Predictor–Corrector Methods for Periodic Second-Order Initial-Value Problems

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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.

1. Introduction

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

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

Relative to a linear test equation, one may distinguish papers which deal with reducing the phase lag (or phase error or dispersion) of the homogeneous solution component (e.g. [3, 8]) and which deal with reducing the phase lag of the inhomogeneous component (e.g. [1, 5, 10, 11]).

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 by Chawla & Rao [3]. Their method is explicit and has algebraic order 4 and phase-lag order 6. Moreover, since only three right-hand-side evaluations per step are involved, the interval of periodicity, which is given by $(0, 7·56)$ (in the sense of Lambert & Watson [9]), is relatively large.

Motivated by the result of Chawla & 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 [6], such methods were analysed for first-order equations; a straightforward modification of these methods make them applicable to second-order equations of the type (1.1) (see also [7]). 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-step and four-step methods are constructed, and in Section 5 we present numerical experiments.

2. Predictor–corrector methods

In [6] a generalization of conventional predictor–corrector methods for first-order ODEs has been proposed; for second-order ODEs such methods are of the form

$$
\left.
\begin{aligned}
& y_{n+1}^{(0)} \text{ is determined by an explicit linear multistep method } \{\bar{\rho}, \bar{\sigma}\}, \\
& y_{n+1}^{(j)} = \sum_{l=1}^{j} (\mu_{jl} y_{n+1}^{(l-1)} + \mu_{jl}' \tau^2 f_{n+1}^{(l-1)}) + \lambda_j \xi_n \quad (j = 1, \ldots, m), \\
& y_{n+1} = y_{n+1}^{(m)}, \qquad f_{n+1}^{(l-1)} := f(t_{n+1}, y_{n+1}^{(l-1)}),
\end{aligned}
\right\}
\quad (2.1a)
$$

where the parameters occurring in this scheme are to be prescribed. Here, $\tau := t_{n+1} - t_n$ is the stepsize, y_{n+1} approximates $y(t_{n+1})$, and ξ_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

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

where E is the forward shift operator ($E\phi_j = \phi_{j+1}$), with $\bar{a}_0$ and $\bar{b}_0$ denoting the coefficients of $z^{\bar{k}}$ in $\bar{\rho}(z)$ and $\bar{\sigma}(z)$. In the following we will assume that $\bar{a}_0 = 1$ and that $\{\bar{\rho}, \bar{\sigma}\}$ is zero-stable. Further, it will be assumed that the parameters of the method satisfy the compatibility conditions

$$
\sum_{l=1}^{j} \mu_{jl} = 1 - \lambda_j, \qquad \sum_{l=1}^{j} \mu_{jl}' = \bar{b}_0 \lambda_j \qquad (j = 1, \ldots, m). \qquad (2.1c)
$$

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

$$
P_0(z) = 1, \qquad P_j(z) = \sum_{l=1}^{j} (\mu_{jl} + \mu_{jl}' z) P_{l-1}(z) \quad (j = 1, \ldots, m). \qquad (2.2)
$$

Notice that $P_m(z)$ satisfies the condition $P_m(1/\bar{b}_0) = 1$.

Suppose that an appropriate iteration polynomial has been constructed (see Sections 3 and 4); then we are faced with the task of deriving 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 μ_{jj}'. Let $P_m(z)$ be given by

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

and set

$$
\mu_{j1} = \mu_j, \qquad \mu_{jj}' = \mu_j'.
$$

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

$$\mu_m = \beta_0, \qquad \mu_{m-j} = \frac{\beta_j}{\mu_m' \mu_{m-1}' \cdots \mu_{m-j+1}'} \qquad (j = 1, \ldots, m-1), \tag{2.1d}$$

$$\mu_1' \mu_2' \cdots \mu_m' = \beta_m.$$

In addition, we have the compatibility condition

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

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

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

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

Returning to the general scheme (2.1a)–(2.1c), the algebraic order of this method and its characteristic equation can be derived in a similar way as done in [6] for first-order equations (a detailed derivation can be found in [7]). The results are given by the Theorems 2.1 and 2.2.

