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DEFECT CORRECTION ITERATION AND SPLITTING METHODS FOR  
TIME-DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

Preprint

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Defect correction iteration and splitting methods for time-dependent partial differential equations<sup>\*)</sup>

by

P.J. van der Houwen

ABSTRACT

Nonlinear defect correction iteration is applied for solving the implicit relations which arise when an implicit linear multistep method is used in order to integrate semi-discrete initial value problems for partial differential equations. The approximate inverse occurring in the defect correction process is obtained by employing splitting methods. In order to accelerate convergence second degree Chebyshev iteration is used which is tuned in such a way that the lower frequencies in the iteration error are strongly damped without using a large number of iterations.

KEY WORDS & PHRASES: *Numerical analysis, method of lines, initial-boundary value problems, defect correction, Chebyshev iteration, splitting methods*

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<sup>\*)</sup> This report will be submitted for publication elsewhere.



## 1. INTRODUCTION

Consider an initial-boundary value problem in two space dimensions and assume that this problem can be semi-discretized (by finite differences or finite element methods) into an explicit system of ordinary differential equations of the form

$$(1.1) \quad \frac{d^v y}{dt^v} = f(t, y), \quad v \geq 1,$$

where the boundary conditions are lumped into the right hand side and the initial condition is of the form

$$(1.2) \quad \frac{d^i y}{dt^i}(t_0) = y_0^{(i)}, \quad i = 0, \dots, v-1.$$

We assume that the Jacobian matrix  $\partial f / \partial y$  has *negative* eigenvalues.

Suppose that a linear multistep method is chosen for the integration of (1.1). Then in each integration step we have to solve a, usually nonlinear, system of equations of the form

$$(1.3) \quad y - b_0 \tau^v f(t_{n+1}, y) = \sum_{\ell=1}^k [a_{\ell} y_{n+1-\ell} - b_{\ell} \tau^v f(t_{n+1-\ell}, y_{n+1-\ell})],$$

where  $\tau$  is the stepsize  $t_{n+1} - t_n$ ,  $y_n$  the numerical approximation to  $y(t_n)$  and  $\{a_{\ell}, b_{\ell}\}$  coefficients specifying the  $k$ -step method chosen. The solution of (1.3) is denoted by  $\eta$ , the approximation to  $\eta$  obtained in actual computation by  $y_{n+1}$ . We will write (1.3) in the compact form

$$(1.3') \quad Ly = \Sigma.$$

In this paper we analyse a special class of nonlinear defect correction iteration methods for solving (1.3'). The special features of this iteration process are (i) the application of second degree Chebyshev iteration, (ii) the use of splitting functions in the definition of the approximate inverse of  $L$ , (iii) the strong damping of the lower frequencies by the amplification operator and (iv) the first order consistency of the iteration

result after (say)  $m$  iterations as  $\tau \rightarrow 0$  for fixed damping factors.

Since for computational reasons, one wishes a relatively low number of iterations, the iteration result may differ considerably from the solution of equation (1.3). Therefore, we will also consider the stability of the iteration result for a class of model problems.

In the near future, numerical experiments will be reported comparing the method proposed in this paper with conventional splitting methods.

## 2. DEFECT CORRECTION ITERATION

Suppose we want to solve the problem

$$(2.1) \quad Ly = \Sigma,$$

where  $L$  is a (nonlinear) operator in  $\mathbb{R}_r$  and  $\Sigma$  a given vector. We will assume that  $L$  has an inverse  $L^{-1}$ . For such problems one may define the (nonlinear) *defect correction step* (cf. STETTER [7] and HEMKER [2])

$$(2.2) \quad y^{(j+1)} = y^{(j)} + \tilde{L}_j^{-1}(\tilde{\Sigma}_j + \Sigma - Ly^{(j)}) - \tilde{L}_j^{-1}\tilde{\Sigma}_j, \quad j = 0, 1, \dots,$$

where  $y^{(0)}$  is an approximation to the solution  $\eta$  of (2.1),  $\tilde{\Sigma}_j$  are approximations to  $\Sigma$  and  $\tilde{L}_j^{-1}$  are approximations to  $L^{-1}$ .

In this paper we will consider the *two-step version* of nonlinear defect correction iteration. This may be defined by

$$(2.3) \quad y^{(j+1)} = \mu_j y^{(j)} + (1-\mu_j)y^{(j-1)} + \lambda_j[\tilde{L}_j^{-1}(\Sigma + \tilde{\Sigma}_j - Ly^{(j)}) - \tilde{L}_j^{-1}\tilde{\Sigma}_j],$$

$$\mu_0 = 1, \quad j = 0, 1, 2, \dots,$$

where  $\mu_j$  and  $\lambda_j$  are parameters which will be used in order to accelerate the convergence.

If the operators  $\tilde{L}_j^{-1}$  and  $L$  are differentiable then the iteration error  $\varepsilon_j = y^{(j)} - \eta$  of (2.3) satisfies a relation of the form

$$(2.4) \quad \varepsilon_{j+1} = [\mu_j - \lambda_j(\tilde{L}_j^{-1})'L']\varepsilon_j + (1-\mu_j)\varepsilon_{j-1} + O(\|\varepsilon_j\|^2),$$

where  $(\tilde{L}_j^{-1})'$  and  $L'$  denote the derivatives (Jacobian matrices) of the operators  $\tilde{L}_j^{-1}$  and  $L$  evaluated at  $\tilde{\Sigma}_j$  and  $\eta$ , respectively. We remark that the second order term in (2.4) vanishes if  $\tilde{L}_j^{-1}$  and  $L$  are affine operators.

In the analysis of the error equation (2.4) it turns out that we often cannot explicitly derive the matrix  $(\tilde{L}_j^{-1})'$  whereas the matrix  $(\tilde{L}_j')^{-1}$  is rather easily obtained. Therefore, we prove the following theorem.

**THEOREM 2.1.** *Let the operators  $L$ ,  $\tilde{L}_j$  and  $\tilde{L}_j^{-1}$  have bounded derivatives and let  $\tilde{L}_j'$  be nonsingular. If we choose*

$$(2.5) \quad \tilde{\Sigma}_j = \tilde{L}_j y^{(j)}$$

*then the iteration error satisfies the recurrence relation*

$$(2.4') \quad \varepsilon_{j+1} = [\mu_j - \lambda_j (\tilde{L}_j')^{-1} L'] \varepsilon_j + (1 - \mu_j) \varepsilon_{j-1} + O(\|\varepsilon_j\|^2),$$

*where  $\tilde{L}_j'$  and  $L'$  are evaluated at  $\eta$ .*

**PROOF.** If  $\tilde{\Sigma}_j$  is of the form (2.5) we can write (2.3) in the form

$$\tilde{L}_j \left( y^{(j)} + \frac{y^{(j+1)} - \mu_j y^{(j)} - (1 - \mu_j) y^{(j-1)}}{\lambda_j} \right) = \Sigma + \tilde{L}_j y^{(j)} - L y^{(j)}.$$

From this representation it is immediate that

$$\begin{aligned} & \tilde{L}_j' \left( \frac{\varepsilon_{j+1} - \mu_j \varepsilon_j - (1 - \mu_j) \varepsilon_{j-1}}{\lambda_j} \right) + O \left( \left\| \frac{\varepsilon_{j+1} - \mu_j \varepsilon_j - (1 - \mu_j) \varepsilon_{j-1}}{\lambda_j} \right\|^2 \right) = \\ & = -L' \varepsilon_j + O(\|\varepsilon_j\|^2), \end{aligned}$$

where  $\tilde{L}_j'$  and  $L'$  are evaluated at  $y^{(j)}$  and  $\eta$ , respectively. Substitution of (2.4) yields

$$\begin{aligned} & \tilde{L}_j' \left( \frac{\varepsilon_{j+1} - \mu_j \varepsilon_j - (1 - \mu_j) \varepsilon_{j-1}}{\lambda_j} \right) + O(\|(\tilde{L}_j^{-1})' L' \varepsilon_j\|^2) = \\ & = -L' \varepsilon_j + O(\|\varepsilon_j\|^2). \end{aligned}$$

From the boundedness of  $L'$ ,  $\tilde{L}_j'$  and  $(\tilde{L}_j^{-1})'$  equation (2.4') is immediate.  $\square$

In this paper it will be assumed that  $\tilde{\Sigma}_j$  is defined by (2.5).

