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PREDICTOR-CORRECTOR METHODS WITH IMPROVED ABSOLUTE STABILITY REGIONS

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Predictor-corrector methods with improved absolute stability regions *)

by

P.J. van der Houwen & B.P. Sommeijer

ABSTRACT

Generalized predictor-corrector methods are studied with extended region of absolute stability. Choosing an extrapolation-predictor and a backward-differentiation-corrector methods are constructed of orders up to 6, the real stability boundaries of which are of magnitude m^2, where m is the number of right-hand side evaluations per integration step. The coefficients of the method can be generated during the computation for arbitrary values of m. The storage requirements are limited and independent of m. The method is particularly suited for the integration of semi-discrete parabolic differential equations in more space dimensions.

KEY WORDS & PHRASES: *predictor-corrector methods; parabolic diffential equations; stability*

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*) This report will be submitted for publication elsewhere.

1. INTRODUCTION

The conventional predictor-corrector methods for solving the initial-value problem

$$(1.1) \qquad \frac{d^\nu y}{dt^\nu} = f(t,y), \ \frac{d^i y}{dt^i}(t_0) \qquad \text{prescribed for } i = 0,1,\ldots,\nu-1;\ \nu \geq 1$$

have rather restricted regions of stability (cf. [7, 10]). In order to improve the region of absolute stability, Stetter [11] proposed a generalization of these methods and showed by a few examples for first order equations ($\nu=1$) that the stability region can be extended considerably. These generalized methods fit into a still more general framework of "hybrid" explicit multistep methods introduced by Gear [3] and by Butcher [1]. Within this class of methods, Verwer [12] studied a family of m-stage three-step Runge-Kutta methods of orders p = 1 and 2 with a real stability boundary $\beta = c_p m^2$, where c_p is slowly varying with m. For these methods Verwer found values $c_1 \cong 5.15$ and $c_2 \cong 2.29$. The code based on this family is rather robust in practice and particularly suited for the integration of semi-discrete parabolic problems in more space dimensions [13]. However, for large values of m ($m \geq 12$) the method becomes unstable because of the development of internal instabilities. As a consequence, the m^2 behaviour of β cannot fully be expoited. In order to overcome this difficulty the present authors [5] derived m-stage (one-step) Runge-Kutta methods of order $p=2$ with stability boundary $\beta \cong 0.66\ m^2$ which are internally stable for arbitrary high m. This derivation is based on recursions of Chebyshev type. Verwer [14] followed this approach and constructed first and second order, three-step methods with $c_1 \cong 5.17$ and $c_2 \cong 2.32$ which also remain stable for arbitrarily large values of m. A further extension to k-step methods with k arbitrary was given in [6].

The order of accuracy of the multistage methods mentioned above does not exceed p=2. In this paper, a family of higher order predictor-corrector type methods with enlarged stability interval is constructed. The local error analysis (section 3) and the (linear)stability analysis (section 4) are given for (1.1) with ν arbitrary. In section 5 implementational details are given.

The general theory is applied to an extrapolation-predictor and backward-differentiation-corrector pair for fist-order systems of differential equations (section 6). Examples are given of methods up to order 6 with $\beta = c_p m^2$, where $c_2 \cong 1.37$, $c_3 \cong 1.01$, $c_4 \cong 0.73$, $c_5 \cong 0.54$ and $c_6 \cong 0.37$. The methods have restricted storage requirements and are internally stable for all m. By means of numerical experiments it is shown that the higher order methods are more efficient than the lower order ones even in the range of low accuracies. The paper is concluded with an application to second-order differential equations (section 7).

2. PRELIMINARIES

Consider a linear k-step method for the numerical solution of the initial-value problem (1.1), then the numerical approximation to $y(t_{n+1})$ is the solution of the equation

$$y - b_0^* \tau^\nu f(t_{n+1},y) = \Sigma_n, \qquad b_0^* > 0, \tag{2.1a}$$

where τ denotes the integration step $t_{n+1} - t_n$ and Σ_n is a sum of known terms, i.e.

$$\Sigma_n = \sum_{\ell=1}^{k} [a_\ell^* y_{n+1-\ell} + b_\ell^* \tau^\nu f(t_{n+1-\ell},y_{n+1-\ell})] \tag{2.1b}$$

with $y_{n+1-\ell}$ denoting the numerical solution at $t_{n+1-\ell}$. The exact solution of (2.1a) will be denoted by η.

In order to solve (2.1a) we consider the following m-point iteration method

$$y_{n+1}^{(0)} = \text{some initial approximation to } \eta,$$

$$y_{n+1}^{(j)} = \sum_{\ell=1}^{m} [\mu_{j\ell} y_{n+1}^{(\ell-1)} + \bar{\mu}_{j\ell} \tau^\nu f(t_{n+1},y_{n+1}^{(\ell-1)})] + \lambda_j \Sigma_n, \qquad j = 1,2,\ldots,m, \tag{2.2}$$

$$y_{n+1} = y_{n+1}^{(m)},$$

where

$$\sum_{\ell=1}^{m} \mu_{j\ell} = 1 - \lambda_j, \quad \sum_{\ell=1}^{m} \bar{\mu}_{j\ell} = b_0 \lambda_j, \quad j = 1,2,\ldots,m$$

(2.3)

$$\mu_{j\ell} = \bar{\mu}_{j\ell} = 0, \quad \ell = j+1,\ldots,m.$$

This scheme is a special case of the general "hybrid" explicit multistep method introduced by Butcher [1] (see also Gear [3] and Stetter [11]). From (2.3) it follows that the iteration method (2.2) is (i) consistent with equation (2.1a) and ii) self-starting provided that $y_{n+1}^{(0)}$ is given by some predictor formula.

The result after m iterations is accepted as the numerical approximation y_{n+1} to $y(t_{n+1})$.

In the analysis of the method (2.2) we will need the polynomials $P_j(z)$ defined by the recurrence relation

$$P_0(z) = 1, \quad P_j(z) = \sum_{\ell=1}^{m} [\mu_{j\ell} + \bar{\mu}_{j\ell} z] P_{\ell-1}(z), \quad j = 1,2,\ldots,m. \tag{2.4}$$

Evidently, $P_j(z)$ is a polynomial of degree $\leq j$ in z. Furthermore, by virtue of (2.3) we have

$$P_j(1/b_0^*) = 1, \quad j = 0,1,\ldots,m. \tag{2.5}$$

These polynomials will be called the *iteration polynomials*.

In addition to the polynomials $P_j(z)$ we define the first and second characteristic polynomials of the *corrector formula* (2.1) by

$$\rho^*(\zeta) = -\sum_{\ell=0}^{k} a_\ell^* \zeta^{k-\ell}, \quad \sigma^*(\zeta) = \sum_{\ell=0}^{k} b_\ell^* \zeta^{k-\ell}, \tag{2.6}$$

where $a_0^* = -1$. Furthermore, it will be assumed that $y_{n+1}^{(0)}$ is obtained by a linear multistep method with characteristic polynomials $\tilde{\rho}(\zeta)$ and $\tilde{\sigma}(\zeta)$ where $\tilde{a}_0 = -1$ and $\tilde{b}_0 = 0$. The orders of accuracy of the predictor formula $\{\tilde{\rho}, \tilde{\sigma}\}$ and the corrector formula $\{\rho^*, \sigma^*\}$ are denoted by $\tilde{p}$ and p^*, respectively. The order of the resulting predictor-corrector method (2.2) is denoted by p.

The method (2.2) contains a number of well-known integration formulas as special cases. In order to characterize these cases it is convenient to introduce the m×m triangular matrices

$$M = (\mu_{j\ell}),\ \bar{M} = (\bar{\mu}_{j\ell}),\ j,\ell = 1,2,\ldots,m. \tag{2.7}$$

Suppose that the predictor $\{\tilde{\rho}, \tilde{\sigma}\}$ and the generating method (2.1) are given and let

$$M = 0,\quad \bar{M} = b_0^* I. \tag{2.8}$$

Then the scheme (2.5) reduces to a predictor-corrector (PC) method in $P(EC)^m E$ mode. The iteration polynomials are given by $P_j(z) = (b_0^* z)^j$ for all j. As a second example, let

$$M = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \\ \mu_1 & \cdots & \mu_m \end{pmatrix},\quad \bar{M} = \begin{pmatrix} b_0^* & & \bigcirc \\ & \ddots & \\ \bigcirc & & b_0^* \end{pmatrix} \tag{2.9}$$

Then the scheme (2.5) becomes the $P(EC)^{m-1}LE$ method of Stetter [11] with the iteration polynomials $P_j(z)=(b_0^* z)^j$, $j=0,1,\ldots,m-1$ and $P_m(z)=\sum_{j=1}^m \mu_j (b_0^* z)^{j-1}$. However, for semi-discrete parabolic equations this scheme is internally unstable unless m is restricted to small values. Such a restriction of m will limit the stability boundary and therefore we study alternative predictor-corrector schemes of the type (2.2) with limited storage requirements whatever the value of m is. Firstly however, the local error and the absolute stability of the general scheme (2.2) will be considered.

3. THE LOCAL ERROR

Suppose that until t_n the integration process has been exact, i.e. $y_i = y(t_i)$, $i \le n$ (localizing assumption [7]). Furthermore, let us define the iteration error

$$\varepsilon_j = y_{n+1}^{(j)} - \eta. \tag{3.1}$$

Then the local error is given bij

$$y_{n+1} - y(t_{n+1}) = [\eta - y(t_{n+1})] + \varepsilon_m, \tag{3.2}$$

that is the sum of the local error of the linear k-step method (2.1) and the final iteration error. From the theory of linear multistep methods (see e.g. [7]) we may derive estimates for the local error $\eta - y(t_{n+1})$. Here, we consider the iteration error

THEOREM 3.1 *Let* $f(t,y)$ *be differentiable with respect to* y *then*

$$\varepsilon_j = P_j(Z)\varepsilon_o + O(\tau^{2s+\nu}) \text{ as } \tau \to 0,$$

where

$$Z = \tau^{\nu} \frac{\partial f}{\partial y}(t_{n+1},\eta), \quad s \geq \nu + \min\{p^*,\tilde{p}\} \qquad \square$$

