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A note on phase-lag computations for multiderivative methods for second order periodic initial value problems.

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Abstract

Phase—lag computations are carried out for a family of two-step multiderivative methods for solving second order initial value problems of the form $y'' = f(t, y)$, $y(t_0) = y_0$, $y'(t_0) = z_0$. The analysis is carried out with respect to the familiar model equation $y'' = -\lambda^2 y$, where λ is real.

Keywords: Phase—lag analysis, two-step multiderivative methods, periodic initial value problems, Pade approximant, PECE mode.

1. Introduction

Periodic initial value problems of the form

$$y'' = f(t,y) \quad , \quad y(t_0) = y_0 \quad , \quad y'(t_0) = z_0 \qquad (1)$$

arise in the theory of orbital mechanics (Lambert and Watson [1]) and have applications in the study of wave equations (Twizell [2]). In orbital mechanics, such problems can be divided into two distinct classes:
(a) problems for which the solution period is known in advance,
(b) problems for which the period is unknown.

Computational methods applied to type (a) which yield a numerical solution that stays on the orbit are described as *orbitally stable;* numerical methods which yield a solution that spirals inwards or outwards are said to be *orbitally unstable.* For the numerical solution of problems of type (b) it is desirable that the method used should be P-stable. Usually, linear multistep methods are considered for solving (1). However, Lambert and Watson [1] have shown that P-stable linear multistep methods cannot have order of accuracy greater than two. This feature is the main motivation for turning to multiderivative methods for the solution of (1), as these methods are able to attain, simultaneously, high accuracy and good stability properties. It is the aim of the present note to reveal the small phase-lags of multiderivative methods.

2. Analyses

The family of multiderivative methods developed by Twizell and Khaliq [3] was based on the formula

$$y(t-\ell) - \{\exp(\ell D) + \exp(-\ell D)\}y(t) + y(t+\ell) = 0 \quad , \qquad (2)$$

where D is the differential operator d/dt. In [3], the exponential terms were replaced by their (m,k) Pade approximants which have the forms

$$\exp(\pm\ell D) = [Q_m(\pm\ell D)]^{-1}P_k(\pm\ell D)0(\ell^{m+k+1}), \qquad (3)$$

where P_k and Q_m are polynomials of degrees k and m, respectively.

These replacements lead to the formula

$$Q_m(\ell D)\,Q_m(-\ell D)y(t-\ell) - \{Q_m(-\ell D)P_k(\ell D)) + Q_m(\ell D)P_k(-\ell D)\}y(t)$$

$$+Q_m(\ell D)\,Q_m(-\ell D)y(t+\ell) + 0(\ell^{m+k+2}) = \qquad (4)$$

which, in turn, leads to the family of two-step multiderivative methods for the solution of (1). Examination of the methods shows that those based on the (0,2), (1,1) and (1,2) Padé approximants can also be classed as linear multistep methods. The method based on the (m,k) Padé approximant has local truncation error with principal part $C_{p+2}\ \ell^{p+2}\, d^{p+2}\ y/dt^{p+2}$, where $p = m+k$ is the order of the method and C_{p+2} is its error constant; for consistency, $p \geq \uparrow$ (see Lambert [4]).

The usual choice of model periodic initial value problem is the test equation

$$y'' = -\lambda^2 y, \quad \lambda > 0 \text{ real} \qquad (5)$$

with initial conditions $y(t_0) = y$, $y'(t_0) = z_0$ as for (1), It was shown in [3] that the periodicity polynomial associated with (4) and (5) is

$$\Omega(s, H^2) = A(H)s^2 - B(H)s + A(H) \qquad (6)$$

where $H = \lambda\ell$, $A(H) = Q_m(iH)Q_m(-iH)$ and $B(H) = Q_m(-iH)P_k(iH) + Q_m(iH)P_k(-iH)$, with $i = +\sqrt{=}1$.

The interval of periodicity of the multiderivative method yielded by (4) is then determined by computing the range of values of H^2 for which s_1 and s_2, the zeros of the periodicity equation

$$\Omega(s, H^2) = 0 \qquad (7)$$

satisfy

$$s_1 = e^{i\theta}(H) \ , \ s_2 = e^{-i\theta}(H) \quad (8)$$

where $0(H)$ is real and is an approximation for H. The multiderivative method is then orbitally stable and those methods for which $H^2 \in (0,\infty)$ are said to be P-stable (Lambert and Watson [1,p.199]).

Having satisfied the conditions (8) for orbital stability, the (consistent) two-step multiderivative methods arising from (4) then have no algorithmic damping and the use of the more general model equation

$$y'' = \lambda - {}^2y + r\, e^{iwt} \quad (9)$$

is not called for (see Gladwell and Thomas [5] and Chawla and Rao [6]).

The phase—lag of the two—step multiderivative method based on the use of the (m,k) Padé approximant is the leading term in the expansion of

$$|\{\theta(H) - H\}/H| \quad (10)$$

see Brusa and Nigro [7]; the phase—lag is denoted by $\Phi(H)$.

It is easy to show from (8) that

$$\tan\theta(H) = [4\{A(H)\}^2 - \{B(H)\}^2]^{\frac{1}{2}} /B(H) \ . \quad (11)$$

Then, using the expansion

$$\tan^{-1} x = x - \frac{1}{3}x^3 + \frac{1}{5}x^5 - \frac{2}{35} + \ldots \ . \quad (12)$$

to determine $\theta(H)$, the phase lag may be determined from (10).

