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IMPROVED ABSOLUTE STABILITY OF PREDICTOR-CORRECTOR METHODS FOR RETARDED DIFFERENTIAL EQUATIONS

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Improved absolute stability of predictor-corrector methods for retarded differential equations \*)

by

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

#### ABSTRACT

The absolute stability of predictor-corrector type methods is investigated for retarded differential equations. The stability test equation is of the form  $dy(t)/dt = \omega_1 y(t) + \omega_2 y(t-\omega)$  where  $\omega_1, \omega_2$  and  $\omega$  are constants ( $\omega$ >0). By generalizing the conventional predictor-corrector methods it is possible to improve the stability region in the ( $\omega_1 \Delta t, \omega_2 \Delta t$ ) - plane considerably. In particular, methods based on extrapolation-predictors and backward differentiation- correctors are studied.

KEY WORDS & PHRASES: retarded differential equations; predictor-corrector methods; absolute stability

\*) This report will be submitted for publication elsewhere.

#### 1. Introduction

Consider the initial value problem for a system of retarded differential equations of the form

(1.1)

$$y(t) = \phi(t), \quad t \leq t_0,$$

 $\dot{y}(t) = f(t,y(t),y(t-\omega)), \quad t_0 \leq t \leq T,$ 

where  $\omega$  is a nonnegative function which may depend on t and y(t). We will study numerical integration methods of the predictor-corrector type as proposed in [7] for ODEs. In particular, the stability of such methods will be investigated with respect to the stability test equation

(1.2)

 $\omega_1, \omega_2, \omega$  real constants,  $\omega > 0$ .

 $\dot{y}(t) = \omega_1 y(t) + \omega_2 y(t-\omega),$ 

Related work on the stability of multistep methods for delay equations can be found in Wiederholt [11], Cryer [4] and Barwell [2].

The results presented in this paper were derived in the institute report [6] where proofs of the theorems can be found.

#### 2. Linear multistep methods

Following Cryer [4] we may define the linear multistep method (LMM)

(2.1)

$$\rho(E)y_{n} - \Delta t\sigma(E)f_{n} = 0, \quad n \ge 0,$$
  
$$f_{n} = f(t_{n}, y_{n}, \hat{y}_{n}(t_{n}-\omega_{n})), \quad \omega_{n} = \omega(t_{n}, y_{n}),$$

where  $\Delta t$  is the integration step,  $y_n$  the numerical approximation to  $y(t_n)$ , E the shift operator defined by  $y_{n+1} = Ey_n$  and  $\{\rho,\sigma\}$  denote the characteristic polynomials of an LMM for ODEs. The polynomial  $\hat{y}_n(t)$  interpolates the values  $y_j, y_{j-1}, \dots, y_{j-\ell}$  with  $t_{j-1} < t_n - \omega_n \leq t_j$ . The value of  $\ell$  determines the accuracy of the interpolation, the order of which is not less than the order of the LMM. In the general case  $f_n$  is a complicated expression in  $\Delta t, t_n$ ,  $y_n, y_j, \dots, y_{j-\ell}$ .

Alternative methods for solving (1.1) are the LMMs of Tavernini [10] and the Runge-Kutta type methods proposed by Arndt [1] and Oppelstrup [8].

When the LMM (2.1) is applied, we are faced in each integration step with the problem to solve an implicit relation of the form

(2.2) 
$$a_0 y_n - b_0 \Delta tf(t_n, y_n, \hat{y}_n(t_n - \omega_n)) = \Sigma_n,$$

where  $\Sigma_n$  is a sum of already computed terms, and  $a_0, b_0$  are the leading coefficients in the polynomials  $\rho$  and  $\sigma$ , respectively. We assume  $a_0 = 1$  and  $b_0 > 0$ . Equation (2.2) will be solved by a predictor-corrector method.