PROOF. Substitution of $y_{n+1}^{(j)} = \eta + \varepsilon_j$ into (2.2) and using (2.3) yields

$$\begin{aligned} \varepsilon_j &= \sum_{\ell=1}^{m} [\mu_{j\ell}\varepsilon_{\ell-1} + \tau^{\nu} \bar{\mu}_{j\ell}(f(t_{n+1},\eta+\varepsilon_{\ell-1}) - f(t_{n+1},\eta))] \\ &= \sum_{\ell=1}^{m} \{[\mu_{j\ell} + \bar{\mu}_{j\ell}\tau^{\nu} \frac{\partial f}{\partial y}(t_{n+1},\eta)]\varepsilon_{\ell-1} + \tau^{\nu} O(\|\varepsilon_{\ell-1}\|^2)\} \\ &= \sum_{\ell=1}^{m} \{[\mu_{j\ell} + \bar{\mu}_{j\ell}Z]\varepsilon_{\ell-1} + \tau^{\nu} \bar{\mu}_{j\ell} O(\|\varepsilon_{\ell-1}\|^2)\}. \end{aligned} \tag{3.3}$$

Let us assume that $\|\varepsilon_j\| = O(\tau^s)$ as $\tau \to 0$ for $j = 0,1,\ldots,m$ and write

$$\varepsilon_j = P_j(Z)\varepsilon_0 + c_j\tau^{2s+\nu}, \tag{3.4}$$

where P_j is the polynomial defined by (2.4). The representation (3.4) for the iteration error is correct if the c_j satisfy the relation (substitute (3.4) into (3.3))

$$c_j = \sum_{\ell=1}^{m} \{[\mu_{j\ell} + \bar{\mu}_{j\ell}Z]c_{\ell-1} + O(1)\} \text{ as } \tau \to 0$$

with $c_0 = 0$. For finite j the c_j will be bounded as $\tau \to 0$ so that

$$\varepsilon_j = P_j(Z)\varepsilon_0 + O(\tau^{2s+\nu}) \text{ as } \tau \to 0,\ j \geq 1. \tag{3.4'}$$

By observing that

$$\varepsilon_0 = y_{n+1}^{(0)} - \eta = y_{n+1}^{(0)} - y(t_{n+1}) + y(t_{n+1}) - \eta = O(\tau^{\tilde{p}+\nu} + \tau^{p^*+\nu}),$$

we deduce from (3.4') that all ε_j are at least of $O(\tau^{\tilde{p}+\nu} + \tau^{p^*+\nu})$ as $\tau \to 0$. Thus $s \geq \nu + \min\{\tilde{p}, p^*\}$ which proves the theorem. □

From this theorem the following corollary is immediate.

COROLLARY 3.1 The local error of $y^{(j)}$ in (2.2) is given by

$$y_{n+1}^{(j)} - y(t_{n+1}) = [I - P_j(Z)](\eta - y(t_{n+1})) + P_j(Z)(y_{n+1}^{(0)} - y(t_{n+1})) + O(\tau^{2s+\nu}) \text{ as } \tau \to 0, \tag{3.5}$$

where $s \geq \nu + \min\{p^*, \tilde{p}\}$ □

We now state the main results of this section.

THEOREM 3.2 *Let the iteration polynomial $P_m(z)$ has a zero of multiplicity r at $z = 0$. Then the method (2.2) has the order*

$$p = \min\{p^*, \tilde{p}+\nu r, 2s\},\ s \geq \nu + \tilde{p}. \quad \square$$

PROOF. From the definition of the matrix Z it follows that

$$Z = O(\tau^{\nu}) \text{ as } \tau \to 0.$$

Hence,

$$P_m(Z) = O(\tau^{\nu r}) \text{ as } \tau \to 0,$$

where r is the multiplicity of the zero $z=0$ of $P_m(z)$. Using corollary 3.1, we obtain for $\tau \to 0$

$$y_{n+1}^{(m)} - y(t_{n+1}) = y_{n+1} - y(t_{n+1}) = O(\tau^{p^*+\nu} + \tau^{\nu r+\tilde{p}+\nu} + \tau^{2s+\nu}).$$

From this expression the theorem is immediate □

It should be remarked that in the case of the conventional predictor-corrector methods where $\mu_{j\ell} = 0$ and $\bar{\mu}_{j\ell} = b_0^*$ the iteration error satisfies $\|\varepsilon_j\| \le L\tau^{\nu}\|\varepsilon_{j-1}\|$, where L is a Lipschitz constant for f; consequently $\varepsilon_m = O(\tau^{\nu m}\|\varepsilon_0\|) = O(\tau^{\tilde{p}+\nu+\nu m})$ so that we obtain the familiar result $p = \min\{p^*, \tilde{p}+\nu m\}$.

The polynomial $P_j(z)$ will be called of *order r* if $z=0$ is a zero of multiplicity r.

4. STABILITY

4.1 The characteristic equation

Applying the method (2.2) to the stability test equation

$$\frac{d^{\nu}y}{dt^{\nu}} = \delta y, \quad \delta \in \mathbb{C} \tag{4.1}$$

we obtain the relations

$$y_{n+1}^{(j)} = \sum_{\ell=1}^{m} [\mu_{j\ell} + \bar{\mu}_{j\ell} z] y_{n+1}^{(\ell-1)} + \lambda_j \Sigma_n, \quad j = 1,\ldots,m, \tag{4.2}$$

where we have written $z = \tau^{\nu}\delta$. Let us write

$$y_{n+1}^{(j)} = P_j(z) y_{n+1}^{(0)} - Q_j(z)\,\Sigma_n. \tag{4.3}$$

It is straightforwardly verified that (4.3) satisfies (4.2) if the function $Q_j(z)$ is defined by

$$Q_j(z) = \frac{P_j(z)-1}{1-b_0^* z}. \tag{4.4}$$

Expressing Σ_n in terms of the characteristic polynomials ρ^* and σ^* we arrive at the formula

$$(4.3') \qquad y_{n+1} = P_m(z)y_{n+1}^{(0)} - Q_m(z)[1 - b_0^*z - (\rho^*(E)-z\sigma^*(E))E^{-k}]y_{n+1},$$

where E denotes the shift operator defined by $y_{n+1} = Ey_n$. Finally, we use the fact that the predictor formula for $y_{n+1}^{(0)}$ is of the linear multistep form, that is when applied to (4.1)

$$(4.5) \qquad y_{n+1}^{(0)} = [1 - \tilde{\rho}(E)E^{-k}]y_{n+1} + z\tilde{\sigma}(E)E^{-k}y_{n+1},$$

where we put $\tilde{a}_0 = -1$. From (4.3'), (4.4) and (4.5) the following theorem is now immediate.

THEOREM 4.1 *The characteristic equation of the generalized predictor-corrector method is given by*

$$(4.6) \qquad \rho^*(\zeta) - z\sigma^*(\zeta) = \frac{(1-b_0^*z)P_m(z)}{P_m(z)-1}\,[\tilde{\rho}(\zeta)-z\tilde{\sigma}(\zeta)] \qquad \square$$

If we substitute for $P_m(z)$ the polynomial corresponding to the conventional predictor-corrector method in $P(EC)^mE$ mode defined by $M = 0$ and $\bar{M} = b_0^*I$, that is we set $P_m(z) = (b_0^*z)^m$, then we obtain the familiar characteristic equation [7, p.97]

$$(4.7) \qquad \rho^*(\zeta) - z\sigma^*(\zeta) = \frac{(1-b_0^*z)(b_0^*z)^m}{(b_0^*z)^m-1}\,[\tilde{\rho}(\zeta)-z\tilde{\sigma}(\zeta)].$$

It is well-known that the stability intervals for predictor-corrector methods are rather modest. For instance, a frequently cited predictor-corrector method for first order equations is the fourth order PECE method of Crane and Klopfenstein [2] which has the relatively large interval of stability $(-2.48,0)$. However, in many applications this interval is still unacceptably small.

In this section we will show that a suitable choice of the polynomial $P_m(z)$ extends the stability interval considerably. Here, we will call the generalized predictor-corrector method *stable* in a point z if (4.6) has for that point z its roots on the unit disk.

The set of all points z for which the method is stable will be called the *stability region;* the set of points of the stability region on the real axis form the *stability interval* and the length of the largest interval $[-\beta,0]$ within the stability interval is called the *stability boundary* β. The method is called *zero-stable* if for $z = 0$ the equation (4.6) has its roots on the unit disk those on the unit circle being simple roots. Furthermore, by writing

$$z^* = P_m(z) \tag{4.8}$$

and by considering z^* as an independent variable we may define in the *real* (z,z^*) -plane a region where the generalized predictor-corrector method is stable. Since this region plays a central rôle in the subsequent analysis we give a formal definition.

DEFINITION 4.1 The region in the (z,z^*) -plane where all roots of the equation

$$\rho^*(\zeta) - z\sigma^*(\zeta) = \frac{(1-b_0^*z)z^*}{z^*-1}\,[\tilde{\rho}(\zeta) - z\tilde{\sigma}(\zeta)] \tag{4.6'}$$

are on the unit disk will be called the *stability domain* $\mathcal{D}$ □

Note that the points in $\mathcal{D}$ on the z -axis form the stability interval of the corrector formula $\{\rho^*,\sigma^*\}$. Finally, we define the *stability constant* $c = \beta/m^2$ and the *effective stability boundary* $\beta_{eff} = [\beta]^{1/\nu}/\bar{m}$, where $\bar{m}$ denotes the number of right-hand side evaluations per step.

The stability domain $\mathcal{D}$ can be determined by applying the Routh-Hurwitz criterion (see e.g. [7, p. 82]) which is more easy applicable by using a computer. A particularly straight forward derivation of $\mathcal{D}$ can be obtained in the case where $\tilde{\sigma}(\zeta) = 0$, i.e. when extrapolation-predictors are used (see appendix A).

Presenting $\mathcal{D}$ in the form

$$-D_1(z) \le z^* \le D_2(z),$$

where $D_1(z)$ and $D_2(z)$ are functions completely determined by $\tilde{\rho},\tilde{\sigma},\rho^*$ and σ^*, we conclude that the method with iteration polynomial $P_m(z)$ has a stability interval $[-\beta,0]$ if

$$(4.7) \qquad -D_1(z) \le P_m(z) \le D_2(z) \quad \text{for} \quad -\beta \le z \le 0.$$

A typical example of a stability domain is given in figure 4.1.

In the next subsection polynomials $P_m(z)$ are constructed of arbitrarily large degree m which "remain" fairly long in the stability domain $\mathcal{D}$. In this construction we will replace condition (4.7) by

$$(4.7') \qquad -D_1 \le P_m(z) \le D_2 \quad \text{for} \quad -\beta \le z \le 0,$$

where D_1 and D_2 denote the minimal values of $D_1(z)$ and $D_2(z)$ in the interval $[-\beta,0]$. It should be remarked, however, that in the case of lower degree polynomials $P_m(z)$ (say $m = 2$ or $m = 3$), the value of β obtained by using (4.7') instead of (4.7) is rather pessimistic, because for small m that part of $\mathcal{D}$ which is close to the origin is only relevant and it is just in this part where the simplification (4.7') is a rather rough approximation to (4.7). Thus, unnecessarily small estimates for β are obtained when using (4.7') for small m (see figure 4.1).