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

THEOREM 2.2 *The characteristic polynomial equation of the predictor–corrector method (2.1), when applied to the test equation*

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

is given by

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

where $z_0 := -\tau^2\delta^2$, $\bar{k}$ is the number of steps of the predictor method, $\bar{l} := \max\{0, \bar{k} - \bar{k}\}$, and $\bar{l} := \max\{0, \bar{k} - \bar{k}\}$. □

The two principal roots of equation (2.3) correspond to the characteristic roots $\exp\{\pm i(-z_0)^{\frac{1}{2}}\}$ 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 $(-z_0)^{\frac{1}{2}} = v_0$. Let us assume that the principal roots of (2.3) are of the form

$$\zeta_\pm = a(v_0)e^{\pm i\theta(v_0)}, \qquad v_0, a, \theta \in \mathbb{R}_+. \tag{2.4}$$

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, 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*

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

and let the order conditions

$$\tilde{\phi}(v)e^{i\bar{l}v} - (1 + \bar{b}_0v^2)\bar{\phi}(v)e^{i\bar{l}v} \approx c_1v^{q_1}, \qquad C_\zeta(e^{iv}, -v^2) \approx c_3v^{q_3},$$
$$P_m(-v^2) - R(v) \approx c_2v^{q_2}, \qquad q_j > 0 \quad (j = 1, 2, 3) \tag{2.7}$$

be satisfied. If $P_m(0) \neq 1$ and $q_1 + q_2 - 2q_3 > 0$ 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_+. Since $C(\zeta_+, -v_0^2) = 0$, we deduce from (2.5) that ε_+ satisfies the equation

$$C(e^{iv_0} - \varepsilon_+, -v_0^2) = 0. \tag{2.8}$$

In order to find the behaviour of ε_+ as a function of v_0 as $v_0 \to 0$, we employ the Newton–Kantorovich theorem for the solution of nonlinear equations (see e.g. [4: Thm 5.3.1]). In the special case (2.8), where ε_+ satisfies a polynomial equation with complex coefficients, we use the Newton–Kantorovich theorem in the following form:

Let $\varepsilon_0 \in \mathbb{C}$ and let there exist constants β and η such that

$$|C_\varepsilon^{-1}(e^{iv_0} - \varepsilon_0, -v_0^2)| \leq \beta,$$
$$|C_\varepsilon^{-1}(e^{iv_0} - \varepsilon_0, -v_0^2)C(e^{iv_0} - \varepsilon_0, -v_0^2)| \leq \eta.$$

Define $\alpha := \beta\gamma\eta$, where γ denotes a Lipschitz constant for C_ε in the closure of the neighbourhood $N(\varepsilon_0, r) := \{\varepsilon \in \mathbb{C} : |\varepsilon - \varepsilon_0| < r\}$, and let

$$r_0 := [1 - (1 - 2\alpha)^{\frac{1}{2}}]/\beta\gamma.$$

If $\alpha \leq \frac{1}{2}$ and $r \geq r_0$, then there is a unique zero ε_+ of (2.8) in the neighbourhood $N(\varepsilon_0, r_0)$.

