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STABILITY OF LINEAR MULTISTEP METHODS ON THE IMAGINARY AXIS

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Stability of linear multistep methods on the imaginary axis *

by

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ABSTRACT

The stability of linear multistep methods of order higher than one is investigated for hyperbolic equations. By means of the Routh array and the Hermite-Biehler theorem, the stability boundary on the imaginary axis is expressed in terms of the error constant of the third order term. As a corollary we state the result that the stability boundary for methods of order higher than two, is at most $\sqrt{3}$, and this value is attained by the Milne-Simpson method.

KEY WORDS & PHRASES: Numerical analysis, Linear multistep methods, Hyperbolic equations, Stability analysis

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* This report will be submitted for publication elsewhere.

1. INTRODUCTION

For the initial value problem

(1.1) $y' = f(x,y), \quad y(0) = y_0,$

the linear k-step method is defined by

(1.2) $$\sum_{j=0}^{k} \alpha_j y_{n+j} - h \sum_{j=0}^{k} \beta_j f(x_{n+j}, y_{n+j}), \quad n=0,1,\ldots \quad .$$

In this paper we will study the behaviour of the difference equation (1.2) on *hyperbolic* problems; thus, the Jacobian of (1.1)

(1.3) $$\frac{\partial f}{\partial y}$$

has purely imaginary eigenvalues. Application of (1.2) to the model equation

(1.4) $y' = \lambda y, \quad y(0) = 1,$

leads to

(1.5) $$(\rho(E) - h\lambda\, \sigma(E))\, y_n = 0, \quad n=0,1,\ldots \quad ,$$

where E denotes the shift operator $Ey_n = y_{n+1}$, and ρ and σ are the polynomials

(1.6) $$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j, \quad \sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j.$$

It is well known that all solutions of (1.5) are bounded if and only if $q = h\lambda$ lies in the stability region S, defined by

(1.7) $$S = \{ q \in \mathbb{C} \mid \rho(\xi) - q\,\sigma(\xi) = 0 \Rightarrow (|\xi| < 1 \text{ or } |\xi| = 1 \text{ and } \xi \text{ is a simple root}) \} .$$

DEFINITION: A linear multistep method is said to be *stable* on the imaginary axis if $\{ iy \mid -\infty < y < \infty \} \subset S$.

DEFINITION: The *imaginary stability boundary* of a multistep method is the largest number w_0, such that $\{ iw \mid -w_0 < w < w_0 \} \subset S$. In the remainder of this paper we will call w_0 briefly the stability boundary.

JELTSCH[5] has proved that the highest order for a consistent linear multistep method which is stable on the imaginary axis, is two; in his proof the well-known theorem of DAHLQUIST[3] about *A-stability* and order of a multistep method is used.

This result is entirely different from those obtained for *parabolic* equations (i.e. the eigenvalues of (1.3) are negative). For instance, CRYER [2] showed that there are linear multistep methods of arbitrarily high order, which are stable along the negative real axis. Of late we have been trying to construct linear multistep methods of order at least three with an optimal stability interval along the imaginary axis. To that end we implemented Routh's algorithm (see BARNETT & SILYAK [1]), using a formula manipulation program (DEKKER [4]) and tried to optimize the stability boundary. Despite many efforts we were not able to exceed $\sqrt{3}$, the stability boundary of the Milne-Simpson method, which has order four. In this paper we proof that the stability boundary of any linear multistep method of order higher than two, is really at most $\sqrt{3}$.

During our investigations, we received a personal communication from Jeltsch, stating the same result. His proofs, based on the algebraic techniques described in JELTSCH & NEVANLINNA [6], will appear in the near future in a joint paper of these authors.