On the other hand, optimal stability intervals defined by (4.7) also mean that the corresponding integration method is rather sensitive to "imaginary noise", that is the method rapidly looses stability if eigenvalues with imaginary parts occur in the spectrum of $\partial f/\partial y$.

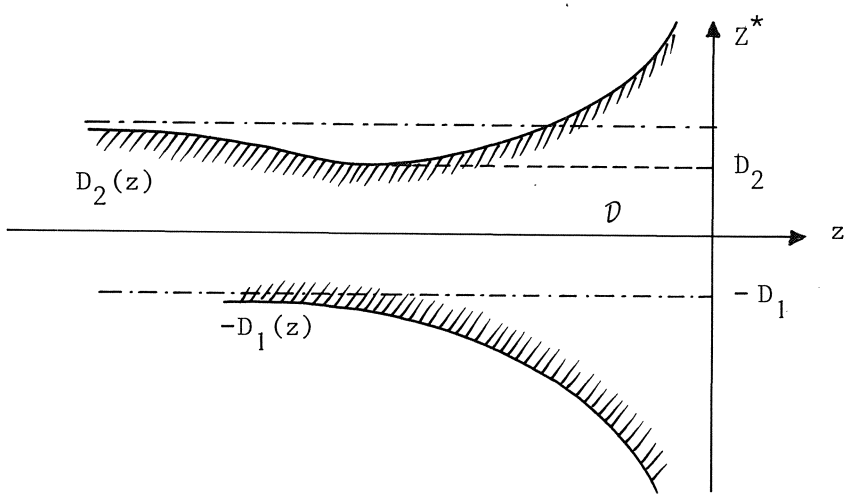


Figure 4.1 Stability domain $\mathcal{D}$

4.2 Construction of polynomials $P_m(z)$ for arbitrary m

We will construct polynomials $P_m(z)$ satisfying (4.7') with the maximal possible value for β . For large m these polynomials approximate the optimal polynomials satisfying (4.7). We consider the case of zero- and first-order iteration polynomials of which the first order polynomials have slightly larger stability intervals. We did not succeed in constructing second order polynomials generating larger intervals of stability than those generated by the first order ones; moreover, only for $D_1=0$ closed expressions can be derived (see appendix B).

It will be assumed that D_1 and D_2 are non-negative.

4.2.1 Zero-order polynomials

It is well known that those polynomials $P_m(z)$ which alternatingly touches the lines $z^* = -D_1$ and $z^* = D_2$ in the (z,z^*) -plane are optimal in the sense that β is as large as possible (see figure 4.2). The polynomial $P_m(z)$ is said to satisfy the *equal ripple property* [4]. Consider the

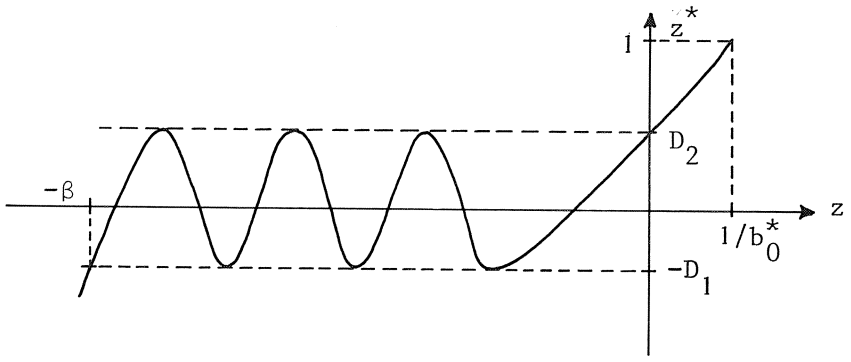


Figure 4.2 Optimal zero- order polynomial $P_m(z)$

shifted Chebyshev polynomial

$$P_m(z) = \frac{1}{2}\,[D_2 - D_1 + (D_2+D_1)T_m(1+\frac{2z}{\beta})] \tag{4.8}$$

,

$$\beta = \frac{2}{b_0^*}\,[T\,\frac{1}{m}\,(\frac{2+D_1-D_2}{D_1+D_2})-1]^{-1}$$

where $T_\mu(x) = \cos(\mu \arccos x)$ if $|x| \leq 1$ and $T_\mu(x) = \cosh(\mu \operatorname{arccosh} x)$ if $x > 1$. Evidently, this polynomial satisfies the equal ripple property with respect to $-D_1$ and D_2, and is such that $P_m(1/b_0^*) = 1$ as required by (2.5).

It is of interest to derive the magnitude of β for $m \to \infty$. From the expansion

$$
\begin{aligned}
T_\mu(x) &= 1 - \tfrac{1}{2}\mu^2[\arccos x]^2 + O(\mu^4) \quad \text{as} \quad \mu \to 0,\ |x| \leq 1 \\
T_\mu(x) &= 1 + \tfrac{1}{2}\mu^2[\ell n(x+\sqrt{x^2-1})]^2 + O(\mu^4) \quad \text{as} \quad \mu \to 0,\ x \geq 1
\end{aligned} \tag{4.9}
$$

we derive that

$$
\beta = \frac{4m^2(1 + O(1/m^2))}{b_0^*\left[\ell_n\left|\dfrac{\sqrt{1+D_1} + \sqrt{1-D_2}}{\sqrt{1+D_1} - \sqrt{1-D_2}}\right|\right]^2} \quad \text{as} \quad m \to \infty. \tag{4.10}
$$

Thus, the stability boundary β shows an $O(m^2)$ behaviour and the order constant is just the stability constant.

4.2.2 First order polynomials

The optimal polynomials are of the form

$$
\begin{aligned}
P_m(z) &= \tfrac{1}{2}\left[D_2 - D_1 + (D_2+D_1)T_m\left(w_0 + \frac{w_0+1}{\beta}z\right)\right], \\
w_0 &= T_{\frac{1}{m}}\left(\frac{D_1-D_2}{D_1+D_2}\right), \quad \beta = \frac{w_0+1}{b_0^*}\left[T_{\frac{1}{m}}\left(\frac{2+D_1-D_2}{D_1+D_2}\right) - w_0\right]^{-1}.
\end{aligned} \tag{4.11}
$$

It is easily verified that $P_m(0) = 0$, $P_m(1/b_0^*) = 1$ and that the equal ripple property is satisfied. From (4.11) it follows that

$$
\beta = \frac{4m^2(1 + O(1/m^2))}{b_0^*\left\{\left[\ell n\left|\dfrac{\sqrt{1+D_1} + \sqrt{1-D_2}}{\sqrt{1+D_1} - \sqrt{1-D_2}}\right|\right]^2 + \left[\arccos\dfrac{D_1-D_2}{D_1+D_2}\right]^2\right\}} \quad \text{as} \quad m \to \infty. \tag{4.12}
$$

4.2.3 Second order polynomials

If $D_1 = 0$ the optimal polynomials are of the form (see appendix B)

$$P_m(z) = \frac{1}{2} D_2\left[1 + T_m\left(\cos\frac{\pi}{m} + \frac{1+\cos\pi/m}{\beta} z\right)\right],$$

(4.13)

$$\beta = \frac{1 + \cos\frac{\pi}{m}}{b_0^*\left[T_{\frac{1}{m}}\left(\frac{2}{D_2} - 1\right) - \cos\frac{\pi}{m}\right]} .$$

It is easily verified that $P_m(0) = P_m'(0) = 0$, $P_m(1/b_0^*) = 1$ and that the equal ripple property is satisfied. From (4.13) it follows that

(4.14)

$$\beta = \frac{4m^2(1 + O(1/m^2))}{b_0\left[\pi^2 + \left(\ell n \frac{2-D_2+2\sqrt{1-D_2}}{D_2}\right)^2\right]} \quad \text{as} \quad m \to \infty.$$

We observe that for $m = 2$ (4.13) yields the conventional PECE method.

5. IMPLEMENTATIONAL DETAILS

In this section the computational scheme is defined based on a predictor $\{\tilde{\rho},\tilde{\sigma}\}$ a corrector $\{\rho^*,\sigma^*\}$ and the first order iteration polynomial $P_m(z)$ defined in (4.11). The scheme is organized in such a way that an arbitrary number of stages are allowed (in order to increase the effective stability boundary) without increasing the storage requirements and without the danger of internal instabilities.

Our starting point is the assumption that the stability domain defined by the predictor-corrector pair (see definition 4.1) contains the set of points

(5.1)

$$\left\{(z,z^*) \mid -D_3 \le z \le 0, \; -D_1 \le z^* \le D_2\right\},$$

where D_1, D_2 are positive and D_3 is sufficiently large (to be specified below). For an example where this assumption is not satisfied see section 7.

5.1 Construction of the scheme

Consider the iteration polynomials

$$(5.2)\qquad P_0(z) = 1,\ P_j(z) = 1 - \frac{1}{d_j}\left[T_j\left(w_0 + \frac{w_0+1}{\beta b_0^*}\right) - T_j\left(w_0 + \frac{w_0+1}{\beta} z\right)\right],\ j \geq 1,$$

where w_0 and β are defined as in (4.11) and $d_m = 2/(D_1+D_2)$. These polynomials satisfy condition (2.5) for all j. Furthermore, $P_m(z)$ is identical to the *first order* polynomial (4.11).