### 2.1. Chebyshev iteration

In the special case where  $\tilde{L}_j^1$  does not depend on  $j$  and  $\tilde{L}_j^{-1}$ ,  $L$  are *affine*, the process (2.3) reduces to the familiar polynomial iteration method [12]. we find

$$(2.4'') \quad \varepsilon_{j+1} = P_{j+1}(\tilde{L}^{'-1}L')\varepsilon_0, \quad j = 0, 1, \dots,$$

where  $P_j$  is a polynomial of degree  $j$  in  $\tilde{L}^{'-1}L'$  generated by the recurrence relation

$$(2.6) \quad P_0(\alpha) = 1, \quad P_{j+1}(\alpha) = (\mu_j - \lambda_j \alpha)P_j(\alpha) + (1 - \mu_j)P_{j-1}(\alpha), \quad j = 0, 1, \dots$$

We will assume that the *iteration matrix*  $\tilde{L}^{'-1}L'$  has its eigenvalues  $\alpha$  in the positive interval  $[\bar{a}, \bar{b}]$ . Then all eigenvector components in the iteration error corresponding to eigenvalues in the interval  $[a, b]$  are maximally damped if we choose

$$(2.7) \quad P_j(\alpha) = \frac{T_j(w_0 + w_1 \alpha)}{T_j(w_0)}, \quad w_0 = \frac{b+a}{b-a}, \quad w_1 = \frac{2}{a-b}.$$

Since  $T_j$  satisfies a recurrence relation of the form (2.6) we can find expressions for the parameters  $\mu_j$  and  $\lambda_j$ . The resulting method is the well-known *Richardson method* [12] (or *Chebyshev iteration method*) applied to the preconditioned problem ( $\tilde{L}_j^{-1}$  does not depend on  $j$  because it is affine)

$$(2.1') \quad \tilde{L}^{-1}Ly = \tilde{L}^{-1}\Sigma.$$

If  $\tilde{L}_j^{'-1}$  does not depend on  $j$  but  $\tilde{L}_j^{-1}$ ,  $\tilde{L}$  are *nonlinear*, we formally may define the parameters  $\mu_j$  and  $\lambda_j$  by (2.6) and (2.7). Then, neglecting second order terms, (2.4'') presents a first order approximation to the error equations. Thus, for *sufficiently close initial approximations*  $y^{(0)}$  the error equation (2.4'') can be used in the analysis of the iteration process.

In this paper it will be assumed that  $\tilde{L}_j^1$  does not depend on  $j$ .



## 2.2. Damping of low frequencies and consistency

In the usual application of iteration processes of the form (2.3), one chooses the parameters such that all frequencies in the initial error  $\varepsilon_0 = y^{(0)} - \eta$  are damped by roughly the same factor. However, if the problem (2.1) originates from a partial differential equation, then often the solution mainly consists of low frequency modes so that one chooses the discrete problem (2.1) such that its solution  $\eta$  does not contain high frequencies (for example, the backward differentiation formulas). Thus, if the initial approximation  $y^{(0)}$  does not contain high frequencies (e.g. if  $y^{(0)}$  is obtained by extrapolation of preceding  $y_n$  values) then  $\varepsilon_0$  will also be free of high frequencies. In such cases only the low frequencies should be strongly damped whereas the high frequencies need only marginal damping. If the low frequencies correspond to large eigenvalues of the iteration matrix this can be achieved by choosing  $a \gg \bar{a}$  and  $b = \bar{b}$  where  $[\bar{a}, \bar{b}]$  denotes the (positive) spectrum of the iteration matrix. As a consequence, the damping of the low frequencies increases considerably as is immediately clear from (2.7) which yields the *damping factor*  $D$  defined by

$$(2.8) \quad D := \max_{a \leq \alpha \leq b} |P_m(\alpha)| = T_m^{-1}\left(\frac{b+a}{b-a}\right) \cong \left\{ \cosh\left(2m \left[ \sqrt{\frac{a}{b-a}} + O\left(\frac{a}{b-a}\right) \right] \right) \right\}^{-1}$$

as  $a/(b-a) \ll 1$  ( $< .025$  say). It turns out that in most applications  $a/(b-a)$  is rather small so that for prescribed damping  $D$  the number of iterations  $m$  can be found from the approximate expression for  $D$ , i.e.

$$(2.8') \quad m \cong \frac{1}{2} \sqrt{\frac{b-a}{a}} \operatorname{arcosh} \frac{1}{D}.$$

It is the purpose of this paper to derive iteration processes of the form (2.3) which strongly damp the low frequency modes and which have a modest damping of the higher frequencies. In the analysis we assume that only a few iterations are performed, otherwise the method becomes too expensive. As a consequence,  $y^{(m)}$  may differ considerably from the solution of (1.3). This implies that one should consider the consistency of the result  $y^{(m)}$  as  $\tau \rightarrow 0$ . Evidently, the local error  $y^{(m)} - y(t_{n+1})$  at  $t_{n+1}$  consists of the local error  $\eta - y(t_{n+1})$  of the generating multistep formula and the iteration error  $\varepsilon_m$ , approximately given by (2.4"). Let the matrix

$\tilde{L}'^{-1}L'$  converge to the matrix  $\alpha_0 I$  as  $\tau \rightarrow 0$ , i.e.

$$(2.9) \quad \tilde{L}'^{-1}L' = \alpha_0 I + \tau^r B(\tau), \quad r \geq 1,$$

where  $B(\tau)$  is a nonvanishing, uniformly bounded matrix as  $\tau \rightarrow 0$ . Then

$$(2.10) \quad \begin{aligned} \varepsilon_m = P_m(\tilde{L}'^{-1}L')\varepsilon_0 = [P_m(\alpha_0)I + \tau^r P'_m(\alpha_0)B(\tau) + \\ + \frac{1}{2}\tau^{2r} P''_m(\alpha_0)B^2(\tau) + \dots]\varepsilon_0 + O(\|\varepsilon_0\|^2). \end{aligned}$$

From the definition (2.7) of  $P_m(\alpha)$  we derive that

$$(2.10') \quad \begin{aligned} \varepsilon_m = T_m^{-1}(w_0)[T_m(w_0+w_1\alpha_0) + w_1 T'_m(w_0+w_1\alpha_0)\tau^r B(\tau) + \\ + \frac{1}{2}w_1^2 T''_m(w_0+w_1\alpha_0)\tau^{2r} B^2(\tau) + \dots]\varepsilon_0 + O(\|\varepsilon_0\|^2). \end{aligned}$$

Introducing the damping factor  $D$  and observing that

$$w_1 = \frac{-2}{b-a} > -\frac{2}{[\sqrt{b}+\sqrt{a}]^2} \sqrt{\frac{m}{2D}}$$

we obtain

$$(2.11) \quad \begin{aligned} \|\varepsilon_m\| \leq D \left[ |T_m(w_0+w_1\alpha_0)| + \frac{\tau^r}{\sqrt{\frac{m}{D/2}}} |T'_m(w_0+w_1\alpha_0)| \|\bar{B}(\tau)\| + \right. \\ \left. + \frac{1}{2} \left( \frac{\tau^r}{\sqrt{\frac{m}{D/2}}} \right)^2 |T''_m(w_0+w_1\alpha_0)| \|\bar{B}(\tau)\|^2 + \dots \right] \|\varepsilon_0\| + O(\|\varepsilon_0\|^2), \end{aligned}$$

where  $\bar{B}(\tau)$  denotes the "normalized" matrix  $2B(\tau)/[\sqrt{a}+\sqrt{b}]^2$  and  $D$  is assumed to be a given number independent of  $\tau$  (e.g.  $D = 1/10$ ).

