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PREDICTOR-CORRECTOR METHODS FOR PERIODIC SECOND-ORDER INITIAL VALUE PROBLEMS

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ABSTRACT Predictor-corrector methods are constructed for the accurate representation of the eigenmodes in the solution of second-order differential equations without first derivatives. These methods have (algebraic) order 4 and 6, and phase errors of orders up to 10. For linear and weakly nonlinear problems where homogeneous solution components dominate, the methods proposed in this paper are considerably more accurate than conventional methods.

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1. Introduction

Recently, various papers have been published dealing with increasing the phase lag order of methods for the special second-order equation

$$y''(t) = f(t,y(t)), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0 . \tag{1.1}$$

Relative to a linear test equation, one may distinguish papers which deal with reducing the phase lag (or: phase error, dispersion) of the homogeneous solution component (e.g., in [3] and [7]) and which deal with reducing the phase lag of the inhomogeneous component (e.g., in [1], [4], [9] and [10]).

Alternatively, one may try to improve the accuracy of the total solution, for instance by increasing the algebraic order of the method (cf. [2] and the references given there).

In this paper, we shall be concerned with methods that produce solutions with small phase lag in the homogeneous solution component. A particularly attractive method of this sort was proposed in Chawla & Rao [3]. Their method is explicit, has algebraic order 4 and phase lag order 6. Moreover, since only 3 right-hand side evaluations per step are involved, the interval of periodicity, which is given by [0,7.56] (in the sense of Lambert and Watson [8]), is relatively large.

Motivated by the result of Chawla and Rao we have looked for methods with both higher algebraic and phase lag order. As starting point we have chosen a generalization of predictor-corrector methods. In [5] such methods were analysed for first-order equations; a straightforward modification of these methods make them applicable to second-order equations of type (1.1) (see also [6]). Within the class of these predictor-corrector methods we shall construct numerical schemes with algebraic order 4 and 6, and with phase lag orders up to 10. In fact, it is possible to obtain arbitrarily high phase lag orders by increasing the number of stages (corrections) in the numerical scheme. Similarly, by starting with a corrector of appropriate algebraic order we can obtain any algebraic order we want.

In Section 2, the phase lag order for predictor-corrector methods is derived. In Sections 3 and 4 optimal two- and four-step methods are constructed, and in Section 5 we present numerical experiments.

2. Predictor-corrector methods

In [5] a generalization of conventional predictor-corrector methods for first-order ODEs has been proposed; for second-order ODEs such methods are of the form

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$$y_{n+1}^{(0)} \quad \text{determined by an explicit LM method } \{\tilde{\rho},\tilde{\sigma}\},$$

$$y_{n+1}^{(j)} = \sum_{\ell=1}^{j} [\mu_{j\ell} y_{n+1}^{(\ell-1)} + \bar{\mu}_{j\ell}\tau^2 f_{n+1}^{(\ell-1)}] + \lambda_j \Sigma_n, \quad j=1(1)m, \tag{2.1a}$$

$$y_{n+1} = y_{n+1}^{(m)}, \quad f_{n+1}^{(\ell-1)} := f(t_{n+1}, y_{n+1}^{(\ell-1)}),$$

where the parameters occurring in this scheme are to be prescribed. Σ_n contains the back values used in the corrector formula. If the corrector formula is defined by a linear $\bar{k}$-step method $\{\bar{\rho},\bar{\sigma}\}$, then

$$\Sigma_n := [\bar{a}_0 E^{\bar{k}} - \bar{\rho}(E)] y_{n+1-\bar{k}} - \tau^2 [\bar{b}_0 E^{\bar{k}} - \bar{\sigma}(E)] f_{n+1-\bar{k}}, \tag{2.1b}$$

with $\bar{a}_o$, $\bar{b}_o$ denoting the coefficients of $z^{\bar{k}}$ in $\bar{\rho}(z)$ and $\bar{\sigma}(z)$. In the following we will assume that $\bar{a}_o = 1$ and that $\{\bar{\rho},\bar{\sigma}\}$ is zero-stable. Furthermore, it will be assumed that the parameters of the method satisfy the compatibility conditions

$$\sum_{\ell=1}^{j} \mu_{j\ell} = 1 - \lambda_j, \quad \sum_{\ell=1}^{j} \bar{\mu}_{j\ell} = \bar{b}_0 \lambda_j, \quad j = 1,2,\ldots,m. \tag{2.1c}$$

The various properties of the method (2.1) are determined by the iteration polynomial $P_m(z)$, which is recursively defined by

$$P_0(z) = 1, \quad P_j(z) = \sum_{\ell=1}^{j} [\mu_{j\ell} + \bar{\mu}_{j\ell} z] P_{\ell-1}(z), \quad j = 1(1)m. \tag{2.2}$$

Notice that $P_m(z)$ satisfies the condition $P_m(1/\bar{b}_o)=1$.