#### 3. Predictor-corrector methods

Predictor-corrector methods will be considered of the general form

(3.1) 
$$y_n^{(0)}$$
 obtained by a predictor formula  $\{\widetilde{\rho}, \widetilde{\sigma}\}$  of explicit LM type,  
 $y_n^{(j)} := \sum_{\ell=1}^{j} [\mu_{j\ell} y_n^{(\ell-1)} + \overline{\mu}_{j\ell} \Delta t f_n^{(\ell-1)}] + \lambda_j \Sigma_n, \quad j = 1, \dots, m,$   
 $y_n^{(j)} := y_m^{(m)}.$ 

Here,  $f_n^{(\ell)}$  is defined by replacing in the expression for  $f_n$  all  $y_n$  by  $y_n^{(\ell)}$ . In the particular case where  $y_n$  is not involved in the interpolation formula

 $\hat{y}_{n}(t)$ , we have

$$f_n^{(\ell)} = f(t_n, y_n^{(\ell)}, \hat{y}_n(t_n - \omega_n)).$$

Requiring that substitution of a fixed vector y for  $y_n^{(\ell)}$  into (3.1) results into an equation of the form (2.2), that is (3.1) is required to be consistent with the corrector formula (2.2), we can express  $\lambda_j$  in terms of  $\mu_{j\ell}$ . The predictor-corrector method (3.1) is then completely determined by the matrices  $(\mu_{j\ell})$  and  $(\bar{\mu}_{j\ell})$ .

The conventional predictor-corrector methods in  $P(EC)^m$  E mode arise for

$$(\mu_{j\ell}) = 0, \quad (\bar{\mu}_{j\ell}) = b_0 I, \quad \lambda_j = 1,$$

where I is the identity matrix. In order to improve the stability behaviour of PC methods we will study generalized predictor-corrector methods (GPC methods) where the matrices  $(\mu_{i\ell})$  and  $(\bar{\mu}_{i\ell})$  have the structure



Notice that the storage requirements when implementing this method are restricted whatever large m is. In this connection, we remark that the P(EC)<sup>m-1</sup> LE mode of a predictor-corrector method defined by (cf. Stetter [9])

$$(\mu_{j\ell}) = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & & \\ 0 & \cdots & 0 \\ \mu_{1} & \cdots & \mu_{m} \end{pmatrix}, \quad (\bar{\mu}_{j\ell}) = \begin{pmatrix} b_{0} & & O \\ & \ddots & \\ O & & b_{0} \\ & & 0 \end{pmatrix} ,$$

will lead to a similar improvement of the stability behaviour but is internally unstable if m is large.

In the following the orders of accuracy of the predictor and the corrector are denoted by  $\widetilde{p}$  and p, respectively.

#### 4. The local error

Before studying stability we first give an expression for the local error of the GPC method in terms of the local errors of the predictor and the corrector formulas (for a discussion of the local and global error of LMMs of type (2.1) we refer to [1,5]). To this end it is convenient to introduce the iteration polynomials

(4.1) 
$$P_0(z) = 1$$
,  $P_j(z) = \sum_{\ell=1}^{j} (\mu_{j\ell} + \overline{\mu_{j\ell}} z) P_{\ell-1}(z)$ ,  $j \ge 1$ .

Furthermore, we define the Jacobian matrix

(4.2) 
$$Z = \Delta t \frac{\partial f_n}{\partial y_n} \Big|_{y_n = \eta_n}$$

where  $\eta_n$  is the exact solution of (2.2). The following theorem holds (cf. [6]).

THEOREM 4.1. If 
$$f(t,u,v)$$
 is sufficiently smooth and  
 $P_j(1/b_0) = 1$ ,  $\lambda_j = \frac{1}{b_0} \sum_{\ell=1}^{j} \overline{\mu}_{j\ell}$ ,  $j = 1, 2, ..., m$ ,

then

$$y_{n} - y(t_{n}) = [I - P_{m}(Z)](\eta_{n} - y(t_{n})) + P_{m}(Z)(y_{n}^{(0)} - y(t_{n}))$$
$$+ \mathcal{O}(\Delta t^{2p+3} + \Delta t^{2p+3}) \quad \underline{as} \quad \Delta t \rightarrow 0. \quad \Box$$

#### 5. Stability region of the stability test equation

The stability region of the differential equation (1.2) is defined by the set of points in the  $(\omega_1, \omega_2)$ -plane where  $y(t) \rightarrow 0$  as  $t \rightarrow \infty$ . It can be shown (see e.g. Bellman & Cooke [3, p.444]) that this region is bounded by the curve

(5.1) 
$$\omega_1 = q \cot \omega q$$
,  $\omega_2 = -\frac{q}{\sin \omega q}$ ,  $0 \le q \le \infty$ .