The iteration polynomials (5.2) satisfy the recurrence relation

$$(5.3)\qquad \begin{aligned} P_0(z) &= 1,\quad P_1(z) = 1 - \frac{w_0+1}{d_1\beta b_0^*}(1-b_0^* z),\\ d_j P_j(z) &= \left\{\left[d_j - 2w_0 d_{j-1} + d_{j-2} - 2\frac{w_0+1}{\beta b_0^*} T_{j-1}\left(w_0 + \frac{w_0+1}{\beta b_0^*}\right)\right]\right.\\ &\quad \left. + 2\frac{w_0+1}{\beta}\left[T_{j-1}\left(w_0 + \frac{w_0+1}{\beta b_0^*}\right) - d_{j-1}\right]z\right\}\\ &\quad + 2\left\{w_0 + \frac{w_0+1}{\beta} z\right\} d_{j-1} P_{j-1}(z) - d_{j-2}P_{j-2}(z),\ j \geq 2. \end{aligned}$$

The matrices M and $\bar{M}$ have the structure

$$(5.4a)\qquad M = \begin{pmatrix} \mu_{11} & & & \\ \mu_{21} & \mu_{22} & & \\ \mu_{31} & \mu_{32} & \mu_{33} & \\ & \ddots & \ddots & \ddots \end{pmatrix},\quad \bar{M} = \begin{pmatrix} \bar{\mu}_{11} & & & \\ \bar{\mu}_{21} & \bar{\mu}_{22} & & \\ & \bar{\mu}_{32} & \bar{\mu}_{33} & \\ & & \ddots & \ddots \end{pmatrix}$$

with

$$\mu_{11} = 1 - \frac{w_0+1}{d_1\beta b_0^*},\quad \mu_{j1} = 1 - 2w_0\frac{d_{j-1}}{d_j} + \frac{d_{j-2}}{d_j} - 2\frac{w_{0+1}}{\beta b_0^*}\frac{\theta_{j-1}}{d_j},\ j \geq 2,$$

$$\mu_{jj} = 2w_0\frac{d_{j-1}}{d_j},\quad \mu_{j,j-1} = -\frac{d_{j-2}}{d_j},\ j \geq 3,$$

$$\bar{\mu}_{11} = \frac{w_{0+1}}{d_1\beta},\quad \bar{\mu}_{j1} = 2\frac{w_0+1}{d_j\beta}(\theta_{j-1}-d_{j-1}),\quad \bar{\mu}_{jj} = 2\frac{w_0+1}{\beta}\frac{d_{j-1}}{d_j},\ j \geq 2,$$

$$\lambda_1 = \frac{w_0+1}{d_1\beta},\quad \lambda_j = 2\frac{w_0+1}{d_j\beta b_0^*}\theta_{j-1},\ j \geq 2,$$

where $\theta_j = T_j(w_0+(w_0+1)/\beta b_0^*), d_0 = 0$ and $d_1,\ldots,d_m$ are still free parameters. A plausible choice for these parameters is such that the $P_j(z)$ have a first order zero at $z=0$, i.e. (use 5.2))

$$(5.4b) \qquad d_j = T_j(w_0 + \frac{w_0+1}{\beta b_0^*}) - T_j(w_0).$$

Then $y^{(j)}$ has the order (by virtue of theorem 3.2)

$$(5.5) \qquad p = \min\{p^*, \tilde{p} + \nu\}.$$

However, for large values of β we obtain rather small values for the first few d_j ($d_j \cong (w_0+1)j^2/\beta b_0^*$ for $\beta >> 1$) and consequently relatively large $\bar{\mu}_{j1}$ -values because $\theta_j - d_j \cong 1$ (note that all other parameters remain of moderate size). Because problems possessing a large Lipschitz constant require relatively small values for the coefficients $\bar{\mu}_{j\ell}$ if we want to integrate with large integration steps, we introduce an index m_0 and only use (5.4b) for $j \geq m_0$ and set $d_j = d_{m_0}$ for $j < m_0$. The index m_0 is chosen in such a way that $d_{m_0} \cong 1$, i.e.

$$d_{m_0} \cong \frac{w_0+1}{\beta b_0^*} m_0^2 = \frac{w_0+1}{c_p b_0^*} \left(\frac{m_0}{m}\right)^2 \cong 1,$$

so that

$$(5.4c) \qquad m_0 \cong m\sqrt{\frac{b_0^* c_p}{w_0+1}}.$$

This choice implies that $\bar{\mu}_{jj} > \bar{\mu}_{j1}$ giving the most recent derivative evaluation the larger weight in the successive iteration steps.

5.2 Internal stability for large m

The stability condition for the scheme generated by (5.4) is given by

$$(5.6) \qquad \tau^\nu \leq \frac{\beta}{S(\partial f/\partial y)},$$

where $S(\partial f/\partial y)$ denotes the spectral radius of the Jacobian matrix $\partial f/\partial y$, and where we have assumed that $D_3 \geq \beta$.

This condition is not sufficient for a stable behaviour if many stages per integration step are used, i.e. if m is large. For a detailed discussion of the phenomenon of *internal instability* we refer to [6] Such instabilities can be suppressed if we require that the homogeneous part of (5.3) is a stable recursion. If d_{j-1}/d_j and d_{j-2}/d_j are constant this is achieved by requiring that the roots of the characteristic equation

$$\zeta^2 - 2\left[w_0 + \frac{w_0+1}{\beta} z\right] \frac{d_{j-1}}{d_j} \zeta + \frac{d_{j-2}}{d_j} = 0$$

are within or on the unit circle, those on the unit circle being simple roots, for all z in the spectrum of $\tau^{\nu}\partial f/\partial y$. We find

$$(5.7) \qquad 2d_{j-1} - d_j \leq d_{j-2} \leq d_j, \; -\beta \leq z \leq 0.$$

It is easily verified that this condition is always satisfied if $j \leq m_0$, that is if $d_j = d_{m_0}$ and if (5.6) holds. For $j > m_0$ the coefficients d_j slowly increase with j sothat d_{j-1}/d_j and d_{j-2}/d_j are also slowly changing. For instance, if β is large we have $d_j \cong 2j^2/\beta b_0^*$ so that

$$\frac{d_{j-1}}{d_j} \cong \left(\frac{j-1}{j}\right)^2, \; \frac{d_{j-2}}{d_j} \cong \left(\frac{j-2}{j}\right)^2, \; j \geq m_0 + 2.$$

Since these quantities are "almost" constant as m large we may expect that (5.7) ensures also stability if $j \geq m_0 + 2$. Evidently, this condition is satisfied for $j \geq m_0 + 2$.

6. EXTRAPOLATION-BACKWARD-DIFFERENTIATION METHODS

In this section we apply the results obtained in preceding sections to the special case where the predictor formula is defined by *extrapolation* and the corrector formula by *backward differentiation*. The considerations are confined to *first order differential equations* (ν=1). The resulting methods will be denoted by *EP-BD methods*. Notice that for these methods the $P(EC)^mE$ and the $P(EC)^m$ mode are identical.

The characteristic polynomials are defined by

$$(6.1) \qquad \tilde{\rho}(\zeta) = (\zeta-1)^{\tilde{p}+1} \cdot \zeta^{k-\tilde{p}-1}, \; \tilde{p} \leq k-1; \; \tilde{\sigma}(\zeta) = 0;$$

$$(6.2)\quad \rho^*(\zeta) = \begin{cases} (3\zeta^2-4\zeta+1)/3 \\ (11\zeta^3-18\zeta^2+9\zeta-2)/11 \\ (25\zeta^4-48\zeta^3+36\zeta^2-16\zeta+3)/25 \\ (137\zeta^5-300\zeta^4+300\zeta^3-200\zeta^2+75\zeta-12)/137 \\ (147\zeta^6-360\zeta^5+450\zeta^4-400\zeta^3+225\zeta^2-72\zeta+10)/147 \end{cases} ; \sigma^*(\zeta) = \begin{cases} 2\zeta^2/3 \\ 6\zeta^3/11 \\ 12\zeta^4/25. \\ 60\zeta^5/137 \\ 60\zeta^6/147 \end{cases}$$

The order of accuracy of these predictor and corrector formulas are respectively $\tilde{p}$ and p^*.

The stability domain $\mathcal{D}$ of these predictor-corrector pairs contain the set (5.1) with $D_3 = \infty$ and (D_1, D_2) listed in table 6.1.

Table 6.1 (D_1, D_2)-values of EP-BD methods

p^*	$\tilde{p} = p^*-2$	$\tilde{p} = p^*-1$	$\tilde{p} = p^*$
2	(1,1)	(1/3,1)	(1/7, $\frac{1}{2}$)
3	(1/3,1)	(1/7,$\frac{1}{2}$)	(1/15, 1/5)
4	(1/7,.4951)	(1/15,.1999)	(1/31, $2/(13+5\sqrt{5})$)
5	(1/15,.1704)	(1/31,.0751)	(1/63, 1/28)
6	(1/31,.0289)	(1/63,.0147)	(1/127,.01128)

6.1 EP-BD methods with only a few stages

We start our discussion with the four-step, fourth order BD formula and the EP formulas of orders $\tilde{p} = 0, 1, 2, 3$. By virtue of theorem 3.2 these predictor-corrector methods are at least of order

$$(6.3)\qquad p = \min\{4, \tilde{p}+r, 2\tilde{p}+2\},$$

where r is the multiplicity of the zero at $z=0$ of $P_m(z)$. In the special case of conventional PC methods we have of coarse

$$(6.4)\qquad p = \min\{4, \tilde{p}+m\}.$$

Let us first consider the conventional predictor-corrector method generated by

$$P_m(z) = \left(\frac{12}{25}\, z\right)^m. \tag{6.5}$$

It is easily verified that $z^* = P_m(z)$ remains within the area (4.7') if

$$-z \le \beta = \begin{cases} \frac{25}{12} D_1^{1/m} & \text{for m odd} \\ \frac{25}{12} D_2^{1/m} & \text{for m even} \end{cases}.$$

In table 6.2 the stability boundaries β_{eff} are listed for a few values of m resulting in p = 4.

Table 6.2 Effective stability boundaries for (6.5)

	$\tilde{p} = 0$	$\tilde{p} = 1$	$\tilde{p} = 1$	$\tilde{p} = 2$	$\tilde{p} = 3$	$\tilde{p} = 3$
m =	4	3	4	2	1	2
p =	4	4	4	4	4	4
β_{eff}	.52	.48	.52	.73	.14	.47

Next we choose $P_m(z)$ optimal with respect to (4.7'). Consider the case m = 2 and $\tilde{p} = 3$, and require that $P_2(z)$ behaves as indicated in figure 6.1. An elementary calculation yields

$$P_2(z) = \frac{1}{5}\, b_0^* z(2+3b_0^* z),\ b_0^* = \frac{12}{25}, \tag{6.6}$$

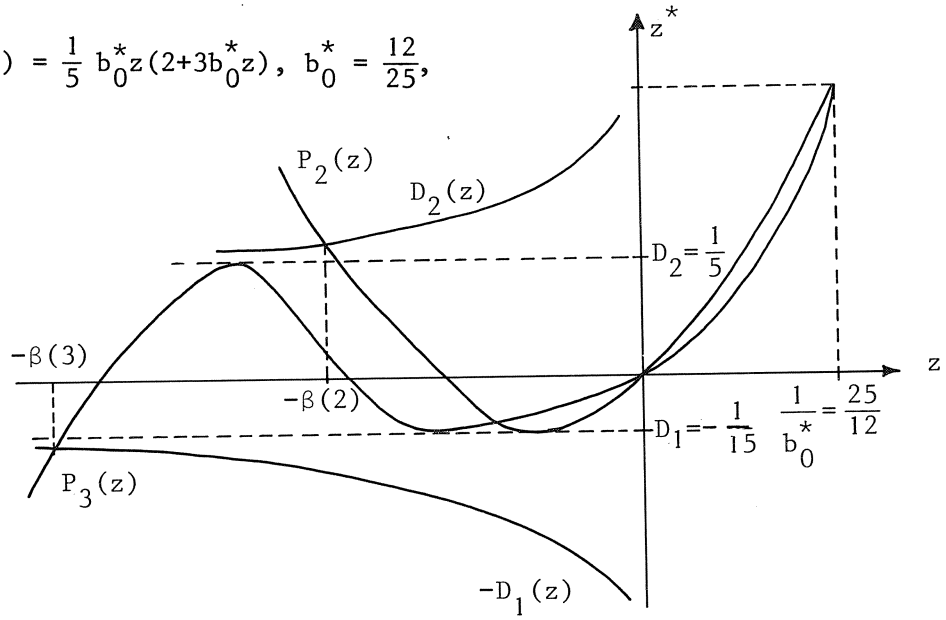


Figure 6.1 Optimal polynomials of first order

with the stability boundary $\beta = 1/b_0^* \simeq 2.08$. According to theorem 3.2 this method is of fourth order. Comparison of this optimized method with the "best" method listed in table 6.2 (i.e. $\tilde{p} = 2$, $m = 2$), we conclude that we already gained a factor 1.4 in the effective stability boundary. In figure 6.2 the stability region is given in the complex z -plane (only half of the stability regions are given as the regions are symmetric about the real axis). Notice that this region extends rather far into the imaginary direction. This is due to the fact that $D_1 = 1/15$ is much smaller that the $D_1(z)$-value at the point where $P_2(z)$ touches the line $z^* = -D_1 = -1/15$ (see figure 6.2).

