

Stage reduction on P-stable Numerov type methods of eighth order.

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Abstract

We present an implicit hybrid two step method for the solution of second order initial value problem. It costs only six function evaluations per step and attains eighth algebraic order. The method satisfy the P-stability property requiring one stage less. We conclude dealing with implementation issues for the methods of this type and give some first pleasant results from numerical tests.

Keywords: Initial Value Problem, Second Order, Oscillatory solutions.

Mathematics Subject Classification: 65L05, 65L06

1 Introduction.

We are interested in solving the initial value problem of second order

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0. \quad (1)$$

where y, y_0 and $y'_0 \in \mathfrak{R}^m$. In this paper we investigate the class of the above problems with periodic solutions. Our result are methods which can be applied to numerous problems in celestial mechanics, quantum mechanical scattering theory, in theoretical physics and chemistry and in electronics [15, 16].

Implicit hybrid two step methods satisfying P-stability property are used for about twenty years for solving (1), [4, 6, 7]. This stability property is particular relevant when (1) is a system whose theoretical solution consists of a periodic part of moderate frequency with a high frequency oscillation of small amplitude superimposed [4].

Implicitness furnishes each step a nonlinear equation in a single unknown $y_{n+1} \approx y(x_{n+1}) = y(x_0 + nh)$. In [19] we used seven stages for achieving P-stability and eighth order of accuracy. Khiyal and Thomas [13] also proposed a seven stage eighth order P-stable method with only the four implicit stages among them.

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The construction this type of methods is usually based on interpolatory nodes. These nodes carry a lot of information which is useless even for conventional methods. So, an alternative implementation of such methods was introduced in [17, 20, 21]. and studied theoretically by Coleman [8] or Chan et. al. [5] through B-series and P-series respectively.

Here we propose a six stage method of the form:

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{j=1}^s b_j f(x_n + c_j h, g_j). \quad (2)$$

with

$$g_i = (1 + c_i) y_n - c_i y_{n-1} + h^2 \sum_{j=1}^s a_{ij} f(x_n + c_j h, g_j), \quad i = 1, 2, \dots, s = 6.$$

Here g_i are only first order approximations of $y(x_n + c_i h)$ while traditional methods demand for most of the $g_i = y(x_n + c_i h) + O(h^8)$. In the following we will present the order conditions for achieving various algebraic orders and after a periodic stability analysis we will derive a P-stable method of eighth order.

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 we consider the matrix of the coefficients

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & a_{56} \\ a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & a_{66} \end{bmatrix},$$

and the vectors

$$b = [w_1 \quad w_2 \quad b_1 \quad b_2 \quad b_3 \quad b_4],$$

and

$$c = [1 \quad 0 \quad c_1 \quad c_2 \quad c_3 \quad c_4]^T.$$

Now the method can be formulated in a table like the Butcher tableau, [1, 2]:

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

Table 1: Equations of condition up to eighth order

$$\begin{aligned}
b \cdot e &= 1, \\
b \cdot c &= 0, \\
b \cdot c^2 &= \frac{1}{6}, \\
b \cdot c^3 &= 0, \\
b \cdot c^4 &= \frac{1}{15}, \\
b \cdot c^5 &= 0, \\
b \cdot c^6 &= \frac{1}{28}, \\
b \cdot A \cdot c^4 &= \frac{1}{840}, \\
b \cdot c^7 &= 0, \\
b \cdot (c A \cdot c^4) &= 0, \\
b \cdot A \cdot c^5 &= 0 \quad \rightarrow\rightarrow \text{Be careful. This equation is missing from JCAM paper}
\end{aligned}$$

Under the simplifying assumptions

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

with

$$e = [1 \ 1 \ 1 \ 1 \ 1 \ 1]^T$$

and

$$c^i = [1 \ 0 \ c_1^i \ c_2^i \ c_3^i \ c_4^i],$$

we get the eighth order conditions given in Table 1 (see [8]):

Our methods include 48 parameters. Thirty five equations are required assuming order conditions and satisfaction of (1). This leaves thirteen coefficients as free parameters.