Suppose that an appropriate iteration polynomial has been constructed (see Sections 3 and 4), then we are faced with the task to derive a scheme of the form (2.1) possessing this particular iteration polynomial. We shall derive an easily implementable scheme with vanishing μ - parameters except for μ_{j1} and $\bar{\mu}_{jj}$. Let $P_m(z)$ be given by

$$P_m(z) = \beta_0 + \beta_1 z + \ldots + \beta_m z^m$$

and set

$$\mu_{j1} = \mu_j, \quad \bar{\mu}_{jj} = \bar{\mu}_j.$$

It follows from (2.2) that the coefficients of the iteration polynomial and the parameters of the method are related by

$$\mu_m = \beta_0; \quad \mu_{m-j} = \frac{\beta_j}{\bar{\mu}_m \cdot \bar{\mu}_{m-1} \cdot \ \dots \ \cdot \bar{\mu}_{m-j+1}}, \qquad j = 1,\dots,m-1; \tag{2.1d}$$

$$\bar{\mu}_1 \cdot \ \dots \ \cdot \bar{\mu}_m = \beta_m .$$

In addition, we have the compatibility condition

$$\bar{\mu}_j = \bar{b}_0(1 - \mu_j), \quad j = 1,\dots,m. \tag{2.1c'}$$

If $P_m(z)$ satisfies $P_m(1/\bar{b}_0)=1$, then the relations (2.1c′) and (2.1d) uniquely define the parameters of the method. The resulting scheme is of the simple form

$$y_{n+1}^{(j)} = [\mu_j y_{n+1}^{(0)} + (1 - \mu_j)\Sigma_n] + (1 - \mu_j)\bar{b}_0\tau^2 f_{n+1}^{(j-1)} \tag{2.1'}$$

for $j=1,\dots,m$.

In a similar way as done in [5] for first-order equations, the algebraic order and the stability polynomial can be derived for the method (2.1) (a detailed derivation can be found in [6]):

Theorem 2.1. Let the predictor $\{\tilde{\rho},\tilde{\sigma}\}$ and the corrector $\{\bar{\rho},\bar{\sigma}\}$ be of order $\tilde{p}$ and $\bar{p}$, respectively, and let the iteration polynomial have a zero of order r at $z=0$. Then the method (2.1) is of order $p := \min\{\bar{p},\tilde{p}+2r,4+2\tilde{p}\}$.#

Theorem 2.2. The characteristic equation of the predictor-corrector method (2.1), when applied to the test equation

$$y''=-\delta^2 y,$$

is given by

$$C(\zeta,z_0):= \bar{\rho}(\zeta) - z_0\bar{\sigma}(\zeta) - \frac{(1-\bar{b}_0 z_0)P_m(z_0)}{P_m(z_0)-1}\,[\tilde{\rho}(\zeta) - z_0\tilde{\sigma}(\zeta)]\zeta^{\bar{k}-\tilde{k}} = 0 \tag{2.3}$$

where $z_0 := -\tau^2\delta^2$ #

The two principal roots of equation (2.3) correspond to the characteristic roots $\exp(\pm i\sqrt{-z_0})$ of the test equation itself. In order to approximate the natural modes of equation (1.1) with improved accuracy, several authors have proposed to increase the order of the phase error introduced by the numerical scheme (cf. [1], [3]). In this paper, we study what can be achieved within the class of methods (2.1).

In the following it is convenient to set $\sqrt{-z_0} = v_0$. Let us assume that the principal roots of (2.3) are of the form

$$\zeta_\pm = a(v_0)\ e^{\pm i\theta(v_0)}; \quad v_0, a, \theta \in R_+. \tag{2.4}$$

Then

$$1 - a(v_0) \quad \text{and} \quad \left| \frac{\theta(v_0) - v_0}{v_0} \right|$$

are respectively called the dissipation error and the phase lag of the method (cf. [1] and [3]). We shall simultaneously reduce these errors by maximizing the order q in the error equation

$$\varepsilon_\pm := e^{\pm iv_0} - \zeta_\pm(v_0) = O(v_0^{q+1}). \tag{2.5}$$

Theorem 2.3. Define the functions

$$\bar{\phi}(v) := \bar{\rho}(e^{iv}) + v^2\bar{\sigma}(e^{iv}), \qquad \tilde{\phi}(v) := \tilde{\rho}(e^{iv}) + v^2\tilde{\sigma}(e^{iv}),$$
$$R(v) := \bar{\phi}(v)/[\bar{\phi}(v) - (1+\bar{b}_0v^2)\tilde{\phi}(v)e^{i(\bar{k}-\tilde{k})v}] \tag{2.6}$$

and let they satisfy the order conditions

$$\bar{\phi}(v) - (1+\bar{b}_0v^2)\tilde{\phi}(v) \approx c_1v^{q_1}, \quad P_m(-v^2) - R(v) \approx c_2v^{q_2},$$
$$C_\zeta(e^{iv}, -v^2) \approx c_3v^{q_3}. \tag{2.7}$$