Similarly, we obtain for $m = \tilde{p} = 3$ and for $P_3(z)$ behaving as in figure 6.1 the stability boundary $\beta \cong 5.7$ which is effectively a factor 2.6 larger than the maximal effective boundary of the conventional methods listed in table 6.2. In figure 6.3 the stability region is shown. The narrowing of this region occurs when $P_3(z)$ touches the line $z^* = D_2 = 1/15$.

We again consider the fourth order EP-BD methods with $k = 4$, $\tilde{p} = 3$ and $m = 2$ and 3. But now the polynomials $P_m(z)$ are chosen in such a way that they approach the boundary curves $z^* = D_2(z)$ and $z^* = -D_1(z)$ rather close but never that close that the characteristic roots (cf. (4.6)) become larger in modulus than .975 in the interval $-\beta(m) < z < 0$. The resulting regions are shown in the figures 6.2 and 6.3 (dotted lines). The

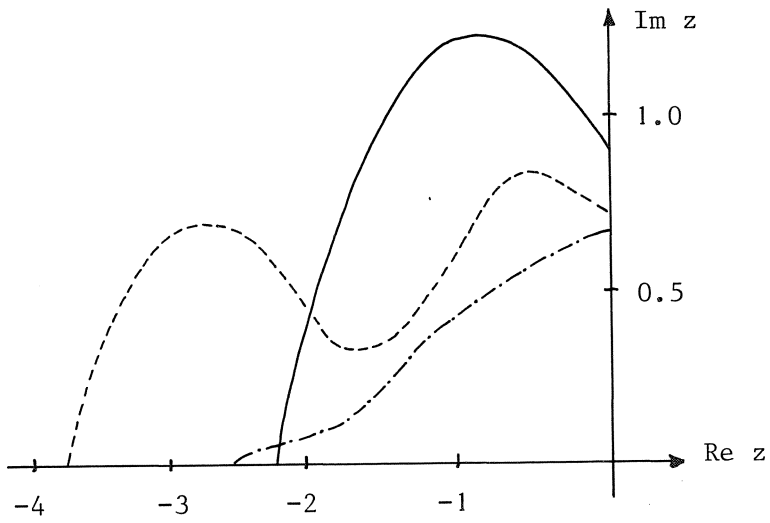


Figure 6.2 ——— EP - BD method ($p^* = 4, \tilde{p} = 3, m = 2$)

------- EP - BD* method ($p^* = 4, \tilde{p} = 3, m = 2$)

-·-·-·- Crane-Klopfenstein method (PECE mode)

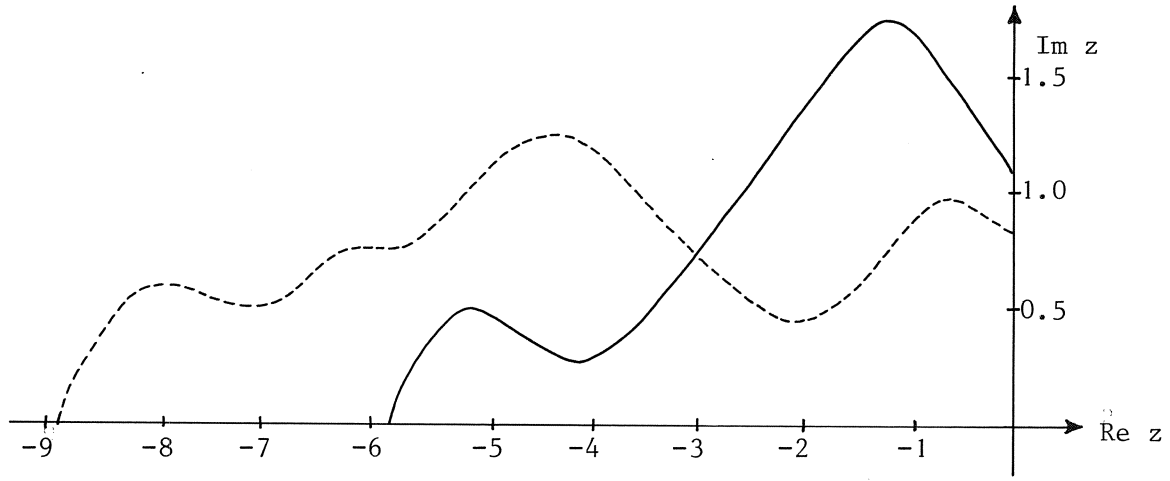


Figure 6.3 ——— EP - BD method ($p^*=4$, $\tilde{p}=3$, m=3)
- - - - - - EP - BD* method ($p^*=4$, $\tilde{p}=3$, m=3)

improvement of the real stability interval of these "optimal" EP-BD methods (indicated by EP-BD*) is considerable whereas the extension of the stability region into the complex plane is still substantial.

6.2 Comparison with conventional PECE methods

Along the lines as indicated in the preceding subsection we can construct EP-BD and EP-BD* methods of orders p = 5 and p = 6. In this subsection we compare the real stability boundaries β and $\beta_{eff} = \beta/m$ of various predictor-corrector methods. In table 6.3 values are listed for the PECE mode of a few Adams-Bashforth-Moulton (ABM) methods,

Table 6.3 Stability boundaries for various predictor-corrector methods

order	ABM		CK		KAM		EP-BD* (m = 2)			EP-BD* (m = 3)		
	β	β_{eff}	β	β_{eff}	β	β_{eff}	β	β_{eff}	D_1	β	β_{eff}	D_1
4	1.3	.65	2.48	1.24	1.8	.9	3.88	1.94	.24	8.90	2.97	.23
5	1.0	.5			1.4	.7	3.15	1.57	.17	7.28	2.42	.16
6	.7	.35			1.0	.5	2.58	1.26	.13	6.03	2.01	.12

the Crane-Klopfenstein (CK) method, the Krogh-Adams-Moulton (KAM) methods and the two-and three-stage EP-BD* methods. In the conventional predictor-corrector methods the predictor and corrector are of the same order.

In order to illustrate the enlarged stability intervals we have integrated the nonlinear problem

$$\frac{dy}{dt} = -y^{4/3} + t^{32/9} + \frac{8}{3}t^{5/3}, \quad 0 \le t \le 10$$

with initial condition $y(0)=0$. The required starting values were taken from the exact solution $y(t)=t^{8/9}$. For the implementation of the EP-BD* methods we refer to the approach in section 5. In table 6.4 we have listed

Table 6.4 Numerical results obtained by various predictor-corrector methods

order	ABM			CK			KAM			EP-BD*(m = 2)			EP-BD*(m = 3)			
	$\tau=\frac{1}{2}$	$\tau=\frac{1}{4}$	$\tau=\frac{1}{8}$	$\tau=\frac{1}{2}$	$\tau=\frac{1}{4}$	$\tau=\frac{1}{8}$	$\tau=\frac{1}{2}$	$\tau=\frac{1}{4}$	$\tau=\frac{1}{8}$	$\tau=\frac{1}{2}$	$\tau=\frac{1}{4}$	$\tau=\frac{1}{8}$	$\tau=1$	$\tau=\frac{1}{2}$	$\tau=\frac{1}{4}$	$\tau=\frac{1}{8}$
4	*	4.2	7.2	*	4.3	7.2	*	0.8	7.0	1.7	4.3	5.2	1.4	3.4	4.2	5.3
5	*	*	8.9				*	*	8.2	1.5	6.1	7.1	*	4.5	5.8	7.1
6	*	*	7.1				*	*	7.3	0.4	7.9	8.7	*	4.3	7.3	8.7

the number of correct digits defined by

(6.7) $$sd = -{}^{10}\log \varepsilon, \quad \varepsilon = \text{absolute error}$$

obtained in the endpoint t = 10.

6.3 EP-BD methods with many stages

Consider the EP-BD-method with the *zero-order* iteration polynomial given in (4.8). In particular we consider the methods of order p = 4,5 and 6. In table 6.5 the stability constants c_p determined by (4.10) are listed for a few values of m where we identified D_1 and D_2 with the values of table 6.1 and where $p = p^* = \tilde{p}$. This table shows the rapid convergence of c to the asymptotic value. We compare

Table 6.5 Stability constants for EP-BD methods of order p = 4, 5, 6

p	m = 1	m = 2	m = 3	m = 4	m = 5	m → ∞
4	.26	.52	.60	.63	.64	.67
5	.12	.33	.40	.44	.45	.48
6	.047	.19	.26	.29	.31	.34

these values with the one-step stabilized Runge-Kutta methods of order 4 derived in [9, 4]. Here it was found that $c_4 \cong 0.24$ for m = 5 and $c_4 \cong 0.34$ as m → ∞. Thus, apart from a faster convergence the present methods also possess substantially larger stability constants.

In a similar way we obtain for EP-BD methods with the *first order* iteration polynomial (4.11) the stability constants listed in table 6.6.

Table 6.6 Stability constants for EP-BD methods of order $p = p^* = \tilde{p} + 1 = 4, 5, 6$

p	m = 1	m = 2	m = 3	m = 4	m = 5	m → ∞
4	.139	.52	.63	.67	.69	.73
5	.074	.34	.44	.48	.50	.54
6	.039	.21	.29	.32	.34	.37

These values are slightly larger than those obtained by zero-order iteration polynomials. We remark that for p = 4 and m = 2 the iteration polynomial is identical to (6.6).