By way of example, consider the multiderivative method based on the (3,3) Pade approximant [3]. Here,

$$A(H) = 1 + \frac{1}{20}H^2 + \frac{1}{600}H^4 + \frac{1}{14400}H^6, \text{and } B(H) = 2 - \frac{9}{10}H^2 + \frac{11}{300}H^4 - \frac{1}{7200}H^6$$

from which it may be shown that

$$\tan\theta(H) = H(1 - \frac{7}{30}H^2 + \frac{61}{3600}H^4 - \frac{7}{18000}H^6 + \ldots)^{\frac{1}{2}} /(1 - \frac{9}{20}H^2 + \frac{11}{600}H^4 - \frac{1}{14400}H^6)$$

and, using (12), that

$$\phi(H) = \frac{1}{100800} H^6$$

This method, which is of order $p = 6$, has a much smaller phase-lag than the recent method of Chawla and Rao [6] for which $\phi(H) = \frac{1}{100800} H^6$. In addition, the method based on the (3,3) Pade approximant is P-stable whereas the method of Chawla and Rao [6], which those authors named $M_4, \frac{1}{200}$, has interval of periodicity for which $H^2 \in (0,20(1 - 0.4^{\frac{1}{2}})) \simeq (0,7.35)$.

The phase-lag of each of the first 14 entries of the Pade Table which lead to consistent two—step multiderivative methods, are given in Tables 1, 2 and 3 for second, third and fourth order methods, respectively. Periodicity intervals for these methods were given in [3] and are reproduced for the convenience of the reader in Tables 1, 2 and 3.

It is noted from [3] and Tables 1, 2 and 3 that the phase-lag of each multiderivative method has the value

$$\frac{1}{2} | C_{P+2} | H^P \tag{13}$$

3. Predictor-corrector combinations

Using the multiderivative method based on the (0,k*) Padé approximant as predictor and the method based on the (m,k) Pade approximant as corrector, the resulting predictor-corrector combination will be denoted by (0,k*); (m,k).

It was found in [3] that the (0,2); (1,2) combination has the greatest interval periodicity, H^2 E (0,9), of the second order combinations in PECE mode. It is easy to verify also that this combination in PECE mode also has the smallest phase-lag with $\Phi(H)^{\frac{1}{2}} = H^2$.

Of the fourth order combinations, it was noted in [3] that the (0,4); (1,2) combination is to be preferred to any other, when used in

PECE mode, to solve linear problems. It may be shown that the phase-lag of this combination in PECE mode is $\Phi(H) = \frac{7}{2880} H^4$, with $H^2 \in (0,4,88)$. When solving non-linear problems, it was seen in [3] that the (0,4); (2,2) combination in PECE mode is to be preferred to any other because it requires no more than the second derivative of $f(t,y)$. It may be shown that the phase-lag for this combination in PECE mode, for which $H^2 \in (0,15.89)$ is $\Phi(H) = \frac{1}{360} H^4$.

It is interesting to note finally that the "Numerov made explicit" method of Chawla [8] has the same phase-lag and periodicity interval as the multiderivative method based on the (0,4) Pade approximant.

4, Summary

This note has been concerned with the determination of the phase-lag of each member of a family of multiderivative methods based on Padé approximants to the exponential function. Each phase-lag was seen to be directly related to the principal part of the local truncation error of the method.

Phase-lag computations were also carried out for predictor-corrector combinations in PECE mode.

Table 1: Phase-lags for second order methods.

Method	Phase-lage	Periodicity
(0,2)	$\frac{1}{24}H^2$	$H^2 \in (0,4)$
(1,1)	$\frac{1}{12}H^2$	P-stable
(1,2)	$\frac{1}{72}H^2$	$H^2 \in (0, \frac{36}{5})$
(2,1)	$\frac{1}{72}H^2$	P-stable
(2,0)	$\frac{1}{24}H^2$	P-stable
(0,3)	$\frac{1}{24}H^2$	$H^2 \in (0,4)$
(3,0)	$\frac{1}{24}H^2$	P-stable

Table 2: Phase-lags for fourth order methods

Method	Phase-lag	Periodicity
(2,2)	$\frac{1}{720}H^4$	P-stable
(1,3)	$\frac{1}{5760}H^4$	$H^2 \in$ (0,6.5) and (29.5,48)
(2,3)	$\frac{1}{7200}H^4$	$H^2 \in$ (0,8.2) and $(14.6, \frac{300}{7})$
(3,2)	$\frac{1}{7200}H^4$	P-stable
(3,1)	$\frac{17}{5760}H^4$	P-stable
(0,4)	$\frac{1}{720}H^4$	$H^2 \in (0,12)$
Numerov	$\frac{1}{480}H^4$	$H^2 \in (0,6)$

Table 3: Phase-lags for sixth order methods.

Method	Phase-lag	Periodicity
(3,3)	$\frac{1}{100800}H^6$	P-stable
Chawla and Rao $M^4\left(\frac{1}{200}\right)$	$\frac{1}{12096}H^6$	$H^2 \in (0,7.35)$

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