If $P_m(0)\neq 1$, then the order q of the error (2.5) is given by $q=q_1+q_2-q_3-1$.

Proof. It follows from our assumption (2.4) that we can restrict our considerations to the error ε_+. Using (2.5) we find the relation

$$C(\zeta_+, -v_0^2) = C(e^{iv_0} - \varepsilon_+, -v_0^2) = C(e^{iv_0}, -v_0^2) - \varepsilon_+ \frac{\partial C}{\partial \zeta}(e^{iv_0}, -v_0^2) + O(\varepsilon_+^2).$$

Since the left-hand side is obviously zero we have

$$\varepsilon_+ = \frac{C(e^{iv_0}, -v_0^2) + O(\varepsilon_+^2)}{\frac{\partial C}{\partial \zeta}(e^{iv_0}, -v_0^2)}. \tag{2.8}$$

Furthermore, it follows from (2.3) and (2.6) that

$$C(e^{iv_0},-v_0^2) = \bar{\phi}(v_0) - \frac{(1+\bar{b}_0 v_0^2)\, P_m(-v_0^2)}{P_m(-v_0^2) - 1} \tilde{\phi}(v_0) e^{i(\bar{k}-\tilde{k})v_0} ,$$

and, using (2.6) and (2.7), we can express $P_m(z)$ in terms of the functions (2.6), so that

$$C(e^{iv_0},-v_0^2) = \frac{\bar{\phi}(v_0) - (1+\bar{b}_0 v_0^2)\tilde{\phi}(v_0) e^{i(\bar{k}-\tilde{k})v_0}}{P_m(-v_0^2) - 1} O(v_0{}^{q_2}).$$

On substitution into (2.8) and using the order conditions (2.7) we obtain

$$\varepsilon_+ = O(v_0{}^{q_1}).O(v_0{}^{q_2}).O(v_0{}^{-q_3})$$

which proves the assertion of the theorem.#

Since the iteration polynomial has to satisfy the compatibility condition $P_m(1/\bar{b}_0)=1$ it follows that in (2.7): $q_2 \leq 2m$. Furthermore, in order to have algebraic order equal to that of the corrector $\{\bar{p},\bar{\sigma}\}$, we should require $r \geq (p-\tilde{p})/2$ (see Theorem 2.1); that is, the polynomial $P_m(-v^2)$, and therefore the function $R(v)$, should have a zero at $v=0$ of multiplicity at least $p-\tilde{p}$. Since

$$\bar{\phi}(v) = O(v^{\bar{p}+2}),$$

it follows from (2.6) and (2.7) that

$$R(v) = O(v^{\bar{p}+2-q_1}), \tag{2.9}$$

so that the order of the corrector is obtained if $q_1 \leq \tilde{p}+2$. Thus, we have proved the following corollary:

Corollary 2.1. Let the conditions of Theorem 2.3 be satisfied and let $q_1 \leq \tilde{p}+2$. Then the algebraic order of the predictor-corrector method is given by $p=\bar{p}$ and the order of the error (2.5) satisfies $q \leq 2m+\bar{p}-q_3+1$.#

In order to obtain the maximal possible order we have to identify the first m terms of the iteration polynomial with the first m terms of the Taylor expansion of $R(v)$ (leaving the last term of the iteration polynomial free to satisfy the compatibility condition). Since $P_m(-v^2)$ is an even function of v we deduce from (2.9) that $\bar{p}-q_1$ should be even. If $\bar{p}>\tilde{p}$, then it follows from the definition of q_1 (cf. (2.7)) that $q_1=\tilde{p}+2$, and consequently, we should choose the generating predictor-corrector pair such that $\bar{p}-\tilde{p}$ is even. If $\bar{p}=\tilde{p}$, then this condition is automatically satisfied.

We shall mainly be interested in methods with zero dissipation. Suppose that we have a zero dissipative method such that

$$|\varepsilon_{\pm}| = c_q v_0^{q+1} + O(v_0^{q+2}).$$

Then it is easily verified that the phase error satisfies

$$\left|\frac{\theta(v_0) - v_0}{v_0}\right| = c_q v_0^{q} + O(v_0^{q+2}).$$

We will call q the phase lag order and c_q the principal phase lag constant.