We apply this theorem with $\varepsilon_0 = 0$ and $r = 1$, and for a fixed value of v_0. From (2.7) it follows that $C_\varepsilon(e^{iv_0}, -v_0^2) = \hat{c}_3(v_0)v_0^{q_3}$, where $\hat{c}_3(v_0) \neq 0$ and is bounded in magnitude. Hence, $\beta = c_\beta v_0^{-q_3}$, where c_β is a bounded constant independent of v_0. In order to express η in terms of v_0, we first derive from (2.3) and (2.6) that

$$C(e^{iv_0}, -v_0^2) = \bar{\phi}(v_0)e^{i\bar{l}v_0} - \frac{(1 + \bar{b}_0v_0^2)P_m(-v_0^2)}{P_m(-v_0^2) - 1}\bar{\phi}(v_0)e^{i\bar{l}v_0};$$

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

$$C(e^{iv_0}, -v_0^2) = \frac{\bar{\phi}(v_0)e^{i\bar{l}v_0} - (1 + \bar{b}_0v_0^2)\tilde{\phi}(v_0)e^{i\bar{l}v_0}}{P_m(-v_0^2) - 1}O(v_0^{q_2}).$$

Since $P_m(0) \neq 1$, it follows from (2.7) that, for sufficiently small values of v_0, $C(e^{iv_0}, -v_0^2) = \hat{c}_0(v_0)v_0^{q_1+q_2}$, where $\hat{c}_0(v_0)$ is bounded in magnitude. Hence, $\eta = c_\eta v_0^{q_1+q_2-q_3}$, where c_η is a bounded constant. Finally, since C_ε is a polynomial in ε, we can always choose the Lipschitz constant γ independent of v_0 in the neighbourhood $N(\varepsilon_0, r) = N(0, 1)$, so that $\alpha = \gamma c_\beta c_\eta v_0^{q_1+q_2-2q_3}$ and

$$r_0 = \frac{1 - (1 - 2\gamma c_\beta c_\eta v_0^{q_1+q_2-2q_3})^{\frac{1}{2}}}{\gamma c_\beta v_0^{-q_3}}.$$

For sufficiently small values of v_0 we achieve that $\alpha \leq \frac{1}{2}$ and $r \geq r_0 \approx c_\eta v_0^{q_1+q_2-q_3}$, so that the Newton–Kantorovich theorem yields $\varepsilon_+ \in N(\varepsilon_0, r_0)$, i.e. $\varepsilon_+ = O(v_0^{q_1+q_2-q_3})$. $\square$

As a corollary of the above theorem, we will derive a lower bound for q in the special case where both the predictor and the corrector are *symmetric* methods (for a definition of symmetry, see Section 3) and have equal stepnumber (i.e. $\bar{k} = \vec{k}$). Then it is easily shown that $R(v)$ is an even function in v. Obviously, the polynomial $P_m(-v^2)$ is also an even function in v. Now, we will identify the first m free coefficients in the iteration polynomial P_m with the corresponding coefficients in the Taylor expansion of R (recall that $R(v)$ differs from the polynomial $P_m(-v^2)$ by a term of order $q_2 > 0$, so that $R(v)$ possesses a Taylor expansion around $v = 0$), whereas the last coefficient (i.e. the one in front of v^{2m}) will be employed to satisfy the compatibility condition $P_m(1/\bar{b}_0) = 1$. As R itself satisfies the compatibility condition (cf. (2.6)), $P_m(-v^2) - R(v)$ behaves as $O(v^{2m})$. Therefore, we can always achieve that $q_2 = 2m$ in (2.7). Further, by the definition of order, we have $\bar{\phi}(v) = O(v^{\bar{p}+2})$ and $\vec{\phi}(v) = O(v^{\vec{p}+2})$, resulting in $q_1 \geq \min\{\bar{p}, \vec{p}\} + 2$. Combining these results, we are led to the following corollary of Theorem 2.3.

COROLLARY 2.1   *Let the order conditions of Theorem 2.3 be satisfied. Further, let the predictor and corrector be symmetric with $\bar{k} = \vec{k}$. Then, the order q in the error equation* (2.5) *satisfies*

$$q \geq \min\{\bar{p}, \vec{p}\} + 2m + 1 - q_3. \quad \square$$

We remark that, for asymmetric methods (i.e. with R not an even function), q will be considerably smaller.