The estimate (2.11) is suitable for practical use if  $\tau$  is sufficiently small, i.e.

$$(2.12) \quad \tau^r \ll \|\bar{B}(\tau)\| \sqrt{\frac{m}{D/2}}.$$

In this range of integration steps the iteration error  $\varepsilon_m$  can be decreased

if we are able to choose  $T_m(w_0 + w_1 \alpha_0) = 0$ , i.e.

$$(2.13) \quad w_0 + w_1 \alpha_0 = \cos \frac{2\ell+1}{2m} \pi, \quad \ell \in \{0, 1, \dots, m-1\},$$

or equivalently

$$(2.13') \quad a = \frac{2\alpha_0 + b[\cos \frac{2\ell+1}{2m} \pi - 1]}{\cos \frac{2\ell+1}{2m} \pi + 1}, \quad \ell \in \{0, 1, \dots, m-1\},$$

where we assume

$$(2.14) \quad b > \alpha_0 > \frac{1}{2}b(1 - \cos \frac{2\ell+1}{2m} \pi).$$

Substitution of (2.13) into (2.11) and using the relation

$$T'_m(w) = m \sqrt{\frac{1 - T_m^2(w)}{1 - w^2}}$$

yields

$$(2.15) \quad \|\varepsilon_m\| \leq D \left[ \frac{m}{\sin \frac{2\ell+1}{2m} \pi} \frac{\tau^r \|\bar{B}(\tau)\|}{\sqrt[m]{D/2}} + O\left(\left[\frac{\tau^r \bar{B}(\tau)}{\sqrt[m]{D/2}}\right]^2\right) \right] \|\varepsilon_0\|, \quad \text{as } \tau \rightarrow 0.$$

Firstly, this estimate shows that for fixed damping factor  $D$

$$\|y^{(m)} - y(t_{n+1})\| = \|\varepsilon_m\| + O(\tau^{p+v}) \leq O(\tau^{p+v} + \tau^{q+v+r}) \quad \text{as } \tau \rightarrow 0,$$

where  $p$  and  $q$  are the orders of consistency of the generating multistep method and of the predictor formula used for  $y^{(0)}$ . Thus the order of consistency  $\tilde{p}$  is given by

$$(2.16) \quad \tilde{p} = \min\{p, q+r\}.$$

Notice that  $\tilde{p} = \min\{p, q\}$  if the consistency condition (2.13) is not satisfied.

Secondly, we observe that for given  $D$  the value of  $m$  should be minimized, that is in (2.8') the value of  $(b-a)/a$  should be made as small as possible. In view of (2.13') this means that

$$\frac{b-a}{a} = 2 \frac{b - \alpha_0}{2\alpha_0 + b(\cos \frac{2\ell+1}{2m} \pi - 1)}$$

should be minimized. This implies that  $\ell = 0$  is the best choice.

### 3. THE APPROXIMATE INVERSE

In order to define the approximate inverse  $\tilde{L}_j^{-1}$  for the problem (1.1) we use the formalism developed in [4] and introduce the *splitting* function  $F(t, u, v)$  which is such that

$$(3.1) \quad F(t, y, y) \equiv f(t, y).$$

This rather general splitting function includes a number of well-known splittings such as the ADI splittings [6] and the hopscotch splittings [1]. It is convenient to introduce the Jacobian matrices

$$(3.2) \quad Z_1 = b_0 \tau^v \frac{\partial F}{\partial u}, \quad Z_2 = b_0 \tau^v \frac{\partial F}{\partial v}, \quad Z = Z_1 + Z_2,$$

which are both evaluated at  $(t_{n+1}, \eta, \eta)$ . The eigenvalues of  $Z_i$ ,  $Z$  will be denoted by  $z_i$  and  $z$ , respectively. We assume that  $Z$  has negative eigenvalues in the interval  $[-S, 0)$  and that the algebraically large eigenvalues correspond to eigenvectors of low frequency. The spectral radius of  $\partial f / \partial y$  is given by  $S/b_0 \tau^v$  and will be denoted by  $\sigma$ .

#### 3.1. Successive corrections

##### 3.1.1. One-stage approximations

A relatively simple class of methods is based on the approximate inverse  $\tilde{L}_j^{-1}: \Sigma \rightarrow y$  defined by the one-stage formula

$$(3.3) \quad \omega y + (1-\omega)y^{(j)} - b_0 \tau^v F(t_{n+1}, y, y^{(j)}) = \Sigma, \quad \omega \neq 0,$$

which leads to the (stationary) iteration matrix

$$(3.4) \quad \tilde{L}'^{-1} L' = [\omega - Z_1]^{-1} [I - Z_1 - Z_2].$$

Examples of splitting functions which are suitable for use in (3.3) are the Jacobi and Gauss-Seidel splittings.

By writing (3.4) in the form (2.9), that is

$$(3.4') \quad \tilde{L}'^{-1} L' = \frac{1}{\omega} - b_0 \tau^v [\omega - b_0 \tau^v \frac{\partial F}{\partial u}]^{-1} [\frac{\omega-1}{\omega} \frac{\partial F}{\partial u} + \frac{\partial F}{\partial v}],$$

we see that  $\alpha_0 = 1/\omega$ ,  $r = v$  and that  $B(\tau)$  is uniformly bounded as  $\tau \rightarrow 0$ . Hence, the error equation (2.15) applies provided that (2.14) holds:

$$(3.5) \quad \frac{1}{b} < \omega < \frac{2}{b(1 - \cos \frac{(2\ell+1)\pi}{2m})}.$$

Within this range of  $\omega$ -values we try to minimize the factor  $(b-a)/b$  in (2.8'). In addition, however, we require that the interval  $[a, b]$  contains sufficiently many eigenvalues of eigenvectors of low frequency.

Let us consider the important case where  $Z_1$  is given by

$$(3.6) \quad Z_1 = -\theta SI.$$

Then

$$(3.7) \quad a = \frac{2 + \omega b (\cos \frac{2\ell+1}{2m} \pi - 1)}{\omega (\cos \frac{2\ell+1}{2m} \pi + 1)}, \quad b = \bar{b} = \frac{1+S}{\omega + \theta S}, \quad \bar{a} = \frac{1}{\omega + \theta S}.$$

The eigenvalues corresponding to the lower frequencies are in the neighbourhood of  $\bar{a}$ . In Figure 3.1 the corresponding polynomial  $P_m(\alpha)$  is illustrated for  $m = 6$ .