Corollary 2.2. Let the conditions of Theorem 2.3 be satisfied and let

$$R(v) \approx c_4 v^{q_4}, \quad \bar{\phi}(v) \approx c_5 v^{\bar{p}+2}. \tag{2.10}$$

If the method has zero dissipation, then the principal phase lag constant and the phase lag order are respectively given by

$$c_q = \left|\frac{c_2 c_5}{c_3 c_4}\right|, \quad q = \bar{p} + q_2 + 1 - q_3 - q_4.$$

Proof. It follows from (2.8), (2.7) and (2.10), and from the identity

$$C(e^{iv}, -v^2) = \frac{\bar{\phi}(v)(P_m(-v^2) - R(v))}{R(v)(P_m(-v^2) - 1)},$$

that

$$\varepsilon_{\pm} \approx \frac{c_5 v_0^{\bar{p}+2} \, c_2 v_0^{q_2}}{c_4 v_0^{q_4} (-1) c_3 v_0^{q_3}}.$$

From this expression and the zero-dissipativity the assertion of the theorem follows.#

3. Construction of two-step methods with minimal phase lag

In this section methods are considered based on the fourth-order Numerov corrector

$$\bar{\rho}(\zeta) = (\zeta-1)^2, \qquad \bar{\sigma}(\zeta) = \frac{1}{12}(\zeta^2+10\zeta+1). \tag{3.1}$$

We shall combine this corrector with a symmetric predictor formula:

$$\tilde{\rho}(\zeta) = \zeta^{\tilde{k}}\tilde{\rho}(1/\zeta) \quad \text{and} \quad \tilde{\sigma}(\zeta) = \zeta^{\tilde{k}}\tilde{\sigma}(1/\zeta)$$

(cf. Lambert & Watson [8]). Since the corrector (3.1) is also symmetric, it follows that the resulting predictor-corrector method itself is symmetric, and consequently a nonempty interval of periodicity is obtained. Thus, we have zero dissipation for all z lying in the interval of periodicity. This property enables us to apply Corollary 2.2 so that the phase lag order and the principal phase lag constant can straightforwardly be calculated.

3.1. Zero-order predictor

Let

$$\tilde{\rho}(\zeta) = (\zeta-1)^2, \qquad \tilde{\sigma}(\zeta) = 0, \tag{3.2}$$

then

$$\tilde{\phi}(v) = (e^{iv}-1)^2 = e^{iv}[e^{iv}-2+e^{-iv}] = 2e^{iv}[\cos(v)-1],$$

$$\begin{aligned}\bar{\phi}(v) &= (e^{iv}-1)^2 + \frac{1}{12}v^2(e^{2iv}+10e^{iv}+1)\\ &= 2e^{iv}[(1+\frac{1}{12}v^2)\cos(v)-1+\frac{5}{12}v^2] \approx \frac{1}{240}v^6,\end{aligned}$$

so that

$$\begin{aligned}R(v) &= \frac{-2}{v^2}[1-\frac{5}{12}v^2-(1+\frac{1}{12}v^2)\cos(v)]\\ &= v^4\sum_{j=2}^{\infty}\left(\frac{1}{6(2j)!}-\frac{2}{(2j+2)!}\right).(-v^2)^{j-2} \approx \frac{1}{240}v^4.\end{aligned}$$

We now define the iteration polynomial

$$P_m(z) := z^2 \sum_{j=2}^{m-1} \left(\frac{1}{6(2j)!} - \frac{2}{(2j+2)!} \right) z^{j-2} + \beta_m z^m, \tag{3.3a}$$

where β_m is determined by the compatibility condition $P_m(12)=1$. By induction it is easily verified that

$$\beta_m = \frac{1}{6(2m)!} \,. \tag{3.3b}$$

Since $P_m(-v^2)=O(v^4)$, we finally have

$$C_\zeta(e^{iv},-v^2) = 2(e^{iv}-1) + \frac{1}{12}v^2(2e^{iv}+10) - \frac{(1+\frac{1}{12}v^2)P_m(-v^2)}{P_m(-v^2)-1}\, 2(e^{iv}-1) \approx 2iv.$$

We now apply Theorem 2.1 and Corollary 2.2 to obtain the following result:

Theorem 3.1. The predictor-corrector method generated by (3.1), (3.2) and (3.3), has algebraic order p=4, phase lag order q=2m, and the principal phase lag constant $c_q = 1/(2m+2)!$.