Apart from a high (phase-lag) order q, the concept of *dissipation* is an important aspect when integrating oscillatory problems. Therefore, we shall only be interested in methods with a nonempty interval of zero-dissipation (see also [9] and Section 3). As symmetry is a necessary condition to obtain a nonempty interval of zero-dissipation, we will confine ourselves to symmetric methods.

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

$$\left| \frac{\theta(v_0) - v_0}{v_0} \right| = c_q v_0^q + O(v_0^{q+1}).$$

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*

$$R(v) \approx c_4 v^{q_4}, \qquad \bar{\phi}(v) \approx c_5 v^{\bar{p}+2}, \qquad P_m(0) \neq 1. \tag{2.9}$$

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

$$c_q = \left| \frac{c_2 c_5}{c_3 (P_m(0) - 1) c_4} \right|, \qquad q = \bar{p} + q_2 + 1 - q_3 - q_4,$$

with $q_4 \leqslant \bar{p} - \min\{\bar{p}, \bar{p}\}$. □

Proof. It follows from (2.8), (2.7), and (2.9), and from the identity

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

that

$$\varepsilon_{\pm} \approx \frac{c_5 v_0^{\bar{p}+2} c_2 v_0^{q_2}}{c_4 v_0^{q_4} [P_m(0) - 1] c_3 v_0^{q_3}}.$$

From this expression and the zero-dissipativity, the assertion of the corollary follows. □

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

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

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

We shall combine this corrector with a symmetric predictor formula:

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

(cf. [9]). Since the corrector (3.1) is also symmetric, it follows that the resulting predictor-corrector method itself is symmetric, and, as the principal roots of $\bar{\rho}$ are the only double roots on the unit circle, a nonempty interval of periodicity is obtained [9]. 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. Finally, in order to have an algebraic order at least equal to that of the corrector, we should have $r \geqslant \tfrac{1}{2}(\bar{p} - \bar{p})$ (cf. Theorem 2.1); consequently, we will use $m \geqslant \tfrac{1}{2}(\bar{p} - \bar{p})$.

3.1 Zero-Order Predictor

Let

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

then

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

$$\bar{\phi}(v) = (e^{iv} - 1)^2 + \tfrac{1}{12}v^2(e^{2iv} + 10e^{iv} + 1)$$

$$= 2e^{iv}[(1 + \tfrac{1}{12}v^2)\cos v - 1 + \tfrac{5}{12}v^2] \approx \tfrac{1}{240}v^6 e^{iv} \approx \tfrac{1}{240}v^6,$$

so that

$$R(v) = \frac{-2}{v^2}[1 - \tfrac{5}{12}v^2 - (1 + \tfrac{1}{12}v^2)\cos v]$$

$$= v^4 \sum_{j=2}^{\infty} \left(\frac{1}{6(2j)!} - \frac{2}{(2j+2)!}\right)(-v^2)^{j-2} \approx \tfrac{1}{240}v^4.$$

We now define the iteration polynomial $(m > 1)$

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

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

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

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* $c_q = 1/(2m + 2)!$. $\square$

Proof. Since $\bar{p} = 4$, $\tilde{p} = 0$, and $r = 2$, Theorem 2.1 states that $p \geqslant 4$. A closer inspection of the local truncation error yields $p = 4$ (cf. [7]). Since $q_2 = 2m$, $q_3 = 1$, and $q_4 = 4$, it follows from Corollary 2.2 that $q = 2m$. Further, since $P_m(0) = 0$ and

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

the principal phase-lag constant is given by

$$c_{2m} = \left|\frac{\tfrac{1}{240}c_2}{2i \cdot \tfrac{1}{240}}\right| = \frac{1}{(2m+2)!}. \quad \square$$