In figure 5.1 this curve is given in the  $(z_1, z_2)$ -plane where  $z_1 = \omega_1 \Delta t$  (the variables  $z_1$  will be used in the plots of the numerical stability region). Stability is obtained in the shaded region. It should be observed that replacing in the stability test equation (1.2) the constants  $\omega_1$  and  $\omega_2$  by matrices  $\Omega_1$  and  $\Omega_2$  with a common eigensystem, will lead to the same stability region as defined by (5.1). Stability is then obtained if all pairs of eigen-

values  $(z_1, z_2)$  of the matrices  $\Delta t\Omega_1$  and  $\Delta t\Omega_2$  (with the same eigenvector) are in the shaded region.

We will now study in what points of the "analytical" stability region the numerical method behaves stable. We will separately treat stability in the "lower" sector and stability in the "left" sector (see figure 5.1). In connection with stability in the left sector it should be remarked that Barwell [2] proved that the test equation (1.2) with  $\omega_1$  and  $\omega_2$  complex, is stable in the region Re  $\omega_1 < - |\omega_2|$ . A numerical method is called <u>P-stable</u> if it is stable in this region. This region reduces to the left sector if  $\omega_1$  and  $\omega_2$  are <u>real</u>. This suggests to call the method <u>P\_0-stable</u> if it is stable in the left sector.



lower sector



### 6. The numerical stability region in the lower sector

By applying the numerical method (2.1) to the stability test equation (1.2) a linear difference equation with constant coefficients is obtained. If we restrict our considerations to the case where  $\omega/\Delta t$  assumes only positive integer values, the corresponding characteristic equation is given by

(6.1) 
$$\rho(\zeta) - (z_1 + z_2 \zeta^{-\frac{\omega}{\Delta t}})\sigma(\zeta) = (1 - b_0 z_1) \frac{P_m(z_1)}{P_m(z_1) - 1} \{ \widetilde{\rho}(\zeta) - (z_1 + z_2 \zeta^{-\frac{\omega}{\Delta t}}) \widetilde{\sigma}(\zeta) \}.$$

Applying the boundary locus method the following theorem can be derived.

THEOREM 6.1. Let  $\{\tilde{\rho}, \tilde{\sigma}\}$  correspond to a  $\tilde{p}$ -th order extrapolation formula, let  $\rho(\zeta)$  be given by  $(\zeta-1)\rho^*(\zeta)$  where  $\rho^*(\zeta)$  is a Schur polynomial, and let  $P_m(z)$  have a zero of order  $r = p - \tilde{p} > 0$  at z = 0. Then the boundary locus of the numerical stability region in the lower sector is given by

(6.2) 
$$z_1 = q\Delta t \operatorname{cotan} \omega q + \mathcal{O}((\frac{\Delta t}{\omega})^{p+1}), \quad z_2 = \frac{-q\Delta t}{\sin \omega q} + \mathcal{O}((\frac{\Delta t}{\omega})^{p+1}).$$

This theorem implies that in the limit (as  $\Delta t \rightarrow 0$ ) the numerical stability region converges to the analytical region. The following theorem provides more detailed information about the way of convergence.

THEOREM 6.2. Let the conditions of theorem 6.1 be satisfied, let  $(z_1(q), z_2(q))$  be a point on the boundary locus (6.2) lying in the lower sector and let

(6.3) 
$$\operatorname{Re}\left\{i^{p+1}\left[1-\frac{\omega q e^{i\omega q}}{\sin \omega q}\right]\left[i^{r} C_{p+1}^{*}+\frac{P_{m}^{(r)}(0)}{r! \sigma(1) \tan^{r} \omega q}\right]\right\} > 0,$$

where  $C_{p+1}^{*}$  is the normalized error constant of the corrector. Furthermore, let  $z_{2} = \alpha z_{1}$  denote the line through the points (0,0) and  $(z_{1}(q), z_{2}(q))$ . Then along the line  $z_{2}=\alpha z_{1}$  the numerical stability interval is larger than the analytical stability interval for sufficiently small  $\frac{\Delta t}{\omega}$ .

