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A Family of Two-step Almost P-stable Methods with Phase-lag of Order Infinity for the Numerical Integration of Second Order Periodic Initial-value Problems

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A family of two-step, almost P-stable methods with phase-lag of order infinity is developed for the numerical integration of second order periodic initial-value problems. The method has algebraic order six. Extensive numerical testing indicates that this family of methods is generally more accurate than other two-step methods, that have been proposed.

Key words: second order periodic initial-value problem, phase-lag

1. Introduction

In the last ten years there has been considerable interest in the numerical solution of initial-value problems of the form:

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

These involve ordinary differential equations of second order in which the first derivative does not appear explicitly. Equations of this type having oscillatory solutions are of particular interest. Examples occur in celestial mechanics, in quantum mechanical scattering problems, and elsewhere.

When deriving efficient numerical methods for the solution of (1.1) it is necessary to consider the phase-lag as well as the algebraic order of the method. The important concept of phase-lag was first introduced by Brusa and Nigro [12].

Recently, several methods with minimal phase-lag have been proposed for the numerical integration of the initial-value problem (1.1).

Chawla and Rao [1, 2, 3, 4] have developed methods with phase-lag of order six and eight. Also, Thomas [6] has given a two-step sixth order method with phase-lag of order eight. Van der Houwen and Sommeijer [7, 8] have derived some methods with minimal phase-lag.

Coleman [9] has given a new approach to constructing methods for the numerical integration of $y'' = f(x, y)$ via a rational approximation to the cosine.

Also, Simos and Raptis [13] have proposed some two-step P-stable Numerov-type methods with minimal phase-lag. Raptis and Simos [14] have derived a four-step method with phase-lag of order infinity. Simos [18, 19] has derived explicit two-step methods with minimal phase-lag and a two-step method with phase-lag of order infinity.

Cash [15] has derived some Runge-Kutta type methods of order four and six.

Qi and Mitsui [17] have proved that the attainable order of these methods is four and it is impossible to construct a sixth order P-stable formula of this type.

The purpose of this paper is to develop a family of two-step almost P-stable Runge-Kutta type methods with phase-lag of order infinity. This method requires an a priori knowledge, or an estimate of, the frequency parameter.

Numerical results presented in Section 3 show that this new method is more accurate than the other methods with minimal phase-lag that have been proposed.

It must be noted that this new method can be useful in cases where a large step-size is to be used; that is, where a modest accuracy is sufficient or in the case of problems where the solution consists of a slowly varying oscillation with a high-frequency oscillation superimposed, having a small amplitude.

2. Derivation of the Family of Two-Step Sixth Order P-Stable Method with Infinite Phase-Lag

For the numerical integration of the initial-value problem (1.1) consider the sixth order discretization developed by Cash [15].

$$y_{n+1} - 2y_n + y_{n-1} = h^2[b_0 f_{n+1} + b_2 f_n + b_0 f_{n-1} + b_1(\overline{f}_{n+a} + \overline{f}_{n-a})] \tag{2.1}$$

where $f_{n\pm a}$ is given by:

$$\begin{aligned} f_{n\pm a} &= f(x_n \pm ah, \overline{y}_{n\pm a}), \\ \overline{y}_{n\pm a} &= a_\pm y_{n+1} + b_\pm y_n + c_\pm y_{n-1} + h^2(d_\pm f_{n+1} + e_\pm f_n + g_\pm f_{n-1}). \end{aligned} \tag{2.2}$$

Consider that:

$$\begin{aligned} \mathrm{TEC}_{n+1} = y(x+h) - 2y(x) + y(x-h) - h^2\{b_0 y''(x+h) + b_2 y''(x) \\ + b_0 y''(x-h) + b_1[y''(x+ah) + y''(x-ah)]\} \end{aligned} \tag{2.3}$$

and

$$\begin{aligned} \mathrm{TEC}_{n\pm a} = y(x \pm a) - a_\pm y(x+h) - b_\pm y(x) - c_\pm y(x-h) \\ - h^2[d_\pm y''(x+h) + e_\pm y''(x) + g_\pm y''(x-h)]. \end{aligned} \tag{2.4}$$

We assume that the solution of (1.1) is sufficiently smooth. So we can have from the above formulae (2.3) and (2.4), using Taylor series expansions, the following system equations, for the method (2.1)–(2.2) to be of algebraic order six.