2. CONSISTENCY CONDITIONS

In the analysis of multistep methods it is convenient to map the unit circle $|\xi| < 1$ onto the left half plane $Re(z)<0$, by the transformations (see CRYER [2], VARAH [10]),

$$z = \frac{\xi + 1}{\xi - 1}, \quad \xi = \frac{z + 1}{z - 1}. \tag{2.1}$$

The polynomials $\rho(\xi)$ and $\sigma(\xi)$ are transformed into

$$(2.2)\qquad \begin{aligned} r(z) &= 2^{-k}\ (z-1)^k \rho\left(\frac{z+1}{z-1}\right) = \sum_{j=0}^{k} a_j\ z^j, \\ s(z) &= 2^{-k}\ (z-1)^k \sigma\left(\frac{z+1}{z-1}\right) = \sum_{j=0}^{k} b_j\ z^j. \end{aligned}$$

The stability region S may be defined in terms of the new polynomials:

$$(2.3)\qquad S = \{q \in \mathbb{C} \mid r(z) - q\ s(z) = 0 \Rightarrow (\mathrm{Re}(z)<0 \text{ or } \mathrm{Re}(z)=0 \text{ and } z \text{ is a simple root})\},$$

which is equivalent to (1.7).

The error constants of a method are usually defined by formulas, linear in the coefficients α_j and β_j (see LAMBERT [7], page 23). For convenience, we introduce the modified error constants $\tilde{C}_j$, defined by

$$(2.4)\qquad \tilde{C}_j = a_{k-j} - 2 \sum_{m=0} \frac{b_{k-j+1+2m}}{1+2m}, \quad j=0,1,\ldots ;$$

these constants differ a factor from the constants given by Lambert. A method is said to be *of order p*, if $\tilde{C}_0,\ldots,\tilde{C}_p$ are equal to zero, and if $\tilde{C}_{p+1} \neq 0$ (cf. CRYER [2]).

REMARK: In equation (2.4) and throughout the remainder of this paper, we omit the upper index of the summation; we intend this to be the largest value, for which the term is non-zero. Moreover, we assume $a_j=b_j=0$ if $j<0$ or $j>k$.
Obviously, for a consistent method a_k equals zero; the scaling factor b_k is chosen equal to 1.

3. STABILITY

In order to determine the stability of a multistep method, we have to locate the zeros of a polynomial in z of degree k

$$(3.1)\qquad f(z,q) = r(z) - q\ s(z).$$

To facilitate the notations, we introduce the following sets in the complex plane:

$$H_- = \{ z \in \mathbb{C} \mid Re(z) < 0 \},$$
$$H_+ = \{ z \in \mathbb{C} \mid Re(z) > 0 \},$$
$$R_- = \{ z \in \mathbb{R} \mid z < 0 \},$$
$$R_+ = \{ z \in \mathbb{R} \mid z > 0 \},$$
$$I = \{ z \in \mathbb{C} \mid Re(z) = 0 \},$$

and we denote their closures by $\overline{H}_-$, $\overline{H}_+$, etc. .

DEFINITION: We call a polynomial *stable* if all its roots lie in $\overline{H}_-$.

Obviously, whenever q lies in S, defined by (2.3), then the polynomial f(z,q) is stable.

Throughout this paper we will assume that r(z) is stable, i.e. that $0 \in S$, that f(z,q) is non-reducible, i.e. r and s have no common roots, and that q is purely imaginary.

The *Routh array* forms a useful tool, to determine whether the zeros of a polynomial lie in H_-, H_+, R_-, R_+, $\overline{H}_-$, etc. . Theorems about the application of the Routh array may be found in MARDEN [8, Chapters 9 and 10] ; BARNETT & SILYAK [1] give a useful survey. According to BARNETT & SILYAK [1, section 3.5] the number of roots in H_- of a complex polynomial, given by

$$f(z) = \alpha_k z^k + (\alpha_{k-1} + i\,\alpha'_{k-1})\, z^{k-1} + \ldots + (\alpha_0 + i\,\alpha'_0) \tag{3.2}$$

may be found by forming Routh's array, with initial rows

$$\begin{array}{lllll} \alpha_k & \alpha'_{k-1} & -\alpha_{k-2} & -\alpha'_{k-3} & \ldots \\ \alpha_{k-1} & \alpha'_{k-2} & -\alpha_{k-3} & -\alpha'_{k-4} & \ldots . \end{array} \tag{3.3}$$