### 7. DA<sub>0</sub>-stability

Cryer [4] called an LMM  $\underline{DA}_0$ -stable if along the line  $z_1 = 0$  the numerical interval of stability is larger than the analytical interval of stability for all positive integer values of  $\omega/\Delta t$ .

By means of theorem 6.2 we can verify whether a method is  $DA_0$ -stable. The condition (6.3) of this theorem reduces to (put  $\omega q = \pi/2$ )

(7.1)  $i^{p}C_{p+1}^{*} > 0$  for p even,  $i^{p+1}C_{p+1}^{*} > 0$  for p odd.

The remaining conditions in theorem 6.2 are easily verified for a given LMM.

EXAMPLE 7.1. Consider the backward differentiation formulas which have the normalized error constant  $C_{p+1}^* = -1/(p+1)$ . Evidently, condition (7.1) is satisfied for  $p = 1,2,5,6,9,10,\ldots$ . The other conditions of theorem 6.2 are satisfied for  $p \le 6$ . Thus, the backward differentiation formulas of orders  $p = 3,4,7,8,9,\ldots$  cannot be DA<sub>0</sub>-stable. For p = 1,2,5,6 all conditions are satisfied so that we have  $DA_0$ -stability for sufficiently large  $\omega/\Delta t$ . For  $\omega/\Delta t \le 80$  we numerically verified the  $DA_0$ -stability. For these high values of  $\omega/\Delta t$  the asymptotic behaviour holds to an high degree of accuracy.  $\Box$ 

#### 8. The numerical stability region in the left sector

Unlike the lower sector, the left hand sector may impose severe restrictions on the integration step  $\Delta t$ . We have the following theorem

<u>THEOREM 8.1.</u> Let  $(z_1, z_2) = \Delta t(\omega_1, \omega_2)$  be a point in the left sector and let the corrector formula be stable at that point  $(z_1, z_2)$ . Then there exists an iteration polynomial  $P_m(z)$  satisfying the conditions

(8.1) 
$$P_m(0) = 0$$
,  $P_m(1/b_0) = 1$ ,

such that the GPC method is stable at  $(z_1, z_2)$  provided that

(8.2) 
$$\Delta t \leq \frac{1 + \cos(\pi/2m)}{-b_0 \omega_1 [\cosh(\frac{1}{m} \ln \frac{2}{\delta}) - \cos\frac{\pi}{2m}]}$$

where  $\delta$  is a positive number independent of m.  $\Box$ 

The quantity  $\delta$  depends on how far the characteristic roots of the corrector formula are away from the unit circle, and is usually rather small. This means that the upper bound for  $\Delta$ t will be small unless m is large. Since large values of m increase the computational effort per step we derive an expression for the maximal <u>effective</u> or <u>scaled</u> integration step  $\Delta$ t/m as  $\delta \rightarrow 0$  and m  $\rightarrow \infty$ . A simple calculation yields

(8.3) 
$$\left(\frac{\Delta t}{m}\right)_{\max} \cong \frac{4m}{-b_0 \omega_1 [\ln(2/\delta)]^2} \text{ as } \delta \to 0, \quad m \to \infty.$$

This formula shows that whatever small  $\delta$  is, by choosing m sufficiently large the effective integration step can be made arbitrarily large.

#### 9. Stability plots

We start with the stability plot of a widely used method based on the fourth-order Adams-Bashforth predictor and the fourth order Adams-Moulton corrector. In the conventional PECE mode, that is the iteration polynomial is given by

(9.1) 
$$P_2(z) = \left(\frac{9z}{24}\right)^2$$
,

we find from (6.1) the regions given in figure 9.1. In order to make the regions mutually comparable we have used scaled coordinates  $z_1/\bar{m}$  and  $z_2/\bar{m}$ , where  $\bar{m}$  denotes the number of right hand side evaluations per step (here  $\bar{m} = 2$ ).