3.2 *Second-Order Predictor*

Let

$$\bar{p}(\zeta) = (\zeta - 1)^2, \qquad \bar{\sigma}(\zeta) = \zeta; \tag{3.4}$$

then

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

so that

$$R(v) = \frac{24}{v^4}[1 - \tfrac{5}{12}v^2 - (1 + \tfrac{1}{12}v^2)\cos v]$$

$$= -12v^2 \sum_{j=2}^{\infty} \left(\frac{1}{6(2j)!} - \frac{2}{(2j+2)!}\right)(-v^2)^{j-2} \approx -\tfrac{1}{20}v^2.$$

We define the iteration polynomial

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

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

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

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

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

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

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

This equation has its roots on the unit circle, which are distinct and complex conjugate, if

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

Remembering that all relevant values of z are real and nonpositive, the interval $0 < -z < H_0^2$ where (3.6) is satisfied is called the interval of periodicity [9].

Since $P_m(z)$ is a Taylor approximation to the function $R((-z)^{\frac{1}{2}})$, and since $R((-z)^{\frac{1}{2}})$ 'touches' the functions $12/z$ and $8(6+z)/z^2$, respectively at the points

$$z_j = -j^2\pi^2 \quad \text{and} \quad z_{j-1} = -(j-1)^2\pi^2 \qquad (j = 2, 4, \ldots), \qquad (3.6')$$

the periodicity condition is easily violated in the neighbourhood of the ₚoints z_l ($l = 1, 2, \ldots$). To check (3.6), we determined numerically the negative real roots of $P_m(z) - 12/z$ and of $P_m(z) - 8(6 + z)/z^2$ for $m = 2, \ldots, 11$. For these m-values, we found that condition (3.6) is violated in neighbourhoods of the 'critical' points (3.6'). The values of these zeros and of the resulting H_0^2-values are given in Table 1. However, for some m-values we have nearly a 'double' zero close to the points (3.6'); or, in other words, one characteristic root ζ assumes values slightly outside the unit circle on these (small) z-intervals. In the right-most column of Table 1, we list the maximal value of $|\zeta|$, assumed on these intervals. Strictly speaking, the scheme is unstable for these z-values and loses its property of zero-dissipation. Thus, if the natural frequencies δ are such that $z_0 := -\tau^2 \delta^2$ lies in these intervals, then there are two consequences.

Firstly, on every step, rounding errors will be amplified by $|\zeta|_{max}$. In actual computation, it is unlikely that this behaviour of $|\zeta(z)|$ will cause instabilities, so that the practical stability limit is determined for each m by the root of largest modulus as listed in Table 1.

The second consequence is that the amplitude of the oscillatory solution will be amplified. Hence, if a strict zero-dissipative behaviour is required, then one should either choose the safe periodicity limit determined by the root of smallest

TABLE 1
Intervals of periodicity $(0, H_0^2)$

| m | Negative real roots of | | H_0^2 | $\|\zeta\|_{max}$ |
	$P_m(z) - 12/z$	$P_m(z) - 8(6 + z)/z^2$		
2	—	$-7\cdot571916$	$7\cdot57$	—
3	$-21\cdot481210$	—	$21\cdot48$	—
4	—	$-9\cdot530082$	$9\cdot53$	$1\cdot0628$
		$-10\cdot306708$		
5	$-30\cdot721458$	$-31\cdot702780$	$30\cdot72$	—
		$-9\cdot851604$		
6	—	$-9\cdot887888$	$9\cdot85$	$1\cdot00289$
		$-50\cdot348639$		
	$-37\cdot075118$			
7	$-46\cdot589878$	—	$37\cdot08$	$1\cdot321$
	$-53\cdot315233$			
		$-9\cdot869077$		
8	—	$-9\cdot870132$	$9\cdot87$	$1\cdot0000840$
		$-67\cdot143093$		
	$-39\cdot182936$			
9	$-39\cdot801579$	—	$39\cdot18$	$1\cdot0249$
	$-88\cdot524508$			
		$-9\cdot869594$		
10	—	$-9\cdot869614$	$9\cdot87$	$1\cdot00000165$
		$-80\cdot367079$		
	$-39\cdot457971$			
11	$-39\cdot499007$	—	$39\cdot46$	$1\cdot00163$
	$-114\cdot724020$			

modulus or one should adapt the stepsize τ such that $-\tau^2\delta^2$ moves away from the critical points.