For a regular array, the number of roots in H_+ equals the number of variations in sign in the sequence formed by the first elements of these rows. However, the array is not regular for a multistep method of order $p \geq 2$, as the first element of the third row, defined by

$$\alpha'_{k-1} - \alpha'_{k-2} \frac{\alpha_k}{\alpha_{k-1}}$$

turns out to be zero. Thus we proceed in a slightly different way. The rows (3.3) may be regarded as a representation of two real polynomials

$$\text{(3.4)} \qquad \begin{aligned} f_0(y) &= \alpha_k y^k + \alpha'_{k-1} y^{k-1} - \alpha_{k-2} y^{k-2} - \alpha'_{k-3} y^{k-3} + \dots, \\ f_1(y) &= \alpha_{k-1} y^{k-1} + \alpha'_{k-2} y^{k-2} - \alpha_{k-3} y^{k-3} - \alpha'_{k-4} y^{k-4} + \dots . \end{aligned}$$

The correspondence between the real variable y and the imaginary variable z, $y=-iz$, will be assumed throughout the rest of this paper.

It is obvious, that the roots of $f(z)$ are purely imaginary, if the roots of $f_0(y)$ are real, and $f_1(y)$ is identically equal to zero. Now we will proof that the stability of $f(z)$ implies that all roots of $f_0(y)$ are real, whether or not $f_1(y)$ is the zero-function. At first, we modify the *Hermite-Biehler theorem* (see OBRESCHKOFF [9, page 106] or MARDEN [8, page 169]).

THEOREM 3.1: *(Hermite-Biehler) All roots of the polynomial* $f(y)=u(y)+iv(y)$, *where* u *and* v *are real polynomials, lie on the same side of the real axis, if and only if* u *and* v *have simple real roots which separate each other.*

As we need a result about the left half-plane H_-, we have to rotate the complex plane.

COROLLARY 3.1: *All roots of the polynomial* $f(z)$, *such that* $f(iy)=u(y)+iv(y)$, *lie on the same side of the imaginary axis, if and only if the real polynomials* $u(y)$ *and* $v(y)$ *have simple real roots which separate each other.*

PROOF: $z=iy$ is a root of f, if and only if y is a root of $u+iv$. □

In the following lemma we include roots lying on the imaginary axis.

LEMMA 3.2: *Let* f *be a complex polynomial, such that* $f(z)=f(iy)=u(y)+iv(y)$, *where* u *and* v *are real polynomials. If all roots of* f *lie in* $\overline{H}_-$, *then all roots of* u *and* v *are real.*

PROOF: Assume that $f(z)$ has m zeros, $z_1,\ldots,z_m$, on the imaginary axis. Obviously, $u(y)$ takes real values and $iv(y)$ purely imaginary values, if $y\in\mathbb{R}$. Thus, the real points $-iz_j$, $j=1,\ldots,m$, are zeros of both u and v.
Now consider the polynomials $\tilde{f}$, $\tilde{u}$ and $\tilde{v}$, which are obtained from f, u and v by dividing these polynomials by the common factors of u and v. The zeros of $\tilde{f}$ are the remaining zeros of f, and lie in H_-. Moreover, $\tilde{u}$ and $\tilde{v}$ are real polynomials, and the relation $\tilde{f}(z)=\tilde{f}(iy)=\tilde{u}(y)+i\tilde{v}(y)$ holds. Thus, according to COROLLARY 3.1, the roots of $\tilde{u}$ and $\tilde{v}$ are real and simple, and separate each other. We conclude that all roots of u and v are simple. □

REMARK 3.1: The roots of u (or v) need not be simple, even if all roots of f are simple; the roots of $\tilde{u}$ (or $\tilde{v}$) may coincide with those produce by the purely imaginary roots of f. For example, $f(z)=(z+1)(z-i)(1-i)$ has simple roots in $\bar{H}_-$, but $u(y)$, obtained from $f(iy)=-(y^2-2y+1)+i(y^2-1)$, has a double root.

