} b \cdot A^2 \cdot c + \frac{1}{6} b \cdot A \cdot c + \frac{1}{120} b \cdot c$$
$$q_{81} = \frac{1}{720} b \cdot c^6 - \frac{1}{20160}$$
$$q_{82} = \frac{1}{24} b \cdot A \cdot c^4 + \frac{1}{720} b \cdot c - \frac{1}{20160}$$
$$q_{83} = \frac{1}{2} b \cdot A^2 \cdot c^2 + \frac{1}{24} b \cdot A \cdot c + \frac{1}{720} b \cdot c - \frac{1}{20160}$$

Table 2. The coefficients of the new method accurate at 16 digits.

$d_{11} = 0.9849042853884411$	$d_{12} = -0.6191851078585296$
$d_{21} = -1.00615149302248$	$d_{22} = 0.8697687073032044$
$g_{21} = 0.01229272944938354$	$d_{31} = 0.6331480169843698$
$d_{32} = -0.3189442671225579$	$g_{31} = 0.1929702170578158$
$g_{32} = 0.2550050264031409$	$c_1 = -0.4906757063034415$
$c_2 = 0.5426601390083943$	$c_3 = -0.8320502943378441$
$w_1 = 0.01207322890110905$	$w_2 = 0.4812388540806565$
$b_1 = 0.2202109686806263$	$b_2 = 0.2432091622840896$
$b_3 = 0.04326778605351844$	

All the other elementary differentials of the principal error are zero. The size of the coefficients in the $O(h^{10})$ term are small enough and do not affect seriously the value of LTE.

The new method is implemented in constant step-size mode. After the evaluation of f_{n+1}, we may use it as an extra fifth stage in an FSAL (first same as last) [16, p. 17] scheme with

$$\hat{b} = [\hat{w}_1 \quad \hat{w}_2 \quad \hat{b}_1 \quad \hat{b}_2 \quad 0 \quad \hat{b}_4],$$

$\hat{c} = [1 \quad 0 \quad c_1 \quad c_2 \quad c_3 \; -1]$, and $a_{61} = w_1$, $a_{62} = w_2$, $a_{63} = b_1$, $a_{64} = b_2$, $a_{65} = b_3$. The new weights can be found satisfying the order conditions up to fourth order $\hat{b} \cdot e = 1$, $\hat{b} \cdot \hat{c} = 0$, $\hat{b} \cdot \hat{c}^2 = 1/6$, $\hat{b} \cdot \hat{c}^3 = 0$, $\hat{b} \cdot A \cdot c = 0$. Following [17], we may deduce an error estimate without cost which produces errors proportional to a requested tolerance when advancing the solution with the higher-order method

$$E = h^3 \left\| \begin{array}{c} (w_1 - \hat{w}_1) f_{n-1} + (w_2 - \hat{w}_2) f_n + \left(b_1 - \hat{b}_1\right) f_a \\ + \left(b_2 - \hat{b}_2\right) f_b + b_3 f_c + \left(b_4 - \hat{b}_4\right) f_{n+1} \end{array} \right\|_2 .$$

Then we may proceed to step adjustment according to the lines introduced in [18]. Actually, Raptis and Cash [18] have restricted all step changes to doubling and halving since they had a high-order midpoint approximation of the solution. An interpolatory technique is more appropriate here. We hope to be able to introduce such a general approach for hybrid Numerov methods in the future.

3. NUMERICAL RESULTS

To illustrate our new seventh-order method, we compare it with the following sixth-order methods:

1. the six-stage two-step method of Chawla and Rao [4],
2. our four-stage method appearing in [7], and
3. the effectively five-stage Runge-Kutta-Nyström pair of orders 6(4) found in [19].

First we solved the linear problem

$$\begin{aligned} y_1'' &= \frac{1}{100}y_1 - \frac{1}{10}y_2, \\ y_2'' &= -\frac{1}{10}y_1 + \frac{1}{100}y_2 + \sin t, \end{aligned}$$

with theoretical solution

$$y_1(x) = \cos\frac{3}{10}t - \frac{1000}{10101}\sin t, \qquad y_2(x) = \cos\frac{3}{10}t - \frac{10100}{10101}\sin t,$$

for $t \in [0, 10\pi]$.