Finally, for reasons of comparison, we remark that the interval of periodicity of the corrector itself is given by $(0, 6)$.

3.2.2 A Two-Stage Method

Let $m = 2$, then (3.5) gives

$$P_2(z) = \tfrac{1}{20}z + \tfrac{1}{360}z^2. \tag{3.5'}$$

Solving all the relations (2.1) leads to the scheme

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

This scheme is of algebraic order $p = 4$ and has phase-lag order $q = 6$; the principal error constant c_6 is $1/40320$ and the periodicity interval is $(0, 7\cdot57)$. 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 all the relations (2.1) leads to the scheme

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

This scheme is of algebraic order $p = 4$ and has phase-lag order $q = 8$; the principal error constant c_8 is $1/3628800$, and the periodicity interval is $(0, 21\cdot48)$. 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 [9: method V with $a = 0$]

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

In this section, we restrict our discussion to methods using the fourth-order predictor [9: method IV with $a = 0$]

$$\bar{\rho}(\zeta) = (\zeta - 1)^2(\zeta^2 + 1), \qquad \bar{\sigma}(\zeta) = \tfrac{1}{6}(7\zeta^3 - 2\zeta^2 + 7\zeta). \tag{4.2}$$

The functions $\vec{\phi}$ and $\vec{\phi}$ respectively corresponding to (4.1) and (4.2), are given by

$$
\begin{aligned}
&\vec{\phi}(v) = 2e^{2iv}[1 + \tfrac{7}{120}v^2 - (2 - \tfrac{13}{15}v^2)\cos v + (1 + \tfrac{3}{40}v^2)\cos 2v], \\
&\vec{\phi}(v) = 2e^{2iv}[1 - \tfrac{1}{6}v^2 - (2 - \tfrac{7}{6}v^2)\cos v + \cos 2v].
\end{aligned}
$$

TABLE 2
Coefficients A_j and B_j

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

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

$$R(v) = \tfrac{16}{3}z\left(\sum_{j=4}^{\infty} A_j z^{j-4}\right)\left(\sum_{j=2}^{\infty} B_j z^{j-2}\right)^{-1} \approx \tfrac{16}{3}\frac{A_4}{B_2}z,$$

where

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

We now define

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

with

$$\beta_0 = 0, \qquad \beta_j = \left(\tfrac{16}{3}A_{3+j} - \sum_{i=0}^{j-1} \beta_i B_{2+j-i}\right)\bigg/ B_2 \qquad (j = 1, \ldots, m - 1) \qquad (4.3c)$$

and with β_m such that $P_m(\tfrac{40}{3}) = 1$. The first few coefficients A_j and B_j are given in Table 2.

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*

In the case of this quartic characteristic equation, we determined numerically the length of the periodicity interval, using an extremely fine mesh on the z-axis. The values of H_0^2 are given in Table 3.

However, similar to the situation encountered with the two-step methods, we again found some values of $-z$, within the interval $(0, H_0^2)$, for which two roots

TABLE 3
Intervals of near-periodicity $(0, H_0^2)$

m	2	3	4	5	6	7	8	9	10	11
H_0^2	7·17	12·93	15·57	15·30	15·60	15·81	15·99	16·13	16·26	16·36
$|\zeta|_{max} - 1$	0	$·53_{10} - 2$	$·31_{10} - 9$	$·20_{10} - 3$	$·59_{10} - 4$	$·19_{10} - 4$	$·63_{10} - 5$	$·21_{10} - 5$	$·11_{10} - 6$	$·16_{10} - 6$

$\zeta(z)$ of the characteristic equation were slightly larger than one in modulus. For $m = 3$, these z-values were situated in the interval $(-2\cdot58, -2\cdot51)$ and, for all $m \geq 4$, these points are in a close neighbourhood of $z = -2\cdot544$. The maximum values of $|\zeta| - 1$ assumed on these intervals, are given in Table 3. For a discussion of the consequences of this behaviour of $|\zeta|$ we refer to Section 3.2.1.