COROLLARY 3.2: *A necessary condition for the stability of* $f(z)$, *given by (3.2), is that all roots of the polynomials* $f_0(y)$ *and* $f_1(y)$, *as defined by (3.4), are real.*

PROOF: It is easily verified that $f(iy)$ equals $i^k f_0(y) + i^{k-1} f_1(y)$, and that both f_0 and f_1 are real polynomials. The stability of f implies that all roots of f lie in $\bar{H}_-$, and thus all roots of f_0 and f_1 are real. □

Now, we apply these results to the polynomial $f(z,q)$, defined by (3.1). Using the expressions (2.2) for $r(z)$ and $s(z)$, and multiplying with i to make the first coefficient real (note that $a_k=0$), we get

$$(3.4')\qquad \begin{aligned} f_0(y,w) &= \sum_{j=0} (a_{k-1-2j} + b_{k-2j}\, w\, y)\, (-1)^j\, y^{k-1-2j}, \\ f_1(y,w) &= \sum_{j=0} (a_{k-2-2j} + b_{k-1-2j}\, w\, y)\, (-1)^j\, y^{k-2-2j}, \end{aligned}$$

where we made the substitution $w=-iq$ to shorten the notation. Thus, according to COROLLARY 3.2, a necessary condition for the stability of $f(z,q)$ is that all roots of $f_0(y,w)$ and $f_1(y,w)$ are real.

EXAMPLE 3.1: The two-step Curtiss-Hirschfelder formula yields the polynomial

$$f(z,q) = 2z + 4 - q(z^2 + 2z + 1).$$

The initial rows of the Routh array are

$-iq$	2	iq
$-2iq$	4	

and the polynomials f_0 and f_1, according to (3.4')

$$f_0(y,w) = w\,y^2 + 2\,y - w,$$

$$f_1(y,w) = 2w\,y + 4.$$

Both polynomials have real zeros for real values of w, so the condition of COROLLARY 3.2 is satisfied. Moreover, the zeros separate each other, which implies, according to COROLLARY 3.1, that all zeros of $f(z,q)$ lie in the same half plane. As the roots are continuous functions of q, and the root of $f(z,0)$ lies in H_-, we conclude that all roots of $f(z,q)$ lie in H_-, for all $q \in I$. We note, that we did not state this stronger result about the separation of the roots in LEMMA 3.2, because we disregard the polynomial f_1 in the sequel.

EXAMPLE 3.2: The three-step Curtiss-Hirschfelder formula yields the polynomials

$$\rho(\xi) = \frac{4}{3}(11\xi^3 - 18\xi^2 + 9\xi - 2), \qquad \sigma(\xi) = 8\xi^3,$$

$$r(z) = 2z^2 + 6z + \frac{20}{3}, \qquad s(z) = z^3 + 3z^2 + 3z + 1,$$

$$f_0(y,w) = w(y^3 - 3y) + 2y^2 - \frac{20}{3}, \qquad f_1(y,w) = w(3y^2 - 1) + 6y.$$

$f_0(y,w)$ has three real roots if $|w| < \frac{1}{3}\sqrt{5}$ or $|w| > \frac{1}{3}\sqrt{32}$; $f_1(y,w)$ has real roots for all values of w. The condition for the roots to separate each other are found by the Routh array, deleting the leading zeros. We get $16w^2 - 60 > 0$, so the formula is unstable on $\{ iw \mid -\frac{1}{2}\sqrt{15} < w < \frac{1}{2}\sqrt{15} \}$.

Observing that the error constants $\tilde{C}_j$, defined by (2.4), contain coefficients of f_0 if j is odd, and coefficients of f_1 if j is even, leads to

THEOREM 3.3: *Suppose there exists a k-step formula of order p (p odd) with stability boundary* w_0. *Then there exists also a k-step formula of order at least p+], whose associated polynomial* $\tilde{f}(z,q)$ *is stable if* $-w_0 < iq < w_0$.