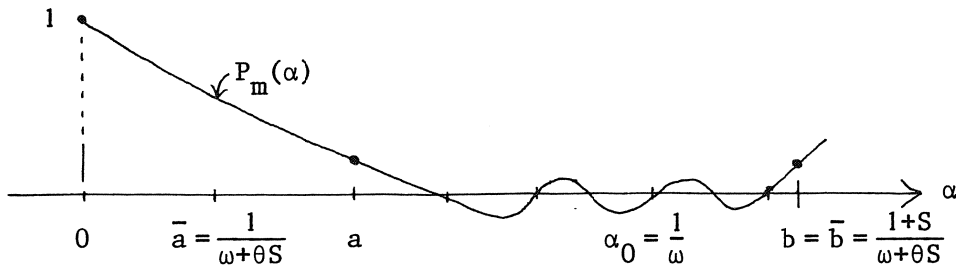


Fig. 3.1 The polynomial  $P_m(\alpha)$  for  $m = 6$ .

If  $\theta = 0$  the iteration process does not contain implicit relations and can be considered as an *explicit Runge-Kutta method* of a special form. Related methods were analysed in [5]. If  $\theta \neq 0$ , e.g.  $\theta = \frac{1}{2}$ , the iteration process only contains *scalarly implicit relations* which may be attractive from a computational point of view (notice that this process is identical to nonlinear Jacobi iteration if  $\text{diag}[\partial f/\partial y] = -\theta SI$ ). However, from Figure 3.1 we conclude that choosing  $(\bar{b}-\bar{a})/\bar{b}$  small means that all eigenvectors of low frequency are not damped unless  $\theta S$  is so small that  $\bar{a} \cong a$ . In practice,  $\theta S = \theta b_0 \tau^\nu \sigma$  is usually rather large because the integration step  $\tau$  is much greater than  $\sigma^{-1/\nu}$ ,  $\sigma$  being the spectral radius of  $\partial f/\partial y$ . Hence in order to damp low frequencies we should choose  $\omega$  such that  $\bar{a} \cong a$ , that is

$$(3.8) \quad \omega = \frac{2\theta}{1 - \cos \frac{2\ell+1}{2m} \pi}.$$

This value for  $\omega$  satisfies the inequality (3.5) for all  $\theta > 0$ . The asymptotic error estimate is given by (2.15) where  $m$  is determined by (2.8'), i.e.

$$(3.9) \quad m = \frac{1}{2}\sqrt{S} \operatorname{arcosh}\left(\frac{1}{D}\right) \cong \frac{1}{2}\sqrt{S} \ln \frac{2}{D} \quad \text{as } S \gg 1 \text{ and } D \ll 1.$$

Unless  $D \cong 1$  this value for  $m$  is extremely large because of the usually large values of  $S$ .

### 3.1.2. Two-stage approximations

In this section iteration matrices are considered of which the large eigenvalues correspond to eigenvectors of low frequency. This enables us to get a strong damping of the lower frequencies without an extremely large number of iterations.

Consider the operator  $\tilde{L}_j^{-1}: \Sigma \rightarrow y$  defined by the two-stage formula

$$(3.11) \quad \begin{aligned} \omega y + (1-\omega)y^* - b_0 \tau^\nu F(t_{n+1}, y, y^*) &= \Sigma, \\ \omega y^* + (1-\omega)y^{(j)} - b_0 \tau^\nu F(t_{n+1}, y^{(j)}, y^*) &= \Sigma, \end{aligned} \quad \omega \neq 0, \frac{1}{2}.$$

An elementary calculation leads to the iteration matrix

$$(3.12) \quad \tilde{L}'^{-1} L' = (2\omega-1)[\omega - Z_1]^{-1}[\omega - Z_2]^{-1}[I - Z_1 - Z_2].$$

By writing (3.11) in the form (2.9) we see that

$$(3.13) \quad \alpha_0 = \frac{2\omega-1}{\omega^2}, \quad r = v$$

and that  $B(\tau)$  is uniformly bounded as  $\tau \rightarrow 0$ . Thus, (2.15) holds provided that inequality (2.14) is satisfied. This inequality gives an interval of  $\omega$ -values and within this interval one should try to minimize the factor  $(b-a)/b$  occurring in (2.8') and at the same time to include sufficiently many eigenvalues of low frequency eigenvectors in the interval  $[a, b]$ .

In the following we consider in more details the model problem where  $Z$  and  $\omega - Z_1$  share the same eigensystem of which the eigenvectors of low frequency correspond to eigenvalues of small magnitude. Then from (2.13') and (3.12) we find (with  $\ell = 0$ )

$$(3.14a) \quad a = \frac{2(2\omega-1) + \omega^2 b (\cos \frac{\pi}{2m} - 1)}{\omega^2 (\cos \frac{\pi}{2m} + 1)},$$

$$(3.15) \quad \bar{a} = (2\omega-1) \frac{2S+1}{(S+\omega)^2}, \quad \bar{b} = \frac{2\omega-1}{\omega} \frac{S+1}{S+\omega},$$

where we have assumed that  $\bar{a} \leq \alpha_0 \leq b$ , that is

$$(3.16) \quad 1 \leq \omega \leq \frac{1}{2}[1 + \sqrt{2S+1}].$$

Since  $S$  is usually rather large we choose instead of  $b = \bar{b}$

$$(3.14b) \quad b = \frac{2\omega-1}{\omega} \geq \bar{b} = \frac{2\omega-1}{\omega} [1 + O(\frac{1}{S})] \quad \text{as } S \rightarrow \infty.$$

In Figure 3.2 the corresponding polynomial  $P_m(\alpha)$  is illustrated for  $S \gg 1$ .

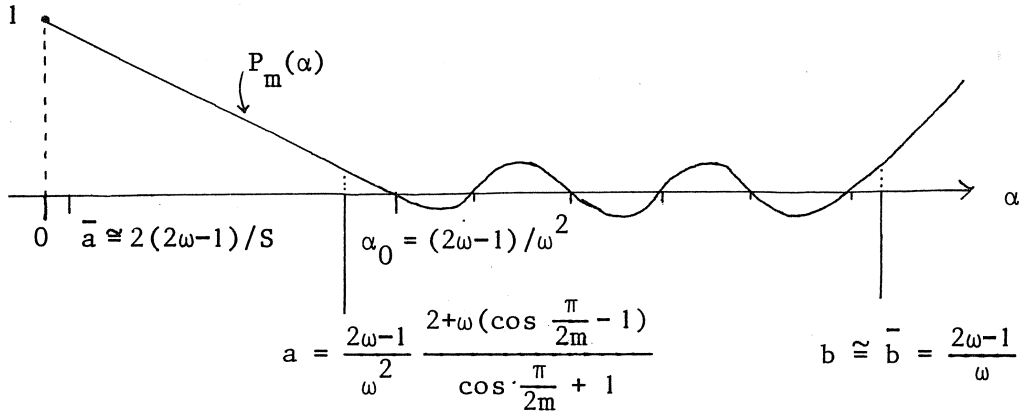


Fig. 3.2 The polynomial  $P_m(\alpha)$  for  $S \gg 1$

Evidently, the low frequency eigenvectors have eigenvalues in the neighbourhood of  $\alpha_0$  which is different from the situation in the preceding section where these eigenvalues are in the neighbourhood of  $\bar{a}$ . In order to see what eigenvalues correspond to the damped eigenvectors we show in Figure 3.3 in the  $(z_1, z_2)$ -plane the region corresponding to the interval  $a \leq \alpha \leq b$ .