We mention that the characteristic equation of this four-step method is of the form

$$\zeta^4 + C_1(z_0)\zeta^3 + C_2(z_0)\zeta^2 + C_1(z_0)\zeta + 1 = 0,$$

which can be written as

$$[\zeta^2 + D_1(z_0)\zeta + a(z_0)][\zeta^2 + D_2(z_0)\zeta + a^{-1}(z_0)] = 0,$$

where one factor determines the principal roots and the other factor determines the spurious roots.

As long as we are in the interval of periodicity (i.e. $-z_0 \in (0, H_0^2)$), we have $a(z_0) \equiv 1$ and $|D_i(z_0)| < 2$ ($i = 1, 2$). Consequently, both principal and spurious roots are *on* the unit circle and both form a complex conjugate pair. It should be observed, however, that only the phase of the principal roots approximates the phase of the true solution. Now, if $-z_0$ becomes larger than H_0^2, we have $a(z_0) \neq 1$, resulting in one pair of roots moving outside the unit circle, while the other pair moves inwards, where the members of each pair still are complex conjugate. (We remark that, if the roots have nonzero imaginary parts, then, if one root leaves the unit circle, they all have to leave, because, if ζ is a root, then $\bar{\zeta}$, $1/\zeta$, and $1/\bar{\zeta}$ are also roots.)

It is of interest to observe that (i) the value of m has only a slight influence on the value of H_0^2 and (ii) the sixth-order methods possess a considerably smaller interval of periodicity than the fourth-order methods.

Finally, we mention that the corrector formula (4.1), when iterated to convergence, possesses the periodicity interval $(0, \frac{60}{11})$.

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 all the relations (2.1), the scheme takes the form

$$\left.\begin{array}{l}
\xi_n = 2y_n - 2y_{n-1} + 2y_{n-2} - y_{n-3} + \frac{1}{120}\tau^2(104f_n + 14f_{n-1} + 104f_{n-2} + 9f_{n-3}), \\[2mm]
y_{n+1}^{(0)} = 2y_n - 2y_{n-1} + 2y_{n-2} - y_{n-3} + \frac{1}{6}\tau^2(7f_n - 2f_{n-1} + 7f_{n-2}), \\[2mm]
y_{n+1}^{(1)} = \frac{1}{1701}(950y_{n+1}^{(0)} + 751\xi_n) + \frac{751}{22680}\tau^2 f_{n+1}^{(0)}, \\[2mm]
y_{n+1} = \xi_n + \frac{3}{40}\tau^2 f_{n+1}^{(1)}.
\end{array}\right\} \tag{4.5}$$

This scheme has algebraic order $p = 6$, phase lag order $q = 8$, and periodicity interval $(0, 7\cdot17)$; it requires three f-evaluations per step.

4.3 A Three-Stage Method

For $m = 3$ we have the iteration polynomial

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

and the corresponding scheme reads

$$\xi_n = 2y_n - 2y_{n-1} + 2y_{n-2} - y_{n-3} + \tfrac{1}{120}\tau^2(104f_n + 14f_{n-1} + 104f_{n-2} + 9f_{n-3}),$$

$$y_{n+1}^{(0)} = 2y_n - 2y_{n-1} + 2y_{n-2} - y_{n-3} + \tfrac{1}{6}\tau^2(7f_n - 2f_{n-1} + 7f_{n-2}),$$