6.4 Application to parabolic initial-boundary value problems

Consider the EP-BD method with first order iteration polynomial (4.11) and implemented as described in section 5.1.

This EP-BD scheme was applied to the semi-discretized version of the parabolic initial-boundary value problem [6]

$$(6.8)\quad \frac{\partial u}{\partial t} = \frac{x_1+x_2}{2(2\pi+t)}\,\Delta(u^3) + \frac{1}{2}(x_1+x_2)\cos t - \frac{3(x_1+x_2)^2}{4(2\pi+t)}\sin^3 t,\quad 0 \le t \le T = 20\pi$$

with Dirichlet-boundary conditions along the square $0 \le x_1, x_2 \le 1$. The initial and boundary values were taken from the exact solution

$$(6.9)\qquad u(t,x_1,x_2) = \frac{1}{2}(x_1+x_2)\sin t.$$

In the semi-discretization we used the conventional five-point molecule on a uniform grid with smesh spacing $h = 1/20$.

The number of stages m in the various EP-BD methods was determined by the stability condition (5.6), i.e.

$$(6.10)\qquad m = m_n \cong \left\lceil \sqrt{\frac{\tau S(\partial f/\partial y)}{c_p}} \right\rceil,\quad S(\partial f/\partial y) = 1.1\,\frac{24}{h^2}\cdot \max_{t\in[t_n,t_n+\tau]}\left(\frac{\sin^2 t}{2\pi+t}\right),$$

where the factor 1.1 in $S(\partial f/\partial y)$ is added to get a safe upperbound. The starting values $y_0,\ldots,y_{k-1}$ were taken from the exact solution (6.9).

For a number of integration steps we defined the accuracy obtained in the endpoint $T = 20\pi$ by means of the number of correct significant digits defined by (6.7). Furthermore, we defined the computational effort by counting the total number of right-hand side evaluations needed in the integration process including the function evaluations required if the starting values were to be computed from points ≤ 0 instead of taking them from the exact solution. This number is given by $N = \sum_{n=1}^{n=T/\tau} m_n$. Using (6.10), N can be expressed in terms of p and τ, and assuming that $\varepsilon = O(\tau^p)$ as $\tau \to 0$, we can express N in terms of p and ε or sd.

We find that N and sd are related by the equation

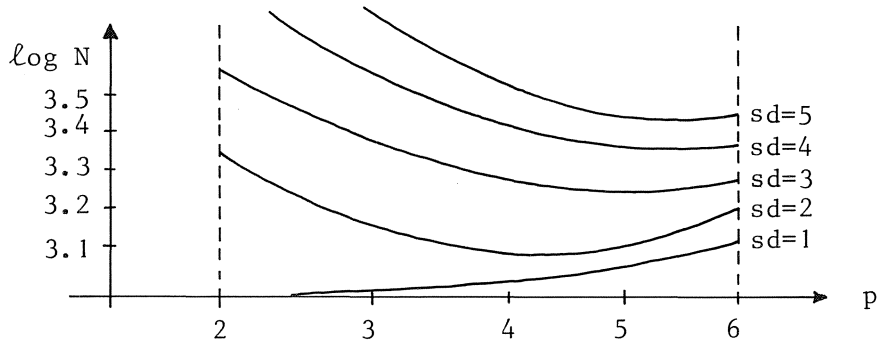
$$(6.11)\qquad \log N = A(p) + \frac{sd}{2p} \text{ as } \tau \to 0$$

where A(p) is a constant only depending on the order p of the method.

Our numerical experiments show that this asymptotic relation is quite good satisfied for rather large integration steps (see appendix D). The constants a(p) and the maximal stable integration steps τ_{max} for problem (5.8) are

	p = 2	p = 3	p = 4	p = 5	p = 6
A(p)	2.72	2.86	2.89	2.99	3.04
τ_{max}	2 π/30	2 π/20	2 π/10	2 π/10	2 π/10

In figure 6.1 the behaviour of log N as a function of p is illustrated for various values of sd. This figure clearly shows that the higher order methods



are the more efficient ones even in the range of low accuracies. The optimal order is clearly the order p for which log N is minimal. In this connection we remark that a lower bound for the optimal order p can be derived which is determined by (see appendix C)

$$(6.12) \qquad pc_p' = c_p \ln \tau,$$

where c_p' denotes the derivative of c_p with respect to p and where it is assumed that the order constant in the relation $\varepsilon = \mathcal{O}(\tau^p)$ is decreasing if p increases. From this relation it can be derived that the optimal order is larger than 3 as soon as $\tau < 0.4$ (see appendix C).

Finally, we compare the results reported above with those obtained if the ADI method of Peaceman-Rachford [8] is applied. From these results it follows that N and sd satisfy the relation (see appendix D)

(6.13) $$\log N = B(i) + \frac{1}{2}\,sd,$$

where i denotes the number of Newton iterations used for solving each implicit relation in the algorithm. The constants B(i) and maximal stable integration step are given by

	i = 1	i = 2
B(i)	1.99	1.67
τ_{max}	$2\pi/80$	$2\pi/80$

From (6.11) and (6.13) it follows that the generalized predictor-corrector methods are cheaper than the ADI method in the accuracy range

(6.14) $$sd > \frac{2p}{p-1}\,[A(p)-B(i)].$$

For instance, the 4-th order method is cheaper than the ADI method using two Newton interations if more than 3.25 correct digits are required.

7. A METHOD FOR SECOND ORDER EQUATIONS

We conclude this paper with the derivation of a generalized predictor-corrector method for *second order ODEs* ($\nu = 2$). We will use the extrapolation predictor and the Störmer-Cowell corrector with k = 2, i.e.

(7.1) $$\tilde{\rho}(\zeta) = (\zeta-1)^2;\ \tilde{\sigma}(\zeta) = 0$$

(7.2) $$\rho^*(\zeta) = (\zeta-1)^2;\ \sigma^*(\zeta) = b_0^*\zeta^2 + (1-2b_0^*)\zeta + b_0^*$$

which have the respective orders $\tilde{p} = 0$ and $p^* \geq 2$ (if $b_0^* = \frac{1}{12}$ then (7.2) defines the fourth-order Numerov corrector).

The stability domain $\mathcal{D}$ of this predictor-corrector pair is given by

$$D_1(z) = \frac{(4b_0^*-1)z-4}{z},\quad D_2(z) = 1.$$

Thus, if $b_0^* \geq \frac{1}{4}$ we have $D_1 = 4b_0^*-1$, $D_2 = 1$ and $D_3 = \infty$.

Using the first order iteration polynomial (4.11) we obtain a *second order* method with the stability boundary β given in (4.11). For m large we have

$$\beta \cong \frac{4m^2}{b_0^* \left[\arccos \frac{2b_0^*-1}{2b_0^*}\right]^2}, \quad b_0^* \geq \frac{1}{4} . \tag{7.3}$$

The stability boundary increases with b_0^* but is bounded above by $4\ m^2$. In view of (3.5) we require, however, $|P_m(z)| \leq 1$, i.e. $D_1 \leq 1$ which yields a stability boundary bounded bij $32\ m^2/\pi^2$.

Finally, consider the Numerov corrector which arises for $b_0^* = 1/12$. Using the second order iteration polynomial (4.13) we obtain a *fourth order* method. Since now $D_1<0$, it is no use to employ large values of m. For m = 2 we find back the conventional $P(EC)^2E$ method based on (7.1) and (7.2) the stability boundary of which equals 12. For m = 3 the stability boundary is determined by the equation

$$-\frac{(4b_0^*-1)z-4}{z} = \frac{1}{2}\left[1+T_3\left(\frac{1}{2}+\frac{3z}{2\beta}\right)\right], \quad b_0^* = 1/12, \tag{7.4}$$

where β is defined in (4.13). Note that here for m odd β is *not* the stability boundary of the method because $D_1<0$ (see figure 7.1). Solving equation (7.4) yields a stability boundary $\cong 32.4$.

In order to compare the efficiency of the methods with regard to stability we compute the effective stability boundaries defined in section 4.1. Taking into account that the number of right-hand side evaluations per step $\bar{m} = m + 1$ (here the $P(EC)^mE$ mode is different from the $P(EC)^m$mode), we arrive at the values listed in table 7.1.

Table 7.1 Effective stability boundaries

b_0^*	r	m	p	β_{eff}
1/2	1	$m \geq 1$	2	$m\sqrt{32}/(m+1)\pi \cong 1.8\ m/(m+1)$
1/12	2	2	4	$\sqrt{12}/3 \cong 1.15$
1/12	2	3	4	$\sqrt{32.4}/4 \cong 1.42$
1/12	m	$m \geq 2$	4	$\leq\sqrt{12}/(m+1) \cong 3.46/(m+1)$
1/12	m	$m \to \infty$	4	$\sqrt{6}/(m+1) \cong 2.45/(m+1)$

We remark that in the three-stage extrapolation-Numerov method the iteration polynomial $P_3(z)$ takes advantage of the special form of the stability domain $\mathcal{D}$ (see figure 7.1) resulting in a stability boundary which is more than 5 times as large as the stability boundary of the Numerov-corrector.

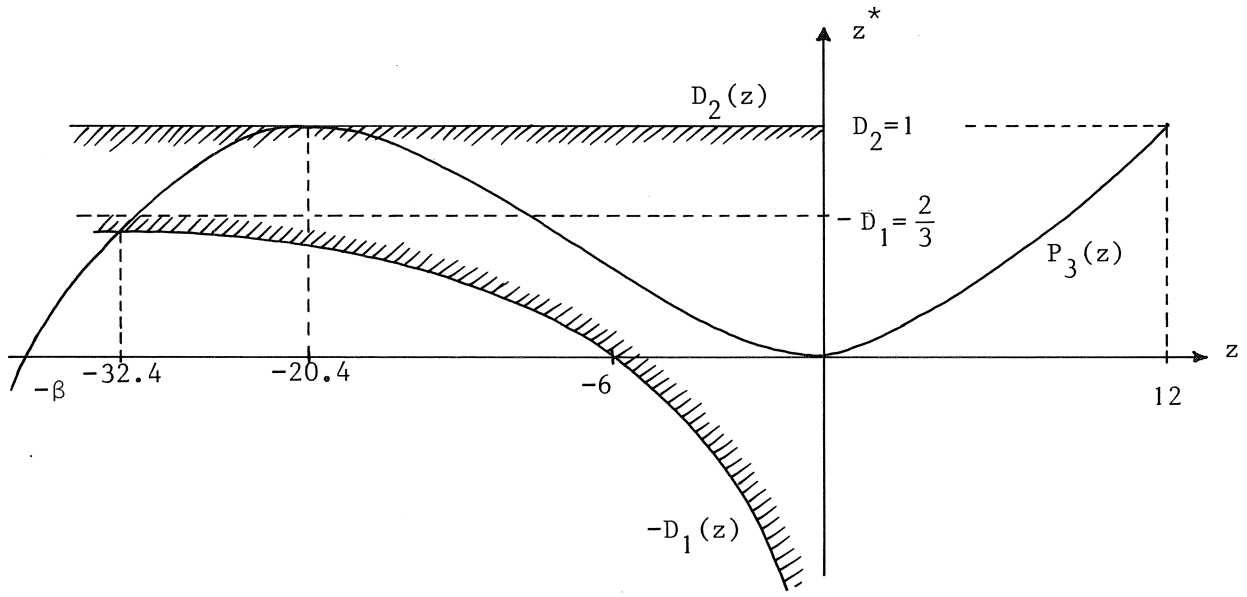


Figure 7.2 Extrapolation- Numerov method with $b_0^* = \frac{1}{12}$, r=2, m=3.