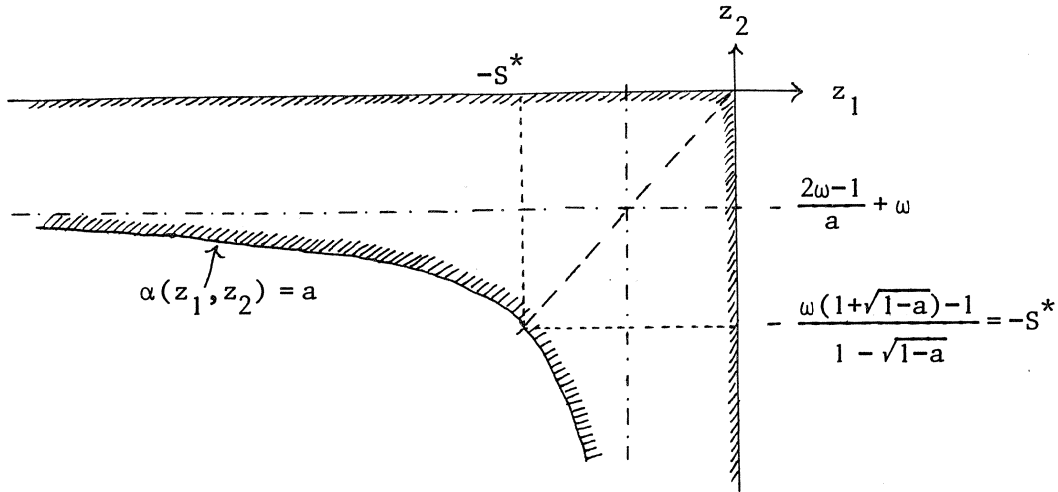


Fig. 3.3 Region of damping in the  $(z_1, z_2)$ -plane.

The magnitude of this damping region can be characterized by the quantity

$$(3.17) \quad S^* := \frac{\omega(1 + \sqrt{1-a}) - 1}{1 - \sqrt{1-a}}, \quad a \leq \frac{2\omega-1}{\omega^2}$$



(the inequality for  $a$  follows from  $\alpha(0,0) \geq a$ ).

Let  $S^*$  be prescribed then

$$(3.17') \quad a = \frac{(2\omega-1)(2S^*+1)}{(S^*+\omega)^2}, \quad 1 \leq \omega \leq \frac{1}{2}[1 + \sqrt{2S^*+1}]$$

and from (3.14a) we find that  $\omega$  should satisfy the (consistency) equation

$$(3.18) \quad (2S^*+1)(\cos \frac{\pi}{2m} + 1)\omega^2 = [2 + \omega(\cos \frac{\pi}{2m} - 1)](S^*+\omega)^2.$$

The error inequality (2.15) holds with  $m$  and  $D$  related to each other by the equation

$$(3.19) \quad D = T_m^{-1} \left( \frac{S^{*2} + 4\omega S^* + \omega^2 + \omega}{S^{*2} + \omega^2 - \omega} \right).$$

In Table 3.1 the values  $(\omega, D)$  are given satisfying (3.18) and (3.19) for various values of  $m$  and  $S^*$ . All  $\omega$ -values turn out to be in the range (3.16). By means of this table we can determine appropriate values for  $m$  and  $\omega$  when  $S^*$  and  $D$  are prescribed.

It may be of interest to determine the minimal damping factor  $D$  if  $\omega$  is not required to satisfy (3.18). An elementary calculation reveals that for given  $m$  and  $S^*$  expression (3.19) decreases as  $\omega$  increases to reach its minimal value at  $\omega = S^*$ . In view of (3.17) the optimal value of  $\omega$  is obviously given by

$$\omega_{\text{opt}} = \frac{1}{2}[1 + \sqrt{2S^*+1}].$$

Table 3.1:  $(\omega; D)$ -values for various values of  $m$  and  $S^*$  with and without satisfying the consistency condition (3.18).

$S^*$	$m=1$	$m=2$	$m=3$	$m=4$	$\omega=\omega_{\text{opt}}$
1	(1.15;.15)	(1.29;.01)	(1.33; $10^{-3}$ )	(1.34; $7_{10}^{-5}$ )	(1.37; $7_{10}^{-5}$ )
2	(1.26;.26)	(1.50;.03)	(1.56; $4_{10}^{-3}$ )	(1.58; $4_{10}^{-4}$ )	(1.62; $4_{10}^{-4}$ )
4	(1.40;.40)	(1.80;.07)	(1.90;.01)	(1.94; $2_{10}^{-3}$ )	(2.00; $2_{10}^{-3}$ )
6	(1.49;.49)	(2.02;.10)	(2.17;.02)	(2.23; $4_{10}^{-3}$ )	(2.30; $4_{10}^{-3}$ )
8	(1.55;.55)	(2.20;.12)	(2.39;.03)	(2.46; $6_{10}^{-3}$ )	(2.56; $6_{10}^{-3}$ )
10	(1.60;.60)	(2.36;.15)	(2.59;.04)	(2.67; $9_{10}^{-3}$ )	(2.79; $8_{10}^{-3}$ )
50	(1.87;.87)	(3.84;.41)	(4.67;.16)	(5.02;.06)	(5.52;.05)
100	(1.93;.93)	(4.58;.55)	(5.99;.26)	(6.63;.11)	(7.59;.10)

The last column of Table 3.1 contains the  $(\omega_{\text{opt}}; D)$ -values for  $m = 4$  showing that even for  $S^*$  as large as 100 the damping factor  $D$  is hardly better by choosing  $\omega = \omega_{\text{opt}}$ . (For  $m < 4$  the damping is slightly weaker if the consistency condition (3.18) is imposed.) Hence, in practice we may proceed as follows. For given values of  $S^*$  and  $D$  we approximate the corresponding value of  $\omega$  by  $\omega_{\text{opt}}$  and determine  $m$  by (3.19), that is

$$(3.19') \quad m \cong \left[ \operatorname{arccosh} \left( 1 + 2 \frac{1 + \sqrt{2S^* + 1}}{S^*} \right) \right]^{-1} \operatorname{arccosh} \frac{1}{D} \\ \cong .42 [S^*]^{1/4} \ln \frac{2}{D} \quad \text{as } D \ll 1 \text{ and } S^* \gg 1.$$

Next the correct value of  $\omega$  is found by solving (3.18) and finally we check whether the damping factor  $D$  defined by (3.19) is acceptable.

A comparison of (3.19') and (3.9) reveals that the number of iterations  $m_1$  of the one-stage operator and the number of iterations  $m_2$  of the two-stage operator, needed to produce the same damping  $D$ , are related by the formula

$$m_2 = .82 \sqrt[4]{\frac{S^*}{S^2}} m_1 \quad \text{as } D \ll 1 \text{ and } S^* \gg 1.$$

Thus, even for  $S^* = S$ , the two-stage formula is usually much more efficient.