Proof. Since $\bar{p}=4$, $\tilde{p}=0$, and r=2, it follows from Theorem 2.1 that p=4, and since $q_2=2m$, $q_3=1$ and $q_4=4$, it follows from Corollary 2.2 that q=2m. Furthermore, since

$$c_2 = -\frac{1}{6(2m)!} + \frac{2}{(2m+2)!} + \beta_m, \quad c_3 = 2i, \quad c_4 = \frac{1}{240}, \quad c_5 = \frac{1}{240},$$

the principal phase lag constant is given by

$$c_{2m} = \left| \frac{1/240}{2i.1/240}\, c_2 \right| = \frac{1}{(2m+2)!} \,.$$

3.2. Second-order predictor

Let

$$\tilde{\rho}(\zeta) = (\zeta-1)^2, \quad \tilde{\sigma}(\zeta) = \zeta, \tag{3.4}$$

then

$$\tilde{\phi}(v) = (e^{iv}-1)^2 + v^2e^{iv} = 2e^{iv}[\cos(v)-1+\tfrac{1}{2}v^2],$$

so that

$$R(v) = \frac{24}{v^2}\,[1-\frac{5}{12}v^2-(1+\frac{v^2}{12})\cos(v)]$$
$$= -12\,v^2\sum_{j=2}^{\infty}[\frac{1}{6(2j)!} - \frac{2}{(2j+2)!}]\,(-v^2)^{j-2} \approx -\frac{1}{20}\,v^2.$$

We define the iteration polynomial

$$P_m(z) = 12\,z\sum_{j=2}^{m}[\frac{1}{6(2j)!} - \frac{2}{(2j+2)!}]\,z^{j-2} + \beta_m z^m, \tag{3.5a}$$

where β_m is again determined by the compatibility condition. By induction it can be shown that

$$\beta_m = \frac{2}{(2m+2)!}\,. \tag{3.5b}$$

Since $P_m(-v^2)=O(v^2)$, we find that

$$c_\zeta(e^{iv},-v^2) = 2(e^{iv}-1) + \frac{v^2}{12}(2e^{iv}+10) - \frac{(1+\frac{v^2}{12})P_m(-v^2)}{P_m(-v^2)-1}\,[2(e^{iv}-1)+v^2] \approx 2iv.$$

Proceeding as in the previous section, the following result can be proved:

Theorem 3.2. The predictor-corrector method generated by (3.1), (3.4) and (3.5), has algebraic order $p=4$, phase lag order $q=2m+2$, and the principal phase lag constant $c_q = 1/(2m+4)!$.#

A comparison with the result stated in Theorem 3.1 reveals that using the second-order predictor (3.4) leads to a higher phase lag order and a smaller phase lag constant as well. Therefore, we shall concentrate on the method described in this section. This method will be denoted by PC4.

3.2.1. The interval of periodicity

The characteristic equation of the method PC4 is given by

$$\zeta^2 - 2\zeta \frac{(1+\frac{5}{12}z)(P_m(z)-1) - (1+\frac{1}{2}z)(1-\frac{1}{12}z)P_m(z)}{(1-\frac{1}{12}z)(P_m(z)-1) - (1-\frac{1}{12}z)P_m(z)} + 1 = 0 .$$

This equation has its roots on the unit circle if

$$\frac{12}{z} \le P_m(z) \le 8\,\frac{6+z}{z^2} . \qquad (3.6)$$

The interval $0 \leqslant |z| \leqslant \beta^2$ where (3.7) is satisfied is called the interval of periodicity [8].

Since $P_m(z)$ is a Taylor approximation to the function $R(\sqrt{-z})$, and since $R(\sqrt{-z})$ 'touches' the functions $12/z$ and $8(6+z)/z^2$, respectively in the points

$$z_j = -j^2\pi^2 \quad \text{and} \quad z_{j-1} = -(j-1)^2\pi^2, \quad j=2,4,\ldots,$$

the periodicity condition is easily violated in the neighbourhood of the points z_ℓ, $\ell=1,2,\ldots$. Therefore, in the numerical verification of (3.6), a rather fine mesh should be used in the neighbourhood of these points. In Table 3.1 the results of such a numerical search are listed.