$$y_{n+1}^{(1)} = \frac{1}{6759}(5230y_{n+1}^{(0)} + 1529\xi_n) + \frac{1529}{90120}\tau^2 f_{n+1}^{(0)},\qquad\qquad (4.7)$$

$$y_{n+1}^{(2)} = \frac{1}{1701}(950y_{n+1}^{(0)} + 751\xi_n) + \frac{751}{22680}\tau^2 f_{n+1}^{(1)},$$

$$y_{n+1} = \xi_n + \tfrac{3}{40}\tau^2 f_{n+1}^{(2)}.$$

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 will place emphasis on the phase errors in the numerical solution. To measure the global phase lag we define

$$a_{\mathrm{cd}} := -\log_{10}|\text{the numerical solution at } t = T|,\qquad\qquad (5.1)$$

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

We will test the PC methods defined in 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.

For reasons of comparison, we also applied two other explicit methods. Firstly, we selected the celebrated fourth-order Runge–Kutta–Nyström method, because it is a widely used method for solving second-order differential equations. Note however, that this method has an empty interval of periodicity.

Secondly, we implemented the fourth-order method of Chawla & Rao [3] already mentioned in the introduction. This method is designed for the same class of problems as the PC methods are; it possesses a relatively large periodicity interval and is quite efficient. Both methods require three right-hand-side evaluations per step.

In the subsequent experiments, these methods are referred to as RKN44 and CR46, respectively.

5.1 Linear Inhomogeneous Perturbation

As a first example we consider the linear equation

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

By specifying the initial conditions $y(0) = [0, 1]^\mathsf{T}$ and $y'(0) = [16, 5]^\mathsf{T}$, we have the solution

$$y(t) = \begin{bmatrix} \sin t \\ \cos t \end{bmatrix} + \begin{bmatrix} \sin 5t + \sin 10t \\ -\sin 5t + \sin 10t \end{bmatrix} =: i(t) + h(t). \quad (5.2b)$$

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 possessing a substantial interval of periodicity. Therefore, since the homogeneous component is the more difficult part in the solution of problem (5.2), we may expect that the PC and CR methods will perform much better than the conventional RKN method.

In Table 4 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.

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

TABLE 4

The a_{cd}-values for the first solution component of problem (5.2) *at*
$T = 40\pi$

Method	N	a_{cd}	N	a_{cd}	N	a_{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

TABLE 5
a_{cd}-values for problem (5.3)

Method	N	a_{cd}	N	a_{cd}	N	a_{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

increases if the phase-lag order increases, provided that the step is sufficiently small to make the higher orders effective (cf. PC424 with $N = 400$).

5.2 Nonlinear Inhomogeneous Perturbation

Our second example is provided by

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

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 $T = 314\cdot161229484 \ldots$.

The results for various steps can be found in Table 5. For large steps, it is the value of q that dictates the order behaviour, and, consequently, large q-values result in efficient schemes. Note, however, that the step should be small enough to present the solution adequately; for example, in the first experiment with the PC424 method, the stepsize $\tau \approx \frac{1}{10}\pi$ is obviously too large for representing a solution which has a period of approximately $\frac{1}{5}\pi$.

On the other hand, when the stepsize decreases, it is the algebraic order that mainly determines the accuracy of the numerical solution. This is most clearly illustrated by the results furnished by the methods PC412 and PC424: for the same stepsize $\tau = T/4000$, equal accuracies are obtained, irrespective of their different phase-lag orders. Obviously, for these extreme q-values, it is the algebraic order that completely determines the error.

Although less obviously so, it is also true that, for more realistic q-values (i.e., $q - p < 5$, say), the influence of the algebraic order becomes more significant as the stepsize tends to zero.

Therefore, in general, we cannot fully benefit from a high phase-lag order when integrating nonmodel problems with very small stepsizes.

Nevertheless, when compared with the RKN44 method, all schemes show a substantial gain in efficiency (higher accuracy at the same costs).

Acknowledgements

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