We conclude this section by writing down explicitly the integration method obtained for the two-stage operator (3.11). From (2.3), (2.5) and (3.11) it follows that the scheme can be simplified to the form

$$(3.20) \quad y^{(j+1)} = (\mu_j - \lambda_j) y^{(j)} + (1 - \mu_j) y^{(j-1)} + \lambda_j \tilde{L}_j^{-1} \Sigma, \quad j = 0, 1, \dots, m.$$

Again using (3.11) yields

$$(3.20'a) \quad y^{(j+1)} = (\mu_j - \lambda_j) y^{(j)} + (1 - \mu_j) y^{(j-1)} + \lambda_j y^{\bullet}, \quad j = 0, 1, \dots, m-1,$$

where  $y^{\bullet}$  is to be computed by solving the system

$$(3.20'b) \quad \omega y^{\bullet} + (1-\omega)y^* - b_0 \tau^v F(t_{n+1}, y^{\bullet}, y^*) = \Sigma,$$

$$\omega y^* + (1-\omega)y^{(j)} - b_0 \tau^v F(t_{n+1}, y^{(j)}, y^*) = \Sigma.$$

As we already observed, the parameters  $\mu_j$  and  $\lambda_j$  are obtained from the Chebyshev recursion formula, i.e.

$$(3.20'c) \quad \mu_0 = \frac{1}{2}(b+a)\lambda_0 = 1, \quad \mu_j = 2w_0 \frac{T_j(w_0)}{T_{j+1}(w_0)}, \quad \lambda_j = \frac{2\mu_j}{b+a}, \quad w_0 = \frac{b+a}{b-a}, \quad j = 1, 2, \dots, m-1,$$

where  $a$  and  $b$  are given by (3.14). We remark that for  $S^* = 0$  the scheme (3.20) reduces to the multistep splitting method analysed in [3]. (By virtue of (3.18)  $S^* = 0$  implies that  $\omega = 1$ ,  $D = 0$ ,  $a = b = 1$  and hence  $\mu_j = \lambda_j = 1$  which leads to [3, scheme (3.3)].)

### 3.1.3. Multistage approximations

Next consider the operator  $\tilde{L}_j^{-1}: \Sigma \rightarrow y$  defined by the  $\tilde{m}$ -stage formula (compare similar operators employed in linear elliptic equations e.g. in [12, p.518])

$$(3.21) \quad y_0^* = y^{(j)}$$

$$\omega_i y_i^* + (1-\omega_i) \bar{y}_{i-1}^* - b_0 \tau^v F(t_{n+1}, y_i, \bar{y}_{i-1}^*) = \Sigma, \quad i = 1, 2, \dots, \tilde{m},$$

$$\omega_i \bar{y}_{i-1}^* + (1-\omega_i) y_{i-1}^* - b_0 \tau^v F(t_{n+1}, y_{i-1}^*, \bar{y}_{i-1}^*) = \Sigma$$

$$y = y_{\tilde{m}}^*.$$

The corresponding iteration matrix is given by

$$(3.22) \quad \tilde{L}^{-1} L = I - \prod_{i=\tilde{m}}^1 [\omega_i - Z_1]^{-1} [\omega_i - Z_2]^{-1} [\omega_i - 1 + Z_2] [\omega_i - 1 + Z_2]$$

which can be written in the form (2.9) with

$$(3.23) \quad \alpha_0 = 1 - \prod_{i=1}^{\tilde{m}} \left( \frac{\omega_i - 1}{\omega_i} \right)^2, \quad r = v$$

and  $B(\tau)$  uniformly bounded in  $\tau$ . Assuming that the parameters  $\omega_i$  satisfy the inequality (3.16) and restricting our considerations to the same class of model problems as in the preceding section, we find that

$$(3.24) \quad \bar{b} \leq 1 + \frac{\omega_\ell - 1}{\omega_\ell} \frac{S - \omega_\ell + 1}{S + \omega_\ell} \prod_{i=\ell} \left[ \frac{S - \omega_i + 1}{S + \omega_i} \right]^2 \cong \frac{2\omega_\ell - 1}{\omega_\ell} \quad \text{as } S \rightarrow \infty,$$

where  $\ell$  is such that  $(\omega_\ell - 1)/\omega_\ell$  is maximal. We define  $a$  by (2.11) and put

$$(3.25) \quad b = \max_i \frac{2\omega_i - 1}{\omega_i}.$$

The damping region  $a \leq \alpha(z_1, z_2) \leq b$  in the  $(z_1, z_2)$ -plane contains the region defined by

$$(3.26) \quad \prod_{i=1}^{\tilde{m}} \left| \frac{\omega_i - 1 + z_\ell}{\omega_i - z_\ell} \right| \leq \sqrt{1-a}, \quad \ell = 1, 2.$$

We now use the following lemma.

LEMMA 3.1. *In the interval  $A \leq x \leq B$  the function*

$$\psi_m(x) = \prod_{i=1}^m \frac{x - \theta_i}{x + \theta_i}, \quad \theta_i = B \left[ \frac{A}{B} \right]^{\frac{i-1}{m-1}}, \quad 0 < A < B, \quad m \geq 2$$

*is bounded by*

$$\left[ \frac{1 - C_m}{1 + C_m} \right]^2, \quad C_m = \left[ \frac{A}{B} \right]^{\frac{1}{2(m-1)}}.$$

PROOF. See YOUNG [12, p.528].  $\square$

The parameters  $\theta_i$  were proposed by WACHSPRESS [10]. We apply this lemma with

$$x = \frac{1}{2} - z_\ell, \quad A = \frac{1}{2}, \quad B = \frac{1}{2} + S^*, \quad m = \tilde{m}, \quad \theta_i = \omega_i - \frac{1}{2}.$$

Thus, if

$$(3.27) \quad \omega_i = \frac{1}{2} + \frac{1}{2}(2S^* + 1)^{\frac{\tilde{m}-i}{\tilde{m}-1}}, \quad i = 1, 2, \dots, \tilde{m} \geq 2,$$

then,

$$\prod_{i=1}^{\tilde{m}} \left| \frac{\omega_i^{-1+z_\ell}}{\omega_i^{-z_\ell}} \right| \leq \left[ \frac{1-C_{\tilde{m}}}{1+C_{\tilde{m}}} \right]^2, \quad C_{\tilde{m}} = [2S^*+1]^{\frac{-1}{2(\tilde{m}-1)}}$$

for  $-S^* \leq z_\ell \leq 0$  (note that the left hand side is bounded by one for all negative values of  $z_\ell$ ). Hence, if  $a$  is chosen such that

$$(3.28) \quad \sqrt{1-a} = \left[ \frac{1-C_{\tilde{m}}}{1+C_{\tilde{m}}} \right]^2,$$

i.e.

$$a = \frac{8C_{\tilde{m}}(1+C_{\tilde{m}}^2)}{(1+C_{\tilde{m}})^4},$$

then (3.26) is satisfied for all  $(z_1, z_2)$  in the square  $-S^* \leq z_1, z_2 \leq 0$ . However,  $a$  is also prescribed by (2.11), so that the consistency equation

$$(3.29) \quad \frac{8C_{\tilde{m}}(1+C_{\tilde{m}}^2)}{(1+C_{\tilde{m}})^4} = \frac{2 + b(\cos \frac{\pi}{2m} - 1)}{\cos \frac{\pi}{2m} + 1}, \quad b = \frac{2}{1 + C_{\tilde{m}}^{2(\tilde{m}-1)}}$$

should be satisfied (notice that  $\alpha_0 = 1$  because  $\omega_{\tilde{m}} = 1$ ). Here,  $S^*$  cannot be chosen freely as in the preceding section. In Table 3.2 a few values of  $(S^*, D)$  are given, where  $S^*$  satisfies (3.19'). The asymptotic

Table 3.2.  $(S^*; D)$  values for various values of  $m$  and  $\tilde{m}$   
with  $S^*$  satisfying (3.29)

	$\tilde{m} = 2$	$\tilde{m} = 3$	$\tilde{m} = 4$
$m = 1$	$(\infty; 1)$	$(\infty; 1)$	$(\infty; 1)$
$m = 2$	$(9; .080)$	$(223; .093)$	$(4805; .094)$
$m = 3$	$(3.7; 8_{10}^{-3})$	$(47; .013)$	$(482; .014)$

error estimate (2.15) holds for the  $(m, D)$ -values occurring in this table.