Table 3.1. Intervals of periodicity $[0,\beta^2]$ of the methods PC4

m	2	3	4	5	6	7	8	9	10	11
β^2	7.56	21.44	9.49	30.69	50.27	36.97	67.08	39.06	80.28	114.70

3.2.2. A two-stage method

Let m=2, then (3.5) gives

$$P_2(z) = \frac{1}{20}\,z + \frac{1}{360}\,z^2. \qquad (3.5')$$

Solving the relations (2.1c)-(2.1d) leads to the scheme

$$\begin{aligned}
\Sigma_n &= 2y_n - y_{n-1} + \frac{1}{12}\tau^2(10f_n + f_{n-1}),\\
y_{n+1}^{(0)} &= 2y_n - y_{n-1} + \tau^2 f_n,\\
y_{n+1}^{(1)} &= \frac{3}{5}y_{n+1}^{(0)} + \frac{2}{5}\Sigma_n + \frac{1}{30}\tau^2 f_{n+1}^{(0)},\\
y_{n+1} &= \Sigma_n + \frac{1}{12}\tau^2 f_{n+1}^{(1)}.
\end{aligned} \tag{3.7}$$

This scheme is of algebraic order p=4, has phase lag order q=6, the principal error constant $c_q=1/40320$, and the periodicity interval [0,7.56]. Three right-hand side evaluations per step are required. It can be verified that its characteristic equation is identical to that of the method of Chawla & Rao [3].

3.2.3. A three-stage method

Let m=3, then (3.5) yields

$$P_3(z) = \frac{1}{20}z + \frac{11}{5040}z^2 + \frac{1}{20160}z^3. \tag{3.5''}$$

Solving the relations (2.1c)-(2.1d) leads to the scheme

$$\begin{aligned}
\Sigma_n &= 2y_n - y_{n-1} + \frac{1}{12}\tau^2(10f_n + f_{n-1}),\\
y_{n+1}^{(0)} &= 2y_n - y_{n-1} + \tau^2 f_n,\\
y_{n+1}^{(1)} &= \frac{11}{14}y_{n+1}^{(0)} + \frac{3}{14}\Sigma_n + \frac{1}{56}\tau^2 f_{n+1}^{(0)},\\
y_{n+1}^{(2)} &= \frac{3}{5}y_{n+1}^{(0)} + \frac{2}{5}\Sigma_n + \frac{1}{30}\tau^2 f_{n+1}^{(1)},\\
y_{n+1} &= \Sigma_n + \frac{1}{12}\tau^2 f_{n+1}^{(2)}.
\end{aligned} \tag{3.8}$$

This scheme is of algebraic order p=4, has phase lag order q=8, the principal error constant $c_q=1/3628800$, and the periodicity interval [0,21.44]. Four right-hand side evaluations per step are required.

4. Construction of four-step methods with minimal phase lag

Consider the symmetric sixth-order corrector formula

$$\bar{\rho}(\zeta) = (\zeta-1)^2(\zeta^2+1), \quad \bar{\sigma}(\zeta) = \frac{1}{120}(9\zeta^4+104\zeta^3+14\zeta^2+104\zeta+9). \tag{4.1}$$

In this section we restrict our discussion to methods using the fourth-order predictor

$$\tilde{\rho}(\zeta) = (\zeta-1)^2(\zeta^2+1), \quad \tilde{\sigma}(\zeta) = \frac{1}{6}(7\zeta^3-2\zeta^2+7\zeta). \tag{4.2}$$

The functions $\bar{\varphi}$ and $\tilde{\varphi}$ respectively corresponding to (4.1) and (4.2), are given by

$$\bar{\phi}(v) = 2e^{2iv}\,[1+\frac{7}{120}v^2-(2-\frac{13}{15}v^2)\cos(v)+(1+\frac{3}{40}v^2)\cos(2v)],$$

$$\tilde{\phi}(v) = 2e^{2iv}\,[1-\frac{1}{6}v^2-(2-\frac{7}{6}v^2)\cos(v)+\cos(2v)].$$

Substitution into the expression for R(v) and writing $-v^2=z$ yields

$$R(v) = \frac{16}{3}\,z\,\Big[\sum_{j=4}^{\infty} A_j z^{j-4}\Big]\,.\,\Big[\sum_{j=2}^{\infty} B_j z^{j-2}\Big]^{-1} \approx \frac{16}{3}\frac{A_4}{B_2}\,z,$$

where

$$\begin{aligned} A_j &:= \frac{1}{(2j)!}\,[15(2^{2j-1}-1) - (9\cdot 2^{2j-5}+13)j(2j-1)], \\ B_j &:= \frac{1}{(2j)!}\,[6 - 7j(2j-1)]. \end{aligned} \tag{4.3a}$$

We now define

$$P_m(z) = \sum_{j=1}^{m-1} \beta_j z^j + \beta_m z^m, \tag{4.3b}$$

with

$$\beta_0 = 0, \quad \beta_j = [\frac{16}{3}A_{3+j} - \sum_{i=0}^{j-1}\beta_i B_{2+j-i}]/B_2, \quad j=1,\dots,m-1 \tag{4.3c}$$

and with β_m such that $P_m(40/3)=1$. The first few coefficients A_j and B_j are given in Table 4.1.