3 Periodic problems.

Following Lambert and Watson [14] and in order to study the periodic properties of methods posed for solving (1), it is constructive to consider the scalar test problem

$$y' = -\omega^2 y, \quad \omega \in \mathfrak{R}. \tag{4}$$

When applying an explicit two step hybrid method of the form (2) to the problem (4) we obtain a difference equation of the form

$$y_{n+1} + S(v^2) y_n + P(v^2) y_{n-1} = 0, \tag{5}$$

where $y_n \approx y(nh)$ the computed approximations at $n = 1, 2, \dots$, $v = \omega h$, h the step size used, and $S(v^2), P(v^2)$ polynomials in v^2 .

Zero dissipation property is fulfilled by requiring $P(v^2) \equiv 1$, and helps a numerical method that solves (4) to stay in its cyclic orbit. We observe that

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

with I_s the identity matrix of dimension $s \times s$. $P(v^2)$ can be written as an infinite series:

$$P(v^2) = 1 + v^9 b \cdot A^4 \cdot c + v^{11} b \cdot A^5 \cdot c + \dots$$

Actually we have to solve only

$$b \cdot A^4 \cdot c = 0,$$

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

and

$$b \cdot A^6 \cdot c = 0,$$

demanding another three coefficients and leaving ten free parameters.

The solution of (4) is

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

and we may write equation (5) as

$$e^{2iv} + S(v^2) \cdot e^{iv} + 1 = O.$$

P-stability means that the numerical solution stays in orbit for ever. Thus we want

$$|S(v^2)| < 2, \quad v \in (0, +\infty)$$

Observe that

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

with $I_s \in \mathfrak{R}^{s \times s}$ the proper identity matrix. After extended search we concluded to a method with coefficients given in Table 2.

4 Implementation issues.

First we introduce

$$z_i = g_i - (1 + c_i) y_n + c_i y_{n-1} = h^2 \cdot \sum_{j=1}^s a_{ij} f(x_n + c_i h, g_j). \quad (6)$$

Similar to implicit Runge-Kutta methods [11, p. 118], we observe that:

Table 2: Coefficients of the new method

$a_{11} = -0.33083649953596372,$	$a_{12} = -0.28554560691201376,$
$a_{13} = 0.096020140660069509,$	$a_{14} = 0.065976488202945502,$
$a_{15} = 0.93159949396176978,$	$a_{16} = -0.25151621006087468,$
$a_{21} = -0.22800572156136017,$	$a_{22} = 0.75775376332106239,$
$a_{23} = 0.044036478175189789,$	$a_{24} = 0.044036478175189789,$
$a_{25} = -0.38981527654872163,$	$a_{26} = -0.22800572156136017,$
$a_{31} = -0.14560363007308039,$	$a_{32} = -1.9592986015796962,$
$a_{33} = -0.024082528198053865,$	$a_{34} = 0.028081493431889852,$
$a_{35} = 2.1942941895272906,$	$a_{36} = -0.18249268029751431,$
$a_{41} = 1.0027874805872521,$	$a_{42} = -1.2518397436149883,$
$a_{43} = -0.092326475684278097,$	$a_{44} = -0.14449049731422181,$
$a_{45} = 0.12503961031290593,$	$a_{46} = 1.0396765308116860,$
$a_{51} = 0.10278432173227921,$	$a_{52} = 0.18924763112443292,$
$a_{53} = 0.019851517364212751,$	$a_{54} = 0.019851517364212751,$
$a_{55} = 0.023382022388299996,$	$a_{56} = 0.10278432173227921,$
$a_{61} = 0.28697954935636091,$	$a_{62} = 0.16149513085428000,$
$a_{63} = 0.085716485163353987,$	$a_{64} = 0.055672832706229981,$
$a_{65} = 0.62654046521477468,$	$a_{66} = 0.20765925988127187,$
$b_1 = 0.29173891914469542,$	$b_2 = 0.12330286145746479,$
$b_3 = 0.084958219397839784,$	$b_4 = 0.084958219397839784,$
$b_5 = 0.12330286145746479,$	$b_6 = 0.29173891914469542,$
$c_1 = c_6 = 0.33749364930837850,$	$c_2 = c_5 = 0,$
$c_3 = c_4 = 0.76794866228752001.$	