In order to compare the efficiency of the two-stage operator and the multistage Wachspress operator we consider the number of iterations given by (3.29) and the quantity  $\tilde{m}m$  giving the number of "iterations" of the present process. In terms of  $S^*$  and  $D$  we have

$$(3.30) \quad \tilde{m}m = \tilde{m} \left[ \operatorname{arccosh} \left( \frac{b+a}{b-a} \right) \right]^{-1} \operatorname{arccosh} \left( \frac{1}{D} \right) \cong \frac{\tilde{m}}{4} [2S^*]^{-\frac{1}{4(\tilde{m}-1)}} \ln \frac{2}{D}$$

as  $D \ll 1$  and  $S^* \gg 1$ .

Taking (3.19') and (3.30) as a measure for the computational effort of the two-stage and multistage methods, we may conclude that the two-stage approximation should be used if (3.19') yields a lower value than (3.30). In particular, we compare the  $D$ -values obtained for the two-stage operator for the same  $S^*$ -value and if the number of iterations equals the value of  $\tilde{m}m$  listed in Table 3.2. Writing  $m = m_1 m_2$  the two-stage operator yields values given by Table 3.2', showing that the two-stage operator has a considerably stronger

Table 3.2'. ( $S^*$ ;  $D$ ) values satisfying (3.18) and (3.19)  
for various values of  $m = m_1 m_2 / 2$

	$m_2 = 2$	$m_2 = 3$	$m_2 = 4$
$m_1 = 1$	$(\infty; 1)$	$(\infty; 1)$	$(\infty; 1)$
$m_1 = 2$	$(9; .008)$	$(223; .05)$	$(4805; .2)$
$m_1 = 3$	$(37; 4_{10}^{-5})$	$(47; 5_{10}^{-4})$	$(482; 4_{10}^{-3})$

damping in the same damping region unless  $S^*$  is extremely large.

### 3.2. Fractional steps

#### 3.2.1. Two-stage approximations

In this section it will be assumed that the splitting function is of the special form (cf. [4])

$$(3.31) \quad F(t, u, v) = f_1(t, u) + f_2(t, v).$$

Examples of such splitting functions are the LOD splittings [11] and the hopscotch splittings [1].

We define the operator  $\tilde{L}_j^{-1}: \Sigma \rightarrow y$  in two steps (cf. (3.11)):

$$\begin{aligned}
 (3.32) \quad & \omega y + (1-\omega)y^* - b_0 \tau^v [f_1(t_{n+1}, y) + f_2(t_{n+1}, y^*)] = \Sigma, \\
 & \omega y^* + (1-\omega)y^{(j)} - b_0 \tau^v f_2(t_{n+1}, y^*) = \Sigma.
 \end{aligned}$$

Notice that the intermediate result  $y^*$  is obtained by using only a "fraction" of the righthand side function  $f(t, y)$ .

A straightforward calculation reveals that the iteration matrix  $\tilde{L}^{-1}L'$  is identical to (3.12). Consequently, the analysis of the Sections 3.1.2 and 3.1.3 also applies to the approximation (3.32) if  $Z_1$  and  $Z_2$  are understood to be the Jacobian matrices of  $b_0 \tau^v f_1(t_{n+1}, y)$  and  $b_0 \tau^v f_2(t_{n+1}, y)$ , respectively.

VERWER [8] studied the special case where  $\omega = 1$ ,  $\Sigma = y_n$ ,  $v = 1$ ,  $b_0 = 1$  (backward Euler) and where  $F(t, u, v)$  corresponds to an LOD splitting [11]. However, in that case only eigenvectors of lowest frequency are damped, and just as in the case of multistep splitting methods considered in [3], the convergence turns out to be rather poor. VERWER therefore proposed the application of line Jacobi iteration after each LOD iteration in order to damp eigenvectors of higher frequencies which indeed improves the rate of convergence [9].

#### 4. STABILITY

We recall that we want a relatively low number of iterations and consequently the stability properties of  $y_{n+1} = y^{(m)}$  may considerably differ from those of the exact solution  $\eta$  of the linear  $k$ -step formula (1.3). Therefore, we investigate the sensitivity of  $y_{n+1}$  against perturbations  $\Delta y_n$  of previous  $y_n$ -values.

Our considerations will be confined to methods based on the two-stage operator (3.11). It is convenient to write  $\tilde{L}_j^{-1}$  as the operator  $K: (y^{(j)}, \Sigma) \rightarrow y$ . Then (2.3) assumes the form (cf. 3.20))

$$(4.1) \quad y^{(j+1)} = (\mu_j - \lambda_j) y^{(j)} + (1 - \mu_j) y^{(j-1)} + \lambda_j K(y^{(j)}, \Sigma),$$

where we used (2.5). Denoting the Jacobian matrices of  $K$  with respect to the successive arguments by  $K'_1$  and  $K'_2$  we obtain the variational equation

$$(4.2) \quad \Delta y^{(j+1)} = [\mu_j - \lambda_j + \lambda_j K_1'] \Delta y^{(j)} + (1 - \mu_j) \Delta y^{(j-1)} + \lambda_j K_2' \Delta \Sigma.$$

From (3.11) it follows that

$$K_1' = [\omega - Z_1]^{-1} [1 - \omega - Z_2] [\omega - Z_2]^{-1} [1 - \omega - Z_1]$$

$$K_2' = [\omega - Z_1]^{-1} [I - [1 - \omega - Z_2] [\omega - Z_2]^{-1}]$$

so that

$$(4.2') \quad \Delta y^{(j+1)} = [\mu_j - \lambda_j \tilde{L}'^{-1} L'] \Delta y^{(j)} + (1 - \mu_j) \Delta y^{(j-1)} + \lambda_j K_2' \Delta \Sigma,$$

where  $\tilde{L}'^{-1} L'$  is given by (3.12).

We now use the following lemma (cf. [5]):

**LEMMA 4.1.** *For arbitrary vectors  $u_0$  and  $v_0$  the recurrence relations*

$$(4.3) \quad v_{j+1} = [\mu_j - \lambda_j \alpha] v_j + (1 - \mu_j) v_{j-1} + \lambda_j u_0, \quad j \geq 0$$