Table 4.1. Coefficients A_j and B_j

j	2	3	4	5	6
A_j	0	0	-475/8!	-5880/10!	-46185/12!
B_j	-36/4!	-99/6!	-190/8!	-309/10!	-456/12!

The methods defined above will be denoted by PC6. For these methods the following theorem holds:

Theorem 4.1. The PC6 method generated by (4.1), (4.2) and (4.3) has algebraic order p=6 and phase lag order q=2m+4.#

4.1. The interval of periodicity

Proceeding as in Section 3.2.1 we found, by a numerical search, the intervals of periodicity listed in Table 4.2.

Table 4.2. Intervals of periodicity of PC6 methods.

m	2	3	4	5	6	7	8	9	10	11
β^2	7.13	2.51	15.52	15.29	15.60	15.76	15.92	16.08	16.24	16.32

A comparison with Table 3.1 reveals that the 6^{th}-order methods possess a considerably smaller interval of periodicity than the fourth-order methods. The length of the intervals shown in Table 4.2 tends to a limit as m increases, contrary to the fourth-order case where the periodicity interval can be made as large as we want by choosing m sufficiently large. The reason for this is the presence of parasitic roots in four-step methods; these roots move away from the unit circle much earlier than the principal roots as m increases.

In connection with the relatively small periodicity interval of the m=3 method, it should be remarked that this method has an additional periodicity interval located at [2.58,12.92].

4.2. A two-stage method

For m=2 we have the iteration polynomial

$$P_2(z) = \frac{1}{756} z \left(\frac{95}{3} + \frac{751}{400} z\right). \tag{4.4}$$

Using (2.1c) and (2.1d), the scheme takes the form

$$\begin{aligned}
\Sigma_n &= 2y_n - 2y_{n-1} + 2y_{n-2} - y_{n-3} + \frac{\tau^2}{120}(104f_n + 14f_{n-1} + 104f_{n-2} + 9f_{n-3}), \\
y_{n+1}^{(0)} &= 2y_n - 2y_{n-1} + 2y_{n-2} - y_{n-3} + \frac{1}{6}\tau^2(7f_n - 2f_{n-1} + 7f_{n-2}), \\
y_{n+1}^{(1)} &= \frac{1}{1701}(950\, y_{n+1}^{(0)} + 751\Sigma_n) + \frac{751}{22680}\tau^2 f_{n+1}^{(0)}, \\
y_{n+1} &= \Sigma_n + \frac{3}{40}\tau^2 f_{n+1}^{(1)}.
\end{aligned} \tag{4.5}$$

This scheme has algebraic order $p=6$, phase lag order $q=8$, and periodicity interval $[0,7.13]$; it requires three f-evaluations per step.

4.2. A three-stage method

For $m=3$ we have the iteration polynomial

$$P_3(z) = \frac{1}{2268} z \left(95 + \frac{523}{120} z + \frac{1529}{16000} z^2\right) \tag{4.6}$$

and the corresponding scheme reads

$$\begin{aligned}
\Sigma_n &= 2y_n - 2y_{n-1} + 2y_{n-2} - y_{n-3} + \frac{\tau^2}{120}(104f_n + 14f_{n-1} + 104f_{n-2} + 9f_{n-3}), \\
y_{n+1}^{(0)} &= 2y_n - 2y_{n-1} + 2y_{n-2} - y_{n-3} + \frac{1}{6}\tau^2(7f_n - 2f_{n-1} + 7f_{n-2}), \\
y_{n+1}^{(1)} &= \frac{1}{6759}(5230\, y_{n+1}^{(0)} + 1529\Sigma_n) + \frac{1529}{90120}\tau^2 f_{n+1}^{(0)}, \\
y_{n+1}^{(2)} &= \frac{1}{1701}(950\, y_{n+1}^{(0)} + 751\Sigma_n) + \frac{751}{22680}\tau^2 f_{n+1}^{(1)}, \\
y_{n+1} &= \Sigma_n + \frac{3}{40}\tau^2 f_{n+1}^{(2)}.
\end{aligned} \tag{4.7}$$

This sixth-order, three-stage method requires four f-evaluations per step; its phase error, however, is of order 10.

It may be remarked that in the construction of methods of still higher order phase lag, only the coefficients in the first stage have to be calculated: in an m-stage scheme the last m-1 stages are identical to the stages in an (m-1)-stage scheme.

5. Numerical illustrations

In testing the PC methods we wil place emphasis on the phase errors in the numerical solution. To measure the global phase lag we define

$$cd := -\log_{10} |\text{ the numerical solution at } t=T\ |, \tag{5.1}$$

where T is a zero of the exact solution. If the numerical solution is small at t=T, then the value of cd is an adequate measure for the phase lag.