Figure 9.1 Fourth-order Adams-Bashforth-Moulton method

Next we try to extend the stability region into the left hand sector by choosing a suitable stability polynomial and by using a corrector formula which itself has a large stability region (cf. theorem 8.1). From ODE stability theory we know that the backward differentiation formulas are highly stable. Choosing the fourth-order formula as corrector with

(9.2) 
$$P_{m}(z) \equiv 0,$$

that is the method is iterated to convergence, we find from (6.1) the regions given in figure 9.2. These regions contain almost the whole left sector (they are "almost"  $P_0$ -stable). Hence, by theorem 8.1 they are an ideal starting point for the construction of GPC methods with extended stability regions.

Firstly, we try a generalized  $P(EC)^2$  mode with third-order extrapolation as predictor and the iteration polynomial

(9.3) 
$$P_2(z) = \frac{24}{125} z[1 + \frac{18}{25} z].$$

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Figure 9.2 Fourth-order backward differentiation corrector

This polynomial satisfies condition (8.1) (for a derivation of (9.3) we refer to [7]). The corresponding stability regions are given in figure 9.3 for a few values of  $\omega/\Delta t$ . Comparison with figure 9.1 reveals that these regions are already considerably larger than those of the Adams-Bashforth-Moulton method.

The stability region can be further extended by choosing higher degree iteration polynomials. We tried [6]

(9.4) 
$$P_8(z) = \delta T_8(\cos \frac{\pi}{16} + \frac{12}{25} z [\cosh(\frac{\arccos 1/\delta}{8}) - \cos \frac{\pi}{16}]),$$

where  $T_8$  denotes the Chebyshev polynomial of degree 8 and  $\delta$  is a constant. For  $\omega/\Delta t = 2$  the stability region is given in figure 9.4 for a few values of  $\delta$ . As  $\delta$  becomes larger the stability region is extended more into the left sector but the "opening" of the inscribed sector becomes smaller. For higher values of  $\omega/\Delta t$  we obtain similar plots [6].

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Figure 9.3 Fourth-order extrapolation-backward differentiation method



Figure 9.4 Fourth-order extrapolation-backward differentiation method with iteration polynomial (9.4)

#### 10. A numerical example

In order to test the stability theory we chose an example with an extremely smooth solution so that accuracy should not restrict the integration step. In fact, we integrated the problem

(10.1) 
$$\dot{y}(t) = -5y(t) - 2y(t-\frac{1}{2}t) + g(t), \quad 200 \le t \le 600,$$

where g(t) is such that  $y(t) = \exp(-t/100)$  is the exact solution. We applied the fourth-order Adams-Bashforth-Moulton method in PECE mode and the fourthorder extrapolation-backward differentiation method in generalized P(EC)<sup>m</sup> mode with  $\delta = .01$  and m such that the prescribed step  $\Delta t$  was just a stable step (for a detailed description of the method applied we refer to [7]). In table 10.1 the total number of right hand side evaluations ( $\Sigma m$ ) and the number of correct digits (cd) obtained at t = 600 are listed. Here, cd is defined by

(10.2) 
$$cd = -\frac{10}{10} \log |error at t = 600|.$$

Although (10.1) is not a model problem, because of the varying delay, the extrapolation-backward differentiation method is stable for every integration step by adjusting m. Furthermore, in this experiment (and also in other problems to be reported in [6]) the number of changes in the sign of the global error was more or less independent of the number of steps. The Adams-Bashforth-Moulton method is stable only for relatively small steps. It yields too much accuracy and costs too many right hand side evaluations.

Table 10.1	(Sm;cd)	)-values
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∆t	Adams-Bashforth-Moulton	extrapolbackw.diff.
100	unstable	(172; 2.3)
50	11	(248;4.6)
25	"	(352;6.0)
.22	"	
.21	(3840 ; 13.2)	

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