Then we consider the linearized wave equation [20]

$$\begin{aligned} &\frac{\vartheta^2 u}{\vartheta t^2} = 4\frac{\vartheta^2 u}{\vartheta x^2} + \sin t \cdot \cos\left(\frac{\pi x}{b}\right), \qquad 0 \le x \le b = 100, \quad t \in [0, 40\pi], \\ &\frac{\vartheta u}{\vartheta x}(t,0) = \frac{\vartheta u}{\vartheta x}(t,b) = 0, \\ &u(0,x) \equiv 0, \quad \frac{\vartheta u}{\vartheta t}(0,x) = \frac{b^2}{4\pi^2 - b^2}\cos\frac{\pi x}{b}, \end{aligned}$$

with theoretical solution

$$u(t,x) = \frac{b^2}{4\pi^2 - b^2} \cdot \sin t \cdot \cos\frac{\pi x}{b}.$$

Discretization of $\vartheta^2 u/\vartheta x^2$ by fourth-order symmetric differences at internal points and one-sided differences of the same order at the boundaries yields the system

$$\begin{bmatrix} y_1'' \\ y_2'' \\ \vdots \\ y_{N+1}'' \end{bmatrix} = \frac{4}{(\Delta x)^2} \begin{bmatrix} -\frac{415}{72} & 8 & -3 & \frac{8}{9} & -\frac{1}{8} & & & \\ \frac{257}{144} & -\frac{10}{3} & \frac{7}{4} & -\frac{2}{9} & \frac{1}{48} & & O & \\ -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} \\ & O & & \frac{1}{48} & -\frac{2}{9} & \frac{7}{4} & -\frac{10}{3} & \frac{257}{144} \\ & & & -\frac{1}{8} & \frac{8}{9} & -3 & 8 & -\frac{415}{72} \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N+1} \end{bmatrix}$$

$$+\sin t \cdot \begin{bmatrix} \cos\left(\frac{0\cdot\Delta x}{b}\cdot\pi\right) \\ \cos\left(\frac{1\cdot\Delta x}{b}\cdot\pi\right) \\ \vdots \\ \cos\left(\frac{N\cdot\Delta x}{b}\cdot\pi\right) \end{bmatrix}.$$

By choosing $\Delta x = 5$, we arrive at a constant coefficients linear system with $N = 20$.

The two-step methods were run with constant step size, and the observed endpoint error e was recorded at a fixed number of stages. Then we computed in Tables 3 and 4 the value $-\log e$, i.e., the number of accurate digits of the solution. The sixth-order RKN method given in [19] was used to propagate the first step.

The Runge-Kutta-Nyström pair was run for tolerances $10^{-3}, 10^{-4}, \dots, 10^{-9}$ using variable step mode, according to the guidelines and step-size control algorithm introduced in [17]. This affects favorably its efficiency [22, p. 334], but we decided to test the methods the way most codes implement them. For reasons of comparison, we estimated the number of accurate digits that might be generated at the same number of stages used by two-step methods. This estimation was done by linear interpolation on decimal digits of accuracy achieved for each tolerance.

Table 3. Accurate digits for the linear system.

	Stages									
	240	360	480	600	720	840	960	1080	1200	1320
Two-step [4]	1.7	2.7	3.4	4.0	4.5	4.9	5.2	5.5	5.8	6.1
Two-step [7]	2.4	3.5	4.2	4.8	5.3	5.7	6.0	6.3	6.6	6.9
RKN [19]	2.3	3.7	4.6	5.4	6.0	6.5	6.9	7.3	7.6	7.8
NEW	4.8	5.8	6.6	7.3	7.8	8.3	8.6	9.0	9.3	9.6

Table 4. Accurate digits for wave equation.

	Stages									
	360	720	1080	1440	1800	2160	2520	2880	3240	3600
Two-step [4]	< 0	2.0	2.7	3.4	3.9	4.4	4.8	5.1	5.4	5.7
Two-step [7]	< 0	2.7	3.7	4.4	4.9	5.4	5.7	5.9	6.2	6.3
RKN [19]	< 0	2.5	3.9	4.3	4.5	4.6	4.6	5.8	6.3	6.3
NEW	< 0	3.8	5.2	6.0	6.2	6.3	6.3	6.3	6.3	6.3

The results show that the new method has a much better performance than the other methods for the problems considered. Obviously, this is due to its special characteristics. For example, in the linear system, 7.8 digits of accuracy were achieved by the RKN pair at a cost of 80% more function evaluations. In the wave equation, the fixed spatial discretization error limits the accuracy to $10^{-6.3}$. The RKN pair needs almost 60–70% more function evaluations to reach this accuracy. In [21], an RKN pair of orders 6(4) was given, but it was especially constructed for oscillatory problems. Here it showed results improving the RKN performance in Tables 3 and 4 by 10–15%, still far in efficiency from our new method.