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APPENDIX A

In this appendix we derive explicit expressions for the boundary curves of the stability domain $\mathcal{D}$ associated with the characteristic equation (4.6') in the special case $\tilde{\sigma}(\zeta) = 0$. The derivation will be along the lines of a particular application of the boundary locus method described in [6].

A.1 The boundary locus method

If $\tilde{\sigma}(\zeta) = 0$ we can write (4.6') in the form

$$z\sigma^*(\zeta) + \tilde{z}\tilde{\rho}(\zeta) = \rho^*(\zeta), \quad \tilde{z} = -\frac{z^*(1-b_0^*z)}{1-z^*}. \tag{A.1}$$

Let us substitute $\zeta = e^{i\psi}$ to obtain for z and $\tilde{z}$ the relation

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix}\begin{pmatrix} z \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} E \\ F \end{pmatrix}, \tag{A.2}$$

where

$$A + iB = \sigma^*(e^{i\psi}),\ C + iD = \tilde{\rho}(e^{i\psi}),\ E + iF = \rho^*(e^{i\psi})$$

with $|\psi| \le \pi$. Let $z = Z(\psi)$ and $\tilde{z} = \tilde{Z}(\psi)$ be the solution of the boundary locus equation (A2). Then the stability domain is bounded by the curves

$$z = Z(\psi),\ z^* = \frac{\tilde{Z}(\psi)}{\tilde{Z}(\psi)+b_0^*Z(\psi)-1}, \quad |\psi| \le \pi. \tag{A.3}$$

(i) For those values of ψ for which

$$AD - CB = ED - CF = AF - EB = 0 \tag{A.4}$$

the solution of (A.3) degenerates to a straight line given by

$$A(\psi^*)z + C(\psi^*)\tilde{z} = E(\psi^*), \tag{A.5}$$

where ψ^* is a root of (A.4). In terms of z and z^* we find the hyperbolas

$$(A.3a') \qquad z^* = \frac{E(\psi^*) - A(\psi^*)z}{-C(\psi^*)+E(\psi^*)-[A(\psi^*)-b_0^*C(\psi^*)]z}$$

(ii) All values of ψ for which $AD - CB \neq 0$ yield the regular solution

$$z = \frac{ED - CF}{AD - CB}$$

$$(A.3b') \qquad z^* = \frac{AF-EB}{(AF-EB)+b_0^*(ED-CF)-(AD-CB)} .$$

Let $\tilde{\psi}$ denote a solution of $AD - CB = 0$. Choose a $\tilde{\psi} \neq \psi^*$. Then it is of interest to know how the solution (A.3b') behaves as $\psi \to \tilde{\psi}$. If $\tilde{\psi}$ is also a zero of $AF - EB$ then $(z,z^*) \to (\pm\infty,0)$ as $\psi \to \tilde{\psi}$. If $\tilde{\psi}$ is also a zero of $ED - CF$ then $(z,z^*) \to (z,1)$ as $\psi \to \tilde{\psi}$. Finally, if $\tilde{\psi}$ is neither a zero of $AF - EB$ or $ED - CF$ (which is the usual situation) then it is easily shown that

$$(A.3b'') \qquad (z,z^*) \to (\pm\infty, \frac{A(\tilde{\psi})}{A(\tilde{\psi})-b_0^*C(\tilde{\psi})}) \text{ as } \psi \to \tilde{\psi}.$$

For given formulas $\{\rho^*,\sigma^*\}$ and $\{\tilde{\rho},0\}$ the regular curve (A.3b') is easily determined in the (z,z^*)-plane. The determination of the hyperbolas (A.3a') requires the solution of (A.4). Evidently, these three equations have the common solution $\psi^*=0$ and $\psi^* = \pi$. Thus, we find

$$(A.6) \qquad z^* = \frac{\rho^*(\pm1)-\sigma^*(\pm1)z}{-\tilde{\rho}(\pm1)+\rho^*(\pm1)-[\sigma^*(\pm1)-b_0^*\tilde{\rho}(\pm1)]z} .$$

In most cases there will be no more solutions ψ^*. Since the functions $Z(\psi)$ and $\tilde{Z}(\psi)$ are even functions, our considerations will be restricted to the interval $0 \leq \psi \leq \pi$.

A.2 EP - BD methods

Let the predictor formula be defined by the extrapolation formula (6.1) and let the corrector be of the backward differentiation type, i.e.

(A.7) $\sigma^*(\zeta) = b_0^* \zeta^k, \ \nu = 1.$

Then

$$A(\psi) = b_0^* \cos k\psi, \ B(\psi) = b_0^* \sin k\psi$$

(A.8) $$C(\psi) = [R(\psi)]^{\tilde{p}+1} \cos[(\tilde{p}+1)\alpha(\psi)+(k-\tilde{p}-1)\psi] \ ,$$

$$D(\psi) = [R(\psi)]^{\tilde{p}+1} \sin[(\tilde{p}+1)\alpha(\psi)+(k-\tilde{p}-1)\psi]$$

where we have written

(A.9) $e^{i\psi} - 1 = Re^{i\alpha}, \ 0 \le \psi \le \pi$

i.e.

(A.9') $\alpha = \pi + \arctan \frac{\sin\psi}{\cos\psi - 1}, \ R = \sqrt{2(1-\cos\psi)}, \ 0 \le \psi \le \pi.$

The determinant AD-CB is given by

(A.10) $AD-CB = b_0^*[R(\psi)]^{\tilde{p}+1} \sin[(\tilde{p}+1)(\alpha(\psi)-\psi)]$

which vanishes if

(A.10') $R(\psi) = 0$ or $\alpha(\psi) - \psi + \frac{j\pi}{\tilde{p}+1} = 0, \ j = 0,\pm1,\ldots$.

An elementary calculation yields that the roots of (A.10') are given by

(A.11) $\tilde{\psi} = 2i\pi; \ \tilde{\psi} = 2j \frac{\pi}{\tilde{p}+1} + (2\ell+1)\pi; \ i,j,\ell = \pm1,\pm2,\ldots$.

The regular curve (A.3b') can now be computed by excluding $\tilde{\psi}$ from $[0,\pi]$.

In order to compute the hyperbolas (A.3a') we have to solve (A.4). The solutions ψ^* in the interval $[0,\pi]$ are included in the set (A.11). Thus, by substituting $\tilde{\psi}$ into (A.4) it can be checked which one is a ψ^* -solution.

It can be verified that

(A.12) $\psi^* = 0, \pi$

are the only values in the set (A.11) which satisfy (A.4). We are now in a position to compute the boundary curves of the stability domain $\mathcal{D}$.

We conclude this appendix with the asymptotic behaviour of the stability domain $\mathcal{D}$ as $z \to -\infty$. From (A.3a') and (A.3b') it follows that the boundary functions $z^* = -D_1(z)$ and $z^* = D_2(z)$ are of the form

$$(A.13) \qquad z^* = \frac{A(\tilde{\psi})}{A(\tilde{\psi}) - b_0^* C(\tilde{\psi})} \quad \text{as } z \to -\infty,$$

where $\tilde{\psi}$ is given by those values in the set (A.11) for which (A.13) is closest to zero. Substitution of (A.11) into (A.8) and (A.8) into (A.13) yields

$$z^* = 1$$

$$(A.14) \qquad z^* = \frac{1}{1-(-1)^j [R(\tilde{\psi})]^{\tilde{p}+1}} = \frac{1}{1-(-1)^j \left[2(1-\cos\tilde{\psi})\right]^{\frac{\tilde{p}+1}{2}}}, \quad \tilde{\psi} = \left(\frac{2j}{\tilde{p}+1} + 2\ell+1\right)\pi,$$

where $0 \le \frac{2j}{\tilde{p}+1} + 2\ell + 1 \le 1$. Evidently, we may restrict ℓ to $\ell=0$ to obtain

$$(A.15) \qquad z^* = 1; \quad z^* = \frac{1}{1-(-1)^j \left[2\cos\frac{j\pi}{\tilde{p}+1}\right]^{\tilde{p}+1}}, \quad -\frac{1}{2}(\tilde{p}+1) \le j \le 0.$$

The two minimal asymptotic values we are looking for are listed in table A.1.

Table A.1 Asymptotic values for EP-BD methods

$z \to -\infty$	$\tilde{p}=0$	$\tilde{p}=1$	$\tilde{p}=2$	$\tilde{p}=3$	$\tilde{p}=4$	$\tilde{p}=5$	$\tilde{p}=6$
$z^* \to$	1	1	1/2	1/5	$2/(13+5\sqrt{5})$	1/28	.01595
$z^* \to$	-1	-1/3	-1/7	-1/15	-1/31	-1/63	-1/127

We observe that these values are independent of b_0^*.

APPENDIX B

In this appendix we consider the construction of second order iteration polynomials. It is not possible to find optimal polynomials of second order in the form $a + bT_m(w_0+w_1z)$ unless $D_1 = 0$. Of course, we can just put $D_1 = 0$, but then we restrict the stability domain considerably (cf table 4.2) and consequently we get unnecessarily small stability boundaries.