$$y_{n+1} = 2y_n - y_{n-1} + \sum_{j=1}^6 d_j z_j,$$

with

$$d = [d_1 \quad d_2 \quad d_3 \quad d_4 \quad d_5 \quad d_6] = b \cdot A^{-1}.$$

For solving nonlinear equations (6) we use modified Newton iteration according to the scheme (brackets in the exponent include the iteration counter):

$$\begin{aligned} (I_{ms} - h^2 A \otimes J) \Delta Z^{[k]} &= -Z^{[k]} + h^2 (A \otimes I_m) \cdot F \left(Z^{[k]} \right) \\ Z^{[k+1]} &= Z^{[k]} + \Delta Z^{[k]}. \end{aligned} \quad (7)$$

Here $J = \frac{\partial f}{\partial y}(x_n, y_n)$ is the Jacobian matrix evaluated at the left point and kept fixed during the hole step (even in a series of consecutive steps),

$$Z^{[k]} = \begin{bmatrix} z_1^{[k]} & z_2^{[k]} & \cdots & z_s^{[k]} \end{bmatrix}^T,$$

is the k -th iteration and $\Delta Z^{[k]}$ are the corresponding increments. The supervector $F(Z^{[k]})$ is an abbreviation for

$$F(Z^{[k]}) = \begin{bmatrix} f\left(x_n + c_1 h, (1 + c_1)y_n - c_1 y_{n-1} + z_1^{[k]}\right) \\ f\left(x_n + c_2 h, (1 + c_2)y_n - c_2 y_{n-1} + z_2^{[k]}\right) \\ \vdots \\ f\left(x_n + c_6 h, (1 + c_6)y_n - c_6 y_{n-1} + z_6^{[k]}\right) \end{bmatrix},$$

see [11, pp. 119-120] for details.

A simple choice for the starting value of $Z^{[0]}$ would be $z_i^{[0]} = 0$ for $i = 1, 2, \dots, s$. A more satisfactory approach uses an $O(h^4)$ interpolation based on known values y_{n-1} , y_n , y_{n-1}'' and y_n'' . So we may evaluate

$$z_i^{[0]} = -\frac{1}{6}h^2(c_i - 1)(c_i + 1)c_i y_{n-1}'' + \frac{1}{6}h^2(c_i + 2)(c_i + 1)c_i y_n''. \quad (8)$$

In view of (3) we may use high order stage values from previous steps forming more accurate interpolants for $z_i^{[0]}$'s, but (8) is efficient enough to get convergence rapidly for many non-linear problems.

The main drawback of the iteration scheme (7) is that requires the LU decomposition of an $(sm) \times (sm)$ matrix. The computational effort of magnitude raises to $O((sm)^3)$ and it is not comparable to diagonally implicit methods suggested until now and need $O(m^3)$ operations [4, 19].

Since the matrix A is invertible we may overcome this disadvantage using an approach similar to the one introduced by Butcher [3] and it is now applied to implicit Runge-Kutta methods [12]. The idea is to premultiply (7) by $h^{-2}A^{-1} \otimes I$, and transform A to a simple matrix

$$T^{-1}A^{-1}T = \Lambda.$$

Using the transformation $W = (T^{-1} \otimes I_m) \cdot Z$, the iteration (7) becomes equivalent to

$$\begin{aligned} (h^{-2}\Lambda \otimes I_m - I_s \otimes J) \Delta W^{[k]} &= -h^{-2}(\Lambda \otimes I_m) W^{[k]} + (T^{-1} \otimes I_m) \cdot F(Z^{[k]}) \\ W^{[k+1]} &= W^{[k]} + \Delta W^{[k]}. \end{aligned}$$