PROOF: Let the associated polynomial (3.1) of the k-step formula of order p be given by f(z,q). According to COROLLARY 3.2, all roots of the polynomial $f_0(y,w)$ are real, if $|w|<w_0$. Now, choose $\tilde{f}(z,q)$ in such a way, that the polynomials $\tilde{f}_0$ and $\tilde{f}_1$, generated by $\tilde{f}$ according to (3.4'), are equal to f_0 and the zero-function, respectivily. Thus

$$\tilde{f}(z,q) = i^{k-1} f_0(-iz,-iq) = i^{k-1} f_0(y,w).$$

If $|q|<w_0$, then all roots of f_0 are real, and all roots of $\tilde{f}$ purely imaginary; thus $\tilde{f}(z,q)$ is stable. Moreover, the error constants $\tilde{C}_j$ are equal to zero, if $j \le p$ or if j is even, so the order of the new formula is at least p+1. □

EXAMPLE 3.3: For the Backward Euler formula we have

$$f(z,q) = 2 - q\ (z + 1);$$

thus, $f_0(y,w) = wy + 2$ and $f_1(y,w) = w$. f(z,q) is stable for imaginary values of q, and we have first order consistency, as is easily checked by using (2.4). Now, we choose $\tilde{f}_0(y,w) = wy + 2$ and $\tilde{f}_1(y,w) = 0$, which yields $\tilde{f}(z,q) = 2 - q\,z$. The resulting formula is the trapezoidal rule, which is known to be stable on I and which is of second order.

When we have a multistep method of second order, we may have stability on the whole imaginary axis. Now, we will investigate what happens if we increase the order. In that case the leading terms of $f_0(y,w)$ are

$$w\,y^k + 2\,y^{k-1} - w\,b_{k-2}\,y^{k-2} - (2b_{k-2} + \tfrac{2}{3})\,y^{k-3} + \dots\ .$$

As the stability interval $\{ iw \mid -w_0 < w < w_0 \}$ is symmetric around the origin, we should consider $f_0(y,w)$ for both positive and negative values of w. It is therefore convenient to form the product of $f_0(y,w)$ and $f_0(y,-w)$; this polynomial is quadratic in y. Depending on the variable, y or y^2, we will denote this polynomial by $g(y,w)$ and $h(x,w)$, respectivily. Finally, separating terms containing the factor w from the other ones, we obtain the following polynomials:

(3.5)
$$g_0(y) = \{ \sum_{j=0} (-1)^j b_{k-2j} y^{k-2j} \}^2,$$
$$g_1(y) = \{ \sum_{j=0} (-1)^j a_{k-1-2j} y^{k-1-2j} \}^2,$$
$$h_0(x) = h_0(y^2) = g_0(y),$$
$$h_1(x) = h_1(y^2) = g_1(y).$$

It is easily verified that g_0 and g_1 satisfy the relation

(3.6) $$g_1(y) - w^2 g_0(y) = f_0(y,w) f_0(y,-w),$$

so that $g(y,w)$ equals $g_1(y) - w^2 g_0(y)$.

LEMMA 3.4: *A necessary condition for the stability of* $r(z)$ $(=f(z,0))$ *is that all roots of* h_1 *are non-negative.*

PROOF: The stability of $f(z,0)$ implies that all roots of $f_0(y,0)$ are real; however, $f_0(y,0)$ is an odd (or even) function, so $-y_0$ is a root of $f_0(y,0)$ if y_0 is a root of $f_0(y,0)$. Assume that $y_1,\ldots,y_{k-1}$ are the real roots of $f_0(y,0)$; then $-y_1,\ldots,-y_{k-1}$ are also roots of $f_0(y,0)$. Hence, using (3.6), we see that the factors of $g_1(y)$ are $(y-y_j)(y+y_j)$, $j=1,\ldots,k-1$, and the factors of $h_1(x)$ are $(x-y_j^2)$. We may conclude that the roots of h_1 are non-negative. □