Let us consider a slightly more complicated family of iteration polynomials defined by

$$P_m(z) = 1 - \frac{1-b_0^*z}{1-c_0z} \frac{T_m(w_0)-T_m(w_0+w_1(1-c_0z))}{T_m(w_0)-T_m(w_0+w_1)}, \quad m \geq 2$$

(B.1)

$$c_0 = b_0^* \left[1+ \frac{w_1T_m'(w_0+w_1)}{T_m(w_0)-T_m(w_0+w_1)}\right]^{-1},$$

where w_0 and w_1 are free parameters. It is easily verified that these polynomials have a double zero at $z = 0$ and satisfy $P_m(1/b_0^*)=1$. In the interval $-1 \leq w_0 + w_1(1-c_0z) \leq +1$ the polynomials $P_m(z)$ assume values which are bounded by the functions

$$B_{\pm}(z) := 1 - \frac{1-b_0^*z}{1-c_0z} \frac{T_m(w_0)\pm 1}{T_m(w_0)-T_m(w_0+w_1)} . \tag{B.2}$$

We will assume that $c_0w_1 < 0$. Then $P_m(z)$ is bounded by $B_{\pm}(z)$ if

$$-\frac{1+w_0+w_1}{-c_0w_1} \leq z \leq \frac{1-w_0-w_1}{-c_0w_1} .$$

This inequality suggests putting

$$\beta = \frac{1+w_0+w_1}{-c_0w_1}, \quad |w_0+w_1| \leq 1, \quad c_0w_1 < 0, \quad w_0 \geq 1$$

$$-D_1 \leq B_{\pm}(z) \leq D_2, \quad -\beta \leq z \leq 0. \tag{B.3}$$

We now consider two cases $b_0^*/c_0 \geq 1$ and $b_0^*/c_0 \leq 1$. In the first case, condition (B.3) is satisfied if (see figure B.1)

$$\text{(B.4a)} \qquad D_2 = \frac{1-T_m(w_0+w_1)}{T_m(w_0)-T_m(w_0+w_1)}, \quad D_1 = -1 + \frac{T_m(w_0)+1}{T_m(w_0)-T_m(w_0+w_1)} \cdot \frac{b_0^*}{c_0}$$

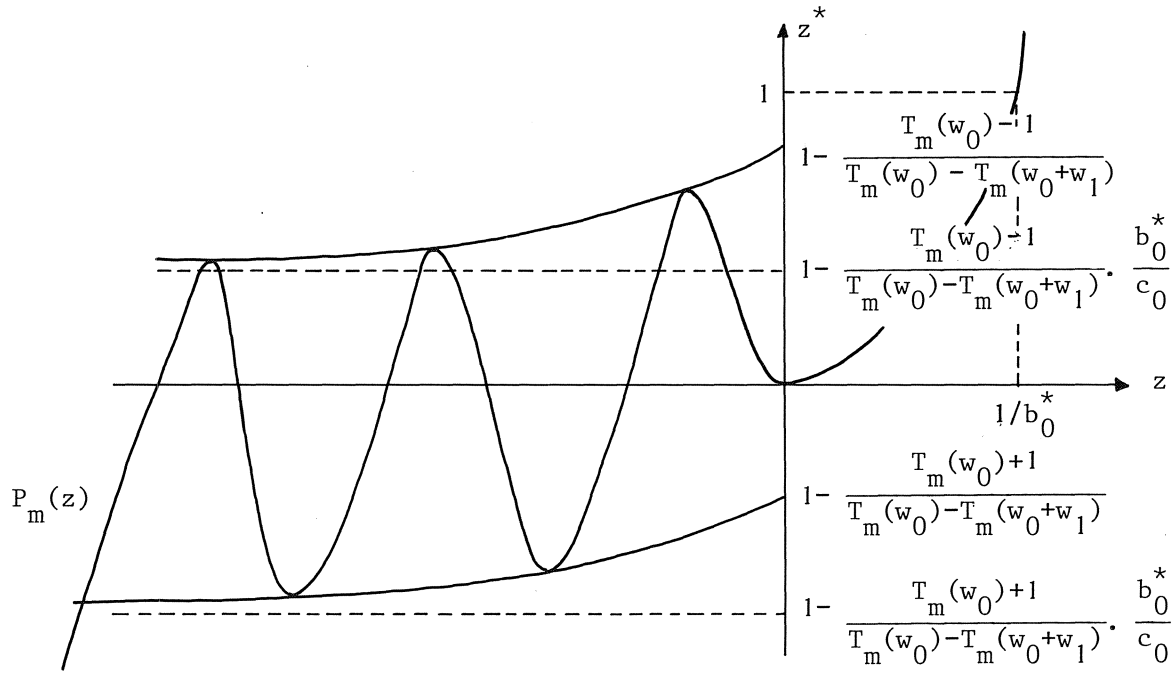

Figure B.1 The polynomial $P_m(z)$ of the family (B.1)

and in the second case we find

$$\text{(B.4b)} \qquad D_2 = 1 - \frac{T_m(w_0)-1}{T_m(w_0)-T_m(w_0+w_1)} \cdot \frac{b_0^*}{c_0}, \quad D_1 = \frac{1+T_m(w_0+w_1)}{T_m(w_0)-T_m(w_0+w_1)} \cdot$$

The equation (B.4) cannot be solved explicitly unless $D_1 = 0$. For $D_1 = 0$ we find the solution

$$w_0 = T_{\frac{1}{m}}\left(\frac{2}{D_2} - 1\right), \; w_1 = \cos\left(\frac{2\ell+1}{m}\pi\right) - w_0, \; \ell = 0, \pm 1, \ldots$$

(B.5)

$$\beta = \frac{1+\cos\left(\frac{2\ell+1}{m}\pi\right)}{b_0^*\left[T_{\frac{1}{m}}\left(\frac{2}{D_2} - 1\right) - \cos\left(\frac{2\ell+1}{m}\pi\right)\right]}, \; c_0 = b_0^* \; .$$

Evidently, one should choose $\ell=0$ in order to maximize β. The resulting values for β are slightly smaller than those listed in table 4.5.

For $D_1 > 0$ we solved (B.4) numerically for various values of D_1 and D_2. These experiments show that for values of $D_2 < \frac{1}{2}$ stability intervals are obtained which are hardly larger than those defined by (B.5). Therefore, we did not pursue the construction of second order iteration polynomials.

APPENDIX C

In order to justify the use of higher order time integrators for parabolic equations we derive an equation for the optimal order of accuracy with respect to the minimization of the number of right-hand side evaluations.

We assume that the integration interval $[0,T]$, the spectral radius $S = S(\partial f/\partial y)$, the stability constant c_p and the desired global error ε over the interval $[0,T]$ are given. Furthermore, we assume that ε and τ are related according to

$$\varepsilon = C(p,T)\tau^p, \tag{C.1}$$

where $C(p,T)$ is a function determined by the numerical method and the problem under consideration. This relation defines τ.

We now try to choose p such that the total number of right-hand side evaluations is minimized. This number is given by $N = Tm/\tau$, where m is the number of stages per integration step. According to the stability condition, m should be at least as large as $\sqrt{\tau S/c_p}$. Expressing τ in term of $C(p,T)$ and ε we find

$$N^2 = S\, T^2\, \frac{[C(p,T)]^{\frac{1}{p}}}{\varepsilon^{1/p}\, c_p}. \tag{C.2}$$

This expression is minimized if p satisfies the equation $dN^2/dp = 0$, which yields

$$p\, c_p' = c_p \left[\ell n\left(\frac{\varepsilon}{C(p,T)}\right)^{\frac{1}{p}} + \frac{C'(p,T)}{C(p,T)}\right], \tag{C.3}$$

where c_p' and $C'(p,T)$ denote the derivatives with respect to p of the functions c_p and $C(p,T)$. Using (C.1) this equation for the optimal order can be written as

$$p\, c' = c_p \left[\ell n\, \tau + \frac{C'(p,T)}{C(p,T)}\right]. \tag{C.3'}$$

Thus, the optimal combination of the order p and the integration step τ is determined by (C.3'). In practice, we usually do not know the function $C(p,T)$. However, in general we have $C'(p,T) \leq 0$ so that the optimal order $\bar{p}$ satisfies the inequality

$$\bar{p}\, c'_{\bar{p}} \leq c_{\bar{p}}\, \ell n\, \tau. \tag{C.4}$$

From this inequality lower bounds can be derived for the optimal order $\bar{p}$ as soon as the integration step τ is determined. In the following example it is shown that, rather surprisingly, this lower bound is relatively high even for large integration steps.

Example C.1 Consider the EP-BD formulas with the first order iteration polynomial (4.11). The asymptotic stability constant c_p can be approximated by

$$c_p = 2.3 - 0.53\,p + 0.035\,p^2, \quad 2 \leq p \leq 6.$$

Substitution into (C.4) yields the values listed in table C.1.

Table C.1 Lower bounds for the optimal order for various values of

τ =	0.568	0.392	0.259	0.180	0.176
$p^* \geq$	2	3	4	5	6

These values indicate that it is advantageous to use higher order EP-BD methods, even for rather large integration steps.

We recall that the values listed in table C.1 present lower bounds only if the error constant $C(p,T)$ is decreasing with p. Otherwise, the values of table C.1 should be considered as upper bounds

APPENDIX D

In this appendix we briefly summarize the numerical results of the EP-BD methods and the ADI method applied to problem (6.8)-(6.9). In table D.1 we list for the EP-BD methods the sd-values (cf. (6.7)) obtained, the required number N of right-hand side evaluations, as well as the functions C(p,T)(cf.(C.1)) and A(p) (cf. (6.11)). In table D.2 results are listed for the ADI method of Peaceman and Rachford (denoted by PR(i), i being the number of Newton iterations)

Table D.1 Results of the EP-BD methods applied to problem (6.8)-(6.9)

p	$\tau/2\pi$	N	sd	$C(p,T)=10^{-sd}/\tau^p$	$A(p)=\log N - sd/2p$
2	1/20		$-\infty$		
	1/30	1725	1.67	0.49	2.82
	1/40	1971	2.23	0.24	2.74
	1/60	2416	2.66	0.20	2.72
3	1/10		$-\infty$		
	1/20	1649	2.13	0.24	2.86
	1/30	1969	2.60	0.27	2.86
	1/40	2249	2.92	0.31	2.86
4	1/10	1472	1.52	0.19	2.98
	1/20	1920	2.89	0.13	2.92
	1/40	2612	4.19	0.11	2.89
5	1/10	1702	1.94	0.12	3.04
	1/20	2220	3.37	0.14	3.01
	1/40	3016	4.86	0.14	2.99
6	1/10	2043	2.13	0.12	3.13
	1/20	2656	4.13	0.08	3.08
	1/40	3587	6.21	0.04	3.04

Table D.2 Results for the ADI method applied to problem (6.8)-(6.9)

PR(i)	τ	N	sd	B(i)
PR(1)	$2\pi/80$	1600	2.42	1.994
PR(2)	$2\pi/80$	3200	3.67	1.670
PR(1)	$2\pi/160$	3200	3.03	1.990
PR(2)	$2\pi/160$	6400	4.28	1.666