4. CONCLUSION

A new approach for the derivation of two-step hybrid methods for inhomogeneous linear problems with constant coefficients was presented. We derived the equations of condition for this type of problem considering, without loss of generality, a scalar problem. Then a new seventh-order method was constructed at the smallest possible cost. The numerical performance of the new method is very promising, especially when applied to semidiscretization of linear wave equation.

REFERENCES

1. E. Hairer, S.P. Norsett and G. Wanner, *Solving Ordinary Differential Equations I*, Springer-Verlag, Berlin, (1987).
2. M.M. Chawla and P.S. Rao, Numerov type method with minimal phase lag for the integration of second order periodic initial value problems, *J. Comput. Appl. Math.* **11**, 277–281, (1984).
3. M.M. Chawla and P.S. Rao, Numerov type method with minimal phase lag for the integration of second order periodic initial value problems II. Explicit method, *J. Comput. Appl. Math.* **15**, 329–337, (1986).
4. M.M. Chawla and P.S. Rao, An explicit sixth-order method with phase-lag of order eight for $y'' = f(t, y)$, *J. Comput. Appl. Math.* **17**, 365–368, (1987).
5. T.E. Simos, Explicit two-step methods with minimal phase-lag for the numerical integration of special second order initial value problems and their application to the one dimensional Schrödinger equation, *J. Comput. Appl. Math.* **39**, 89–94, (1992).
6. Ch. Tsitouras, Dissipative high phase-lag order methods, *Appl. Math. Comput.* **117**, 35–43, (2001).
7. Ch. Tsitouras, Explicit Numerov type methods with reduced number of stages, *Computers Math. Applic.* (to appear).
8. W.H. Enright, The efficient solution of linear constant-coefficient systems of differential equations, *Simulation* **30**, 129–133, (1978).
9. L.F. Shampine, Cheaper integration of linear systems, *Simulation* **20**, 17, (1973).
10. D.W. Zingg and T.T. Chisholm, Runge-Kutta methods for linear ordinary differential equations, *Appl. Numer. Math.* **31**, 227–238, (1999).
11. J.C. Butcher, Implicit Runge-Kutta processes, *Math. Comput.* **18**, 50–64, (1964).
12. J.C. Butcher, On Runge-Kutta processes of high order, *J. Austral. Math. Soc.* **4**, 179–194, (1964).
13. E. Fehlberg, Classical eighth and lower order Runge-Kutta-Nyström formulas with stepsize control for special second order differential equations, NASA Tech. Rep. 381, (March 1972).
14. T. Coleman, M.A. Branch and A. Grace, *Optimization Toolbox User's Guide*, The MathWorcs, Natick, (1999).
15. S. Wolfram, *Mathematica Book, Volume 4.0*, Wolfram Med. and Cambridge Univ. Press, (1999).
16. E. Fehlberg, Low order classical Runge-Kutta formulas with step-size control and their application to some heat transfer problems, NASA Tech. Rep. 315, (1969).
17. Ch. Tsitouras and S.N. Papakostas, Cheap error estimation for Runge-Kutta methods, *SIAM J. Sci. Comput.* **20**, 2067–2088, (1999).
18. A.D. Raptis and J.R. Cash, A variable step method for the numerical integration of the one-dimensional Schrödinger equation, *Comput. Phys. Commun.* **36**, 113–119, (1985).
19. J.R. Dormand, M.E. El-Mikkawy and P.J. Prince, Families of Runge-Kutta-Nyström formulae, *IMA J. Numer. Anal.* **7**, 235–250, (1987).
20. P.J. Van Der Houwen and B.P. Sommeijer, Explicit Runge-Kutta (-Nyström) methods with reduced phase errors for computing oscillating solutions, *SIAM J. Numer. Anal.* **24**, 595–617, (1987).
21. S.N. Papakostas and Ch. Tsitouras, High algebraic order, high phase-lag order Runge-Kutta and Nyström pairs, *SIAM J. Sci. Comput.* **21**, 747–763, (2000).
22. L.F. Shampine, *Numerical Solution of Ordinary Differential Equations*, Chapman & Hall, New York, (1984).