We will test the PC methods defined in the Sections 3.2 and 4 for various values of m (recall that an m-stage method requires m+1 right-hand side evaluations). In the tables of results these methods are denoted by PCpq, where p and q indicate the algebraic and phase lag order, respectively.

As a comparison, we also applied the classical fourth-order Runge-Kutta-Nystrom method and the fourth-order method proposed by Chawla and Rao [3]; these methods are denoted by RKN44 and CR46, respectively. Both methods require three f-evaluations per step.

5.1. Linear inhomogeneous perturbation

As a first example we consider the linear equation

$$2\, y''(t) + \begin{pmatrix} 125 & 75 \\ 75 & 125 \end{pmatrix} y(t) = \begin{pmatrix} 123\sin(t) + 75\cos(t) \\ 75\sin(t) + 123\cos(t) \end{pmatrix}, \quad 0 \le t \le 40\pi. \tag{5.2a}$$

By specifying the initial conditions $y(0)=(0,1)^T$ and $y'(0)=(16,5)^T$ we have the solution

$$y(t) = \begin{pmatrix} \sin(t) \\ \cos(t) \end{pmatrix} + \begin{pmatrix} \sin(5t) + \sin(10t) \\ -\sin(5t) + \sin(10t) \end{pmatrix} =: I + H. \tag{5.2b}$$

This equation differs slightly from the model equation because it includes an inhomogeneous term. The exact solution consists of a slowly oscillating component (the inhomogeneous solution I), and a rapidly oscillating component (the homogeneous solution H). In order to approximate the slowly oscillating component, relatively large time steps can be used and no special properties of the ODE solver are required. However, in order to approximate the rapidly oscillating component, either small steps are required or one should use a method that has small phase errors with respect to homogeneous solution components and, in addition, to make large steps possible, a method with a substantial interval of periodicity. Therefore, since the homogeneous component is dominating in problem (5.2), we may expect that the PC and CR methods will perform much better than the conventional RKN method.

In Table 5.1 we have listed the accuracies produced by the various schemes; here, N denotes the number of steps performed in the integration interval [0,T]. The value of N is such that the results in each column required the same number of f-evaluations.

Table 5.1. cd-values for the first solution component of problem (5.2)

Method	N	cd	N	cd	N	cd
RKN44	1600	0.25	3200	1.03	6400	2.22
CR46	1600	2.09	3200	3.93	6400	5.74
PC46	1600	2.09	3200	3.93	6400	5.74
PC48	1200	3.22	2400	5.69	4800	8.12
PC412	800	5.30	1600	9.10		
PC424	400	1.53	800	10.22		
PC68	1600	2.55	3200	5.09	6400	7.56
PC610	1200	3.25	2400	6.52	4800	9.44

It may be concluded from this table that, for the linear problem (5.2), all methods show their phase lag order q rather than their algebraic order p (note that the CR46 method and the PC46 method yield identical results because of their identical characteristic polynomials). In general, the efficiency of the methods increases if the phase lag order increases, provided that the step is sufficiently small to make the higher orders effective.

5.2. Nonlinear inhomogeneous perturbation

Our second example is provided by

$$y''(t) + 100\, y(t) = \sin(y(t)), \qquad 0 \le t \le T, \qquad y(0) = 0, \quad y'(0) = 1. \tag{5.3}$$

Because of the nonlinear perturbation, the exact solution of this problem is not available; however, the solution is clearly oscillating. The endpoint of the integration interval was chosen at the thousandth zero and was found to occur at T=314.161229484... .

The results for various steps can be found in Table 5.2. For large steps it is the value of q that dictates the order behaviour, and, consequently, large q-values result in efficient schemes. However, when the step tends to zero, it is the algebraic order that determines the accuracy of the numerical solution and we can no longer benefit from a high order phase lag. Nevertheless, when compared with the RKN method, all schemes show a substantial gain in accuracy.

Table 5.2. cd-values for problem (5.3)

Method	N	cd	N	cd	N	cd
RKN44	4000	2.30	8000	1.67	16000	2.85
CR46	4000	2.71	8000	4.55	16000	6.38
PC46	4000	2.71	8000	4.55	16000	6.38
PC48	3000	3.83	6000	5.85	12000	7.13
PC412	2000	5.26	4000	5.51	8000	6.48
PC424	1000	1.14	2000	5.37	4000	5.51
PC68	4000	3.17	8000	5.71	16000	8.17
PC610	3000	3.87	6000	6.70	12000	8.79

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