$$2b_0 + 2b_1 + b_2 = 1$$

$$12a^2 b_1 + 12b_0 = 1$$

$$30a^4 b_1 + 30b_0 = 1$$

$$
\begin{aligned}
&a_+ + b_+ + c_+ = 1\\
&a - a_+ + c_+ = 0\\
&a_+ + c_+ + 2(d_+ + e_+ + g_+) = a^2\\
&a_+ - c_+ + 6(d_+ - g_+) = a^3\\
&a_+ + c_+ + 12(d_+ + g_+) = a^4\\
&a_- + b_- + c_- = 1\\
&a + a_- - c_- = 0\\
&a_- + c_- + 2(d_- + e_- + g_-) = a^2\\
&a_- - c_- + 6(d_- - g_-) = a^3\\
&a_- + c_- + 12(d_- + g_-) = a^4.
\end{aligned}
\tag{2.5}
$$

Taking a, c_+ and c_- as free parameters and solving system (2.5) we have that:

$$
\begin{aligned}
&b_0 = (5a^2 - 2)/[60(a^2 - 1)]\\
&b_1 = -1/[20a^2(a^2 - 1)]\\
&b_2 = (25a^2 - 3)/(30a^2)\\
&a_+ = a + c_+\\
&a_- = -a + c_-\\
&b_- = a - 2c_- + 1\\
&b_+ = -a - 2c_+ + 1\\
&d_+ = (a^4 + 2a^3 - 3a - 2c_+)/24\\
&d_- = (a^4 - 2a^3 + 3a - 2c_-)/24\\
&e_+ = -(a^4 - 6a^2 + 5a + 10c_+)/12\\
&e_- = -(a^4 - 6a^2 - 5a + 10c_-)/12\\
&g_+ = (a^4 - 2a^3 + a - 2c_+)/24\\
&g_- = (a^4 + 2a^3 - a - 2c_-)/24
\end{aligned}
\tag{2.6}
$$

and then the local truncation error is given by:

$$
\begin{aligned}
\text{L.T.E.}(h) = \frac{h^8}{302400a^2(a^2-1)}\{&(-55 + 13a^2 + 42a^6)y_n^{(8)}\\
&+ [63(c_+ + c_-) - 105a^4 + 42a^6)]y_n^{(6)}\}.
\end{aligned}
\tag{2.7}
$$

We apply these methods to the test equation $y'' = -k^2 y$. Setting $H = kh$ we obtain the following polynominal as the characteristic one of the second order linear difference equation:

$$P(w) = A(H)w^2 - 2B(H)w + A(H) \tag{2.8}$$

where:

$$\begin{aligned} A(H) &= 1 + H^2[5a^4 - 2a^2 - 3(c_+ + c_-)]/[60a^2(a^2-1)] \\ &\quad + H^4(a^4 - c_+ - c_-)/[240a^2(a^2-1)] \\ B(H) &= 1 - H^2[25a^4 - 28a^2 + 3(c_+ + c_-)]/[60a^2(a^2-1)] \\ &\quad + H^4[a^4 - 6a^2 + 5(c_+ + c_-)]/[240a^2(a^2-1)]. \end{aligned} \tag{2.9}$$

We call the polynominal $P(w)$ the *stability polynominal*.

DEFINITION 1. The method with stability polynominal given by (2.8) is said to have interval of periodicity $(0, {H_0}^2)$ if, for all $H^2 \in (0, {H_0}^2)$ the roots w_i, $i = 1, 2$ of (2.8) satisfy:

$$w_1 = e^{iv(H)} \quad \text{and} \quad w_2 = e^{-iv(H)}. \tag{2.10}$$

It is obvious that if w is a root of $P(w)$ then so is w^{-1}.

Also, from Definition 1 we have that all the roots of $P(w)$ have moduli equal to 1.

DEFINITION 2. We call a method *P-stable* if its interval of periodicity is $(0, \infty)$.

DEFINITION 3. We call a method *almost P-stable* if its interval of periodicity is $(0, \infty) - W$, where W is a set of distinct points.

We note that Thomas [6] has defined "almost P-stable methods", as the methods which are stable for small and large values of $H = kh$.

DEFINITION 4. (van der Houwen et al. [8]). For any method corresponding to the stability polynominal (2.8) the quantity:

$$T(H) = H - \cos^{-1}[Q(H)], \quad \text{where} \quad Q(H) = B(H)/A(H), \tag{2.11}$$

is called the *dispersion, phase error* or *phase-lag*. If $T(H) = O(H^{t+1})$ as $H \to 0$ the order of dispersion is t.

From (2.11) it is obvious that the phase-lag of a method is the leading term in the expansion of:

$$[\cos(H) - Q(H)]/H^2. \tag{2.12}$$

DEFINITION 5. We call a method *phase-fitted* if it has a phase-lag of order infinity.