*is satisfied by*

$$(4.4) \quad v_j = P_j(\alpha) v_0 + Q_j(\alpha) u_0,$$

*where  $P_j(\alpha)$  is defined by (2.6) and  $Q_j(\alpha)$  by*

$$Q_j(\alpha) = \frac{1 - P_j(\alpha)}{\alpha}.$$

**PROOF.** By substitution of (4.4) into (4.3).  $\square$

Applying this lemma to (4.2) leads to the variational equation

$$\Delta y^{(j+1)} = P_{j+1}(A) \Delta y^{(0)} + Q_{j+1}(A) K_2' \Delta \Sigma,$$

$$(4.5) \quad A = \tilde{L}'^{-1} L' = (2\omega - 1) [\omega - Z_1]^{-1} [\omega - Z_2]^{-1} [I - Z_1 - Z_2],$$

$$K_2' = (2\omega - 1) [\omega - Z_1]^{-1} [\omega - Z_2]^{-1}.$$



#### 4.1. Stability analysis for model problems

In this section we assume that  $Z$  and  $\omega - Z$  share the same eigensystem with eigenvalues  $z_1$  and  $z_2$ . Assuming that  $y^{(0)}$  is computed by a formula of the form

$$(4.6) \quad y^{(0)} = \sum_{\ell=1}^k [\hat{a}_\ell y_{n+1-\ell} - \hat{b}_\ell \tau^v f(t_{n+1-\ell}, y_{n+1-\ell})]$$

and substituting  $\Sigma$  into (4.5) according to (1.3), we arrive after  $m$  iterations at the characteristic equation

$$(4.7) \quad \zeta^k = \sum_{\ell=1}^k \left\{ P_m(\alpha) \left[ \hat{a}_\ell - \frac{\hat{b}_\ell}{b_0} (z_1 + z_2) \right] + [1 - P_m(\alpha)] \frac{a_\ell - \frac{b_\ell}{b_0} (z_1 + z_2)}{1 - (z_1 + z_2)} \right\} \zeta^{k-\ell},$$

where  $\alpha$  is given by

$$(4.8) \quad \alpha = \frac{(2\omega-1)(1-z_1-z_2)}{(\omega-z_1)(\omega-z_2)}.$$

We define the *stability region* by the set of points  $(z_1, z_2)$  where (4.7) has its roots on the unit disk.

An important class of methods uses extrapolation formulas for  $y^{(0)}$ , i.e.  $\hat{b}_\ell = 0$  for  $\ell = 1(1)k$ , and back differentiation formulas for  $\Sigma$ , i.e.  $b_\ell = 0$  for  $\ell = 1(1)k$ . Then (4.7) reduces to

$$(4.7') \quad \zeta^k = \sum_{\ell=1}^k \left\{ \hat{a}_\ell P_m(\alpha) + \frac{a_\ell}{1-z_1-z_2} [1 - P_m(\alpha)] \right\} \zeta^{k-\ell}.$$

In order to illustrate this characteristic equation we derive the stability regions of two well-known iterated integration formulas for first order equations.

EXAMPLE 4.1. Consider Euler's backward formula as the generating formula, i.e.  $k = 1$  and  $a_1 = 1$ , and  $y^{(0)} = y_n$  as predictor formula, i.e.  $\hat{a}_1 = 1$ . Evidently, the stability region consists of the set of points  $(z_1, z_2)$  where

$$(4.9) \quad |\zeta| = \left| P_m(\alpha) + \frac{1 - P_m(\alpha)}{1 - z_1 - z_2} \right| \leq 1.$$

For  $z_1, z_2 \leq 0$  this yields the inequality

$$\frac{2 - z_1 - z_2}{z_1 + z_2} \leq P_m(\alpha) \leq 1$$

which is satisfied if  $0 \leq \alpha \leq b$  (see Figure 3.2). Since  $\bar{a} \leq \alpha \leq \bar{b}$  and  $\bar{a} > 0$ ,  $\bar{b} \leq b$  provided  $\omega \geq 1$  we find that (4.9) is satisfied for all negative  $z_1$  and  $z_2$ . Furthermore, by virtue of (2.16) the method is first order consistent.

**EXAMPLE 4.2.** Next we consider the two-step backward differentiation formula as the generating formula, i.e.  $k = 2$ ,  $a_2 = 4/3$ ,  $a_1 = -1/3$ , and the predictor formula  $y^{(0)} = 2y_n - y_{n-1}$ , i.e.  $\hat{a}_1 = 2$ ,  $\hat{a}_2 = -1$ , to obtain the characteristic equation

$$\zeta^2 - \left\{ 2P_m(\alpha) + \frac{4[1 - P_m(\alpha)]}{3(1 - z_1 - z_2)} \right\} \zeta + \left\{ P_m(\alpha) + \frac{1 - P_m(\alpha)}{3(1 - z_1 - z_2)} \right\} = 0.$$

This equation has its roots on the unit disk if

$$-\frac{3(z_1 + z_2) - 8}{9(z_1 + z_2) - 4} \leq P_m(\alpha) \leq 1,$$

which is certainly satisfied for all negative  $z_1$  and  $z_2$  if  $-\frac{1}{3} \leq P_m(\alpha) \leq 1$ . From Figure 3.2 and the discussion in the preceding example it follows that this inequality holds if  $\omega \geq 1$  and  $D \leq \frac{1}{3}$ . Using Table 3.1 we can determine stable values for  $(m, S^*)$ . The order of consistency equals 2 according to (2.16). We remark that  $D$  is not restricted if the predictor  $y^{(0)} = y_n$  would be used.

Generally, the root condition for the characteristic equation (4.7) is satisfied if the polynomial  $P_m(\alpha)$  satisfies the condition

$$(4.13) \quad -D_1 \leq P_m(\alpha) \leq D_2, \quad 0 < D_1 \leq D_2 \leq 1$$

for  $\bar{a} \leq \alpha \leq \bar{b}$ . From Figure 3.2 it is clear that this condition is satisfied if

$$(4.14a) \quad D \leq D_1$$

$$(4.14b) \quad \alpha \geq \tilde{a} \quad \text{where} \quad P_m(\tilde{a}) = D_2$$

or in terms of the eigenvalues  $z_1$  and  $z_2$  (compare Figure 3.3)

$$(4.14'a) \quad D \leq D_1$$

$$(4.14'b) \quad z_i \geq -\frac{\omega(1+\sqrt{1-\tilde{a}})-1}{1-\sqrt{1-\tilde{a}}}, \quad P_m(\tilde{a}) = D_2.$$

Condition (4.14a) can always be satisfied by choosing  $D$  sufficiently small (at the cost of additional iterations (cf. (3.19'))). Condition (4.14b) is in fact a condition on the integration step; from the definition of  $z_i$  and  $P_m(\alpha)$  it follows that

$$(4.14''b) \quad \tau^v \leq \frac{\beta}{\sigma},$$

$$\beta = \frac{\omega(1+\sqrt{1-\tilde{a}})-1}{b_0(1-\sqrt{1-\tilde{a}})}, \quad \tilde{a} = \frac{2\omega-1}{\omega^2(\cos \frac{\pi}{2m}+1)} \left[ 1+\omega \cos \frac{\pi}{2m} - (\omega-1) \cosh\left(\frac{1}{m} \operatorname{arch} \frac{D_2}{D}\right) \right].$$

The quantity  $\beta$  is usually called the *real stability boundary*.

For smooth problems the stability condition (4.14a) seems to be the most important one, because violating this condition means that instabilities are developed in the *low frequency components* of the solution (recall that these components correspond to eigenvalues  $\alpha$  in the damping interval  $[a, b]$ ). If (4.14a) is satisfied but (4.14b) is not, then instabilities are developed only in the *high frequency components* of the solution. Since we assumed the solution to be smooth these instabilities will not directly ruin the numerical solution. Moreover, the characteristic roots do not increase polynomially with  $z_1$  and  $z_2$  as the region of instability is entered, a situation which occurs in explicit methods (all coefficients in (4.7) are bounded as  $z_1, z_2 \rightarrow -\infty$ ). Therefore, the effect of instabilities due to too large a time step can be removed by now and then performing a smoothing operation on the numerical solution  $y_n$ . In a forthcoming report numerical experiments will be presented where the effect of violating condition (4.14b) is illustrated.

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