Observe that now we have only s matrices of dimension $m \times m$ to factor. A real LU decomposition uses $\frac{2}{3}m^3$ flops [10], while a complex LU decomposition needs $\frac{4}{3}m^3$ flops. Matrix A has four real eigenvalues and one pair of conjugate complex ones. According to analysis in [11, pg 122], we sum to $4 \cdot \frac{2}{3}m^3 + \frac{4}{3}m^3 = \frac{16}{3}m^3$ flops for the new method neglecting operations like

back substitution with cost of $O(m^2)$. Notice that transformations such as $Z = (T \otimes I_m) \cdot W$ cost only $O(m)$.

The main competitor of our new suggestion here is the seven stage method given in [19]. Transforming the later to the form (2), we observe that its corresponding matrix A , has one real and three conjugate complex pairs of eigenvalues. Thus its cost raises to $1 \cdot \frac{2}{3}m^3 + 3 \cdot \frac{4 \cdot 2}{3}m^3 = \frac{26}{3}m^3$ flops. It would be desirable for A to have seven real eigenvalues to reduce the cost to $\frac{14}{3}m^3$ flops only. But A is not invertible and this option is meaningless. The classical iteration scheme for this method has the form

$$\begin{aligned} & (I_m + \rho_1 h^2 J + \rho_2 h^4 J^2 + \rho_3 h^6 J^3 + \rho_4 h^8 J^4) \cdot \left(y_{n+1}^{[k+1]} - y_{n+1}^{[k]} \right) \\ & = F \left(y_{n+1}^{[k]}, y_{n+1}''^{[k]} \right), \end{aligned} \quad (9)$$

with

$$y_{n+1}^{[0]} = 2y_n - y_{n-1} + h^2 y_n''$$

an initial iteration corresponding to (8).

We must avoid the evaluation of J^2 , J^3 and J^4 , because these computations use $2m^3$ flops each [10], giving a total of $\frac{18}{3}m^3$ operations.

Factoring the polynomial (9) in $h^2 J$, we get the scheme

$$\begin{aligned} & (I_m - \xi_1 h^2 J) (I_m - \xi_2 h^2 J) (I_m - \xi_3 h^2 J) (I_m - \xi_4 h^2 J) \cdot \left(y_{n+1}^{[k+1]} - y_{n+1}^{[k]} \right) \\ & = F \left(y_{n+1}^{[k]}, y_{n+1}''^{[k]} \right) \end{aligned}$$

This can be solved by four consecutive LU decompositions of the corresponding factors. If the roots $\xi_1, \xi_2, \xi_3, \xi_4$ were real then the hole procedure would sum to a total cost of only $4 \cdot \frac{2}{3}m^3 = \frac{8}{3}m^3$ operations as $m \rightarrow \infty$. But these roots form a set of two complex conjugate pairs $\xi_1 = \bar{\xi}_2$ and $\xi_3 = \bar{\xi}_4$. We have then to perform two complex LU decompositions since $LU = (I_m - \xi h^2 J)$ implies $\bar{L} \bar{U} = (I_m - \bar{\xi} h^2 J)$. The cost in this case is $2 \cdot \frac{4 \cdot 2}{3}m^3 = \frac{16}{3}m^3$.

The final observation of our analysis is that our new fully implicit method has the same cost of $\frac{16}{3}m^3$ operations per step with the older diagonally implicit method given in [19].