To have a phase-lag of order infinity, it is obviuos that the equation

$$[\cos(H) - Q(H)]/H^2 = 0 \text{ i.e. } A(H)\cos(H) = B(H) \tag{2.13}$$

holds.

THEOREM 1. *The method* (2.1)–(2.2) *has a phase-lag of order infinity if*:

$$\begin{aligned} c_+ = a^4 - c_- &+ \frac{20a^2(a^2-1)}{H^2} - \frac{12a^2(a^2-1)}{H^2+12} \\ &- \frac{6a^2(a^2-1)(H^2-12)}{(H^2+12)\cos(H)+5H^2-12} \\ &- \frac{864a^2(a^2-1)}{[(H^2+12)\cos(H)+5H^2-12](H^2+12)}. \end{aligned} \tag{2.14}$$

For this value of c_+ the above method is almost P-stable.

Proof. From (2.13) with the help of (2.9) it is easy to see that $B(H) = A(H)\cos(H)$ for the value of c_+ given by (2.14).

It is well known that a symmetric two-step method with stability polynominal given by (2.8) has an interval of periodicity $(0, H_0{}^2)$ if $A(H) \pm B(H) > 0$ for all $H^2 \in (0, H_0{}^2)$.

Now if we substitute (2.14) into (2.9) we have that:

$$\begin{aligned} A(H) - B(H) &= -H^6[\cos(H) - 1]/\{40[(H^2+12)\cos(H) + 5H^2 - 12]\} \\ A(H) + B(H) &= H^6[\cos(H) + 1]/\{40[(H^2+12)\cos(H) + 5H^2 - 12]\}. \end{aligned} \tag{2.15}$$

It is easy to see that $A(H) \pm B(H) > 0$ for all $H^2 \in (0, \infty) - W$, where $W = \{H;\ H = 2m\pi,\ m = 1, 2, \ldots\}$.

So the method (2.1)–(2.2) is almost P-stable.

3. Numerical Illustration

We illustrate the new method proposed in this paper by considering two problems: (1) the *well known "almost periodic problem of Stiefel and Bettis"* and (2) the *"resonance problem" of the radial Schrödinger equation.*

3.1. Problem 1.

We consider the following almost periodic problem studied by Stiefel and Bettis [16]:

$$z'' + z = 0.001e^{ix},\ z(0) = 1,\ z'(0) = 0.9995i, \quad z \in \mathbf{C} \tag{3.1}$$

whose theoretical solution is:

$$z(x) = u(x) + iv(x), \quad u, v \in \mathbf{R}$$
$$u(x) = \cos x + 0.0005x \sin x \tag{3.2}$$
$$v(x) = \sin x - 0.0005x \cos x$$

The solution (3.2) represents motion on a perturbation of a circular orbit in the complex plane. The point $z(x)$ spirals outwards so that at time x its distance from the origin is:

$$g(x) = \sqrt{[u^2(x) + v^2(x)]} = \sqrt{[1 + (0.0005x)^2]}. \tag{3.3}$$

We write (3.1) in the equivalent form:

$$\begin{aligned} u'' + u &= 0.001 \cos x, \quad u(0) = 1, \quad u'(0) = 0 \\ v'' + v &= 0.001 \sin x, \quad v(0) = 0, \quad v'(0) = 0.9995. \end{aligned} \tag{3.4}$$

The actual system was solved numerically for $0 \leq x \leq 40\pi$ (which corresponds to 20 orbits of the point $z(x)$) using:

Method 1: Two-step P-stable fourth-order with phase-lag of order six developed by Chawla and Rao, [3].

Method 2: Fourth order method with phase-lag of order six developed by Thomas [6].

Method 3: Sixth order method with phase-lag of order eight developed by Thomas [6].

Method 4: The two-step method with phase-lag of order infinity of Simos [19].

Method 5: Two-step sixth-order phase fitted P-stable method which was developed in Section 2. In this problem we take $H = h$.

In Table 1 we present the absolute errors $g(x) - g$ produced by using these methods with step sizes $h = \pi/4, \pi/8$ and $\pi/16$.