LEMMA 3.5: *Assume that* g_0 *and* g_1 *do not have common roots. A necessary condition for the stability of* $f(z,q)$, *for all* $q \in I$, $|q|<\varepsilon$, *for some small* $\varepsilon>0$, *is that all roots of* g_1 *are double.*

PROOF: Let y_0 be a zero of g_1 of order at least 4. By assumption, y_0 is not a zero of g_0. As g_0 is a quadratic function, we have $g_0(y_0)>0$, so that there are only two real zeros of $g(y,w)$ in the neighbourhood of y_0, if w^2 is small enough. As the roots of $g(y,w)$ are continuous functions of w, we must have two complex(non-real) zeros of g; thus at least one of the functions $f_0(y,w)$ and $f_0(y,-w)$ has a non-real zero, which, according to COROLLARY 3.2, would imply that $f(z,q)$ is not stable, if $q=iw$ or $q=-iw$. As a consequence, the stability of $f(z,q)$ for all $q,|q|<\varepsilon$, implies that the zeros of g_1 are of order less than 4. Moreover, by definition (3.5), the roots of g_1 are of even order, so they are of order 2. □

REMARK 3.2: We can not replace g_1 by h_1 in this lemma, because 0 can be a single root of h_1. The non-zero roots of h_1, however, are always double, so it depends on the degree of the polynomial h_1, whether 0 is a (single) root or not. According to (3.5), the degree of h_1 is $k-1$.

LEMMA 3.6: *A necessary condition for the stability of the polynomials* $f(z,q)$ *and* $f(z,-q)$, *for a fixed* $q\in I$, *is that all roots of* $g(y,w)$, $w=-iq$, *are real.*

PROOF: COROLLARY 3.2 states that the stability of $f(z,q)$ implies that all roots of $f_0(y,w)$ are real. Likewise, all roots of $f_0(y,-w)$ are real as a consequence of the stability of $f(z,-q)$. Thus, according to relation (3.6), all roots of $g(y,w)$ are real. □

In order to get an idea of the behaviour of the zeros of g for various values of w, it is convenient to consider the function

$$(3.7) \qquad Q(y) = \frac{g_1(y)}{g_0(y)} = w^2 + \frac{g(y,w)}{g_0(y)}.$$

It is clear that all zeros of $g(y,w)$ are real, if and only if the function $Q(y)$ has $2k$ points in common with the constant function w^2. In figure 3.1 we have plotted the function $\{Q(y)\}^{\frac{1}{2}}$ for the three-step Curtiss-Hirschfelder formula (see EXAMPLE 3.2).

When we look at the plot of figure 3.1, we get an idea of the intervals of stability and instability of the three-step Curtiss-Hirschfelder formula.