5 Numerical Tests.

Two problems are chosen for our comparisons that are well known in the relevant literature. These problems were run for our new method and its main competitor [19]. We ran both formulas for the same number of steps within the integration step and recorded the end point global errors. We

Table 3: Accurate digits for the Duffing equation

steps	correct digits	
	New	[19]
450	3.8	2.9
900	6.1	5.4
1350	7.5	6.7
1800	8.5	7.7
2250	9.2	8.5
2700	9.8	9.2
3150	10.3	9.7
3600	10.7	10.2
4050	11.2	10.5

avoid recording computer times since they heavily depend on programming defects. The iteration schemes for the two methods are somewhat different and small programming modifications may give considerable differences in the efficiency.

5.1 Duffing equation

First we considered the following problem

$$y'' = -y - y^3 + \frac{1}{500} \cdot \cos(1.01x),$$

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

with theoretical solution

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

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

We solved the above equation in the region $x \in [0, \frac{120.5}{1.01}\pi]$ because $y(\frac{120.5}{1.01}\pi) = 0$.

The results are given in Table- 3 where a gain of more than a half digit is shown.

5.2 Elastodynamics problem

Our second test problem was the linear elastodynamics stiff model [9]:

$$\frac{\partial^2 u}{\partial t^2} + \frac{\partial^4 u}{\partial x^4} - x(1-x) \frac{\partial^2 u}{\partial x^2} - u = 0, \quad 0 < x < 1, \quad t > 0,$$

$$u(0, t) = u(1, t) = 0,$$

$$\frac{\partial^3 u}{\partial x^3}(0, t) = \frac{\partial^3 u}{\partial x^3}(1, t) = 0$$

$$u(x, 0) = x(1-x), \quad \frac{\partial u}{\partial t}(x, 0) = 0$$

with analytical solution

$$u(x, t) = x(1 - x) \cos(t).$$

Using the method of lines we consider an approximation on a uniform grid $y_i(t) \approx u(i\Delta x, t)$ with $\Delta x = 1/N$. Then we semidiscretize on the spatial variable by second order symmetric differences. The final linear equation has the form

$$\begin{bmatrix} y_1'' \\ y_2'' \\ \vdots \\ y_{N-1}'' \end{bmatrix} = \left(-\frac{1}{h^4} A_4 + I_{N-1} + \frac{1}{h^2} U A_2 \right) \cdot \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \end{bmatrix},$$

with

$$A_4 = \begin{bmatrix} 2 & -2 & -2/3 & & \cdots & O \\ -4 & 6 & -4 & 1 & & \\ 1 & -4 & 6 & -4 & 1 & \\ & & & \ddots & & \\ \vdots & & & & 1 & -4 & 6 & -4 \\ O & & & & -2/3 & -2 & 2 & \end{bmatrix} \in \mathfrak{R}^{(N-1) \times (N-1)},$$

$$A_2 = \begin{bmatrix} -2 & 1 & & \cdots & O \\ 1 & -2 & 1 & & \\ & & & \ddots & \\ \vdots & & & 1 & -2 & 1 \\ O & & & & 1 & -2 \end{bmatrix} \in \mathfrak{R}^{(N-1) \times (N-1)},$$

and $U = \text{diag}(\Delta x, 2\Delta x, \dots, (N-1)\Delta x)$.

We integrated that stiff problem in the interval $x \in [0, 20\pi]$ for $N = 40$. This type of problem is very interesting since no high oscillations are present in the solution while its eigenvalues are all negative real laying in the interval

$[-4.1 \cdot 10^7, -1]$. The results are shown in Table 4. The spatial discretization error is fixed since $\Delta x = 1/40$, and limits the accuracy to $10^{-7.8}$. The new method needs almost half steps to achieve this accuracy. The method given in [19] failed to convergence for large steps.

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Table 4: Accurate digits for the Duffing equation.(nc) means not convergence

steps	correct digits	
	New	[19]
90	4.4	(nc)
180	6.7	(nc)
270	7.7	(nc)
360	7.8	(nc)
450	7.8	(nc)
540	7.8	5.6
540	7.8	7.8
630	7.8	7.8
720	7.8	7.8
810	7.8	7.8

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