Table 1. Comparison of the absolute errors $|g(x) - g|$ for the methods 1–5.

h	Method 1	Method 2	Method 3	Method 4	Method 5
$\pi/4$	$0.470\ 10^{-4}$	$0.715\ 10^{-4}$	$0.561\ 10^{-5}$	$0.733\ 10^{-7}$	$0.853\ 10^{-9}$
$\pi/8$	$0.104\ 10^{-5}$	$0.794\ 10^{-6}$	$0.145\ 10^{-7}$	$0.193\ 10^{-9}$	$0.875\ 10^{-11}$
$\pi/16$	$0.347\ 10^{-7}$	$0.135\ 10^{-7}$	$0.760\ 10^{-8}$	$0.326\ 10^{-10}$	$0.954\ 10^{-13}$

3.2. Problem 2.

The radial or one-dimensional Schrödinger equation may be written as:

$$y''(x) = f(x) \cdot y(x), \quad x \in [0, \infty), \tag{3.5}$$

where $f(x) = W(x) - E$, and $W(x) = l(l+1)/x^2 + V(x)$ is an effective potential with $V(x) \to 0$ as $x \to \infty$, l is an integer, and E is a real number denoting the energy.

The problem is one of boundary-value type, with $y(0) = 0$, and a second boundary condition for large values of x determined by physical considerations.

If $E = \varphi^2 > 0$, then, in general, the potential funciton $V(x)$ dies away faster than the term $l(l+1)/x^2$; equation (3.5) then effectively reduces to $y''(x) + (E - l(l+1)/x^2)y(x) = 0$, for x greater than some value R depending on the potential function $V(x)$. The above equation has linearly independent solutions $\varphi x j_l(\varphi x)$ and $\varphi x n_l(\varphi x)$, where $j_l(\varphi x)$ and $n_l(\varphi x)$ are the spherical Bessel and Neumann functions respectively. Thus the solution of equation (3.5) has the asymptotic form:

$$\begin{aligned} y(x) &\underset{x\to\infty}{\simeq} A\varphi x j_l(\varphi x) - B\varphi x n_l(\varphi x) \\ &\underset{x\to\infty}{\simeq} C[\sin(\varphi x - l\pi/2) + \tan\delta_l \cos(\varphi x - l\pi/2)], \end{aligned}$$

where δ_l is the *phase shift* which may be calculated from the formula:

$$\tan\delta_l = [y(x_2)S(x_1) - y(x_1)S(x_2)]/[y(x_1)C(x_2) - y(x_2)C(x_1)]$$

for x_1 and x_2 distinct points on the asymptotic region with $S(x) = \varphi x j_l(\varphi x)$ and $C(x) = -\varphi x n_l(\varphi x)$.

In our numerical example we have used the Woods-Saxon potential with $l = 0$ potential i.e.

$$W(x) = V(x) = u_0/(1+t) - (u_0/a)t/(1+t)^2$$

where $t = \exp[(x - x_0)/a]$ and $u_0 = -50.0$, $a = 0.6$, $x_0 = 7.0$ and $x \in [0, \infty)$. We consider, in particular, the resonance problem for $E \in [1,\ 1000]$ with boundary conditions $y(0) = 0$ and $y(x) \simeq \sin(\sqrt{E}x + \delta)$ at large values of x.

The resonance problem consists in finding values E_j of E (eigenenergies) at which the phase shift $\delta(E_j)$ equals $\pi/2$.

In our numerical test we shall use, for convenience, the exact eigenenergies E_j with six decimal digits accuracy and successively compute the phase shifts by the five techniques denoted in Problem 1. The deviations of the computed phase shifts from the exact value $\pi/2$ are presented in Table 2.

From the results obtained we conclude that the new method 5 is more accurate than the other methods especially in cases of large step sizes.

All computations were carried out on an IBM PC-AT 80386 with an 80387 mathcoprocessor of the Informatic Laboratory of the Agricultural University of Athens, using double precision arithmetic with 14 digits accuracy.

Table 2. Deviations of the computed phase shifts from the exact value $\pi/2$, in 10^{-6} units for various choices of step size shown in the second column. The empty areas indicate that the corresponding variations are larger than the format allowed in the table.

E	h	Method 1	Method 2	Method 3	Method 4	Method 5
53.588872	1/8	3140	44854	2036	89	12
	1/16	199	157	39	0	0
	1/32	4	3	1	0	0
	1/64	1	0	0	0	0
163.215341	1/8	25436	36347	90191	3216	985
	1/16	3454	3005	479	10	1
	1/32	58	49	8	0	0
	1/64	2	1	0	0	0
341.495874	1/8	340798	----	----	189123	18485
	1/16	33940	23547	4309	296	27
	1/32	571	487	69	1	0
	1/64	11	9	5	0	0
989.701916	1/8	----	----	----	----	48325
	1/16	----	----	448431	65095	1652
	1/32	19566	11543	9904	135	7
	1/64	324	275	85	0	0

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