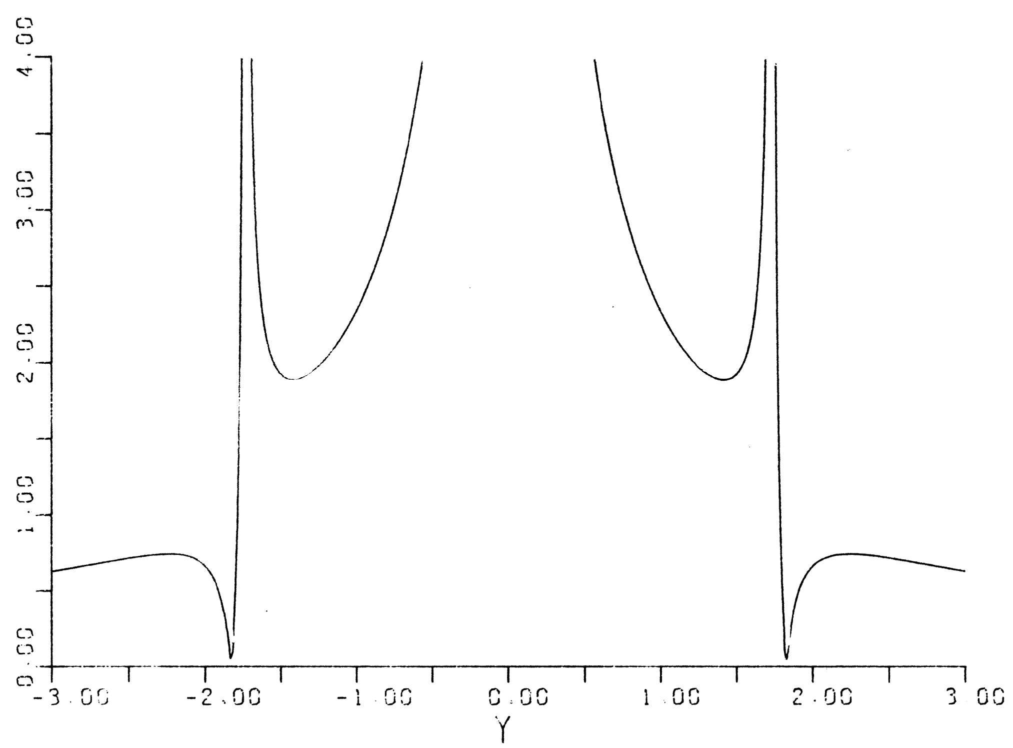

Fig. 3.1 The function $(Q(y))^{\frac{1}{2}} = \left(\frac{(y^2 - 10/3)^2}{y^2\,(y^2 - 3)^2}\right)^{\frac{1}{2}}$.

$Q(y)$ has two double zeros, and $\lim_{y\to-\infty} Q(y) = \lim_{y\to\infty} Q(y) = 0$; this indicates that $g(y,0)$ has two double real zeros, whereas the degree is 4 (=2k-2). Thus, all roots of $g(y,0)$ are real. For small values of w ($|w|<\sqrt{5}/3$), there are 6 points of intersection between $Q(y)$ and the constant function w^2; hence, all roots of $g(y,w)$ are real for these values of w. We remark that each of the intervals $(-\infty,-\sqrt{30}/3)$, $(-\sqrt{30}/3,+\sqrt{30}/3)$ and $(\sqrt{30}/3,\infty)$ contains exactly two intersection points. For values of $w>\sqrt{5}/3$, these intersection points vanish in two of those intervals. These intersection points can not "jump" at once into the other interval (otherwise $g(y,\sqrt{5}/3)$ would have had 4 double and two single roots), so $\sqrt{5}/3$ is an upperbound for the stability boundary of the formula

In the remainder of this section we will prove that the stability boundary can be bounded by the top of the lowest "hill" of the function $\sqrt{Q(y)}$, and we will calculate an upperbound for this top. At first we give four lemma's for rather general polynomials satisfying some conditions. These lemma's can be applied to the real polynomials $h_0(x)$ and $h_1(x)$ as defined in (3.5), and the reader may keep them in mind. We note that h_1 has

$(k-1)\div 2$ double roots, if the conditions of LEMMA 3.5 are satisfied. We denote them by $\tilde{c}_2,\ldots,\tilde{c}_m$, where m equals $(k+1)\div 2$.

Let $c_1,\ldots,c_m$ be real constants, ordered in such a way that $c_1<c_2<\ldots<c_m$. Then we define the open intervals I_j, $j=1,\ldots,m$, by

$$(3.8)\qquad \begin{aligned} I_j &= (\ c_j,\ c_{j+1}\ ), \quad j=1,\ldots,m-1, \\ I_m &= (\ c_m,\ \infty\ ). \end{aligned}$$

In the following four lemma's we assume these constants and intervals be given.

LEMMA 3.7: *Let* $h(x)$ *be a real polynomial of degree* m,

$$(3.9)\qquad h(x) = x^m + \sum_{j=1}^{m}(-c_j)\ x^{m-1} + h_{m-2}x^{m-2} + \ldots + h_0.$$

such that c_j, $j=1,\ldots,m$, *is not a zero of* $h(x)$.
Define the polynomial $P(x)$ *by*

$$(3.10)\qquad P(x) = \prod_{j=1}^{m}(x - c_j)^2 - \{h(x)\}^2.$$

Then there exists an interval I_j, $1\le j\le m$, *such that* $P(x)<0$, $\forall x \in I_j$.

PROOF: $P(x)$ is a polynomial of degree less than or equal to 2m-2; thus, P has at most 2m-2 roots. As $P(c_j)<0$, for all j, the number of zeros in each of the intervals I_j, $j<m$, is even. Thus, in at least one interval P has no roots and is consequently strictly negative. □

REMARK 3.3: The assumptions of this lemma can be satisfied only, if $m>1$. If $m=1$, we have $h(x) = x - c_1$, which contradicts the assumption that c_1 is not a root of $h(x)$.

REMARK 3.4: In the interval I_j indicated in this lemma, the function $\{h(x)\}^2$ is obviously positive; hence, the function $1 + P(x)/\{h(x)\}^2$ has at least one hill with a top less than 1. If we choose $c_2,\ldots,c_m$ equal to the double roots of $h_1(x)$, $h(x)$ equal to $\sqrt{h_0(x)}$ if $k=2m$, else equal to $\sqrt{x\ h_0(x)}$, and c_1 such that the second coefficient of $h(x)$ equals $\sum_{j=1}^{m}(-c_j)$, then $Q(y)$ and $1 + P(y^2)/\{h(y^2)\}^2$ differ a factor $(y^2-c_1)^2/(4y^2)$, as the reader may verify easily. This factor is bounded by $|c_1|$ for $y \in \mathbb{R}$, if c_1 is negative. In that case, $Q(y)$ can be bounded by $|c_1|^{-1}(1 + P(y^2)/\{h(y^2)\}^2)$.

LEMMA 3.8: *Let* $h(x)$ *be a real polynomial of degree* m, *with leading terms given by (3.9). Let* c_1 *be negative, and* $c_2,\ldots,c_m$ *be positive. Define* $R(x,w)$ *by*

$$(3.11) \qquad R(x,w) = 4\,x \prod_{j=2}^{m}(x - c_j)^2 - w^2\,\{h(x)\}^2.$$

Define $\tilde{w}_0 = |c_1|^{-\frac{1}{2}}$. *Then there exists an interval* I_j, $1\le j\le m$, *such that* $R(x,w)$ *does not have roots in* I_j, *if* $|w|>\tilde{w}_0$. *Moreover, if* $h(c_{j'})\neq 0$, *for some* j' , $2\le j'\le m$, *then also* $R(x,\tilde{w}_0)$ *does not have roots in the interval* I_j.

PROOF: For all x the relation $4x \le \tilde{w}_0^2\,(x-c_1)^2$ holds; equality occurs for $x=-c_1$. Using this relation, we get the inequalities, assuming $|w| \ge \tilde{w}_0$,

$$\frac{R(x,w)}{\tilde{w}_0^2} \le \prod_{j=1}^{m}(x-c_j)^2 - \frac{w^2}{\tilde{w}_0^2}\{h(x)\}^2 \le \prod_{j=1}^{m}(x-c_j)^2 - \{h(x)\}^2.$$

If $h(c_j)\neq 0$, for all j, then we apply the previous theorem, and conclude that $R(x,w)$ does not have zeros in I_j, for some j, if $|w| \ge \tilde{w}_0$.
If $h(c_j)=0$, for some j, we may cancel the factors $(x-c_j)^2$, and arrive at the same result, as is easily verified.
If $h(c_j)=0$, for all j, we obtain after division of R by $\prod_{j=2}^{m}(x-c_j)^2$ the function $4x - w^2(x-c_1)^2$; obviously, there is no zero if $|w|>\tilde{w}_0$, and $-c_1$ is a zero if $|w|=\tilde{w}_0$. Thus, there are no roots of $R(x,w)$ in I_1, if $|w| > \tilde{w}_0$. □

EXAMPLE 3.4: The Milne-Simpson method yields the polynomials

$$\rho(\xi) = 2\,(\xi^2-1), \qquad \sigma(\xi) = \frac{2}{3}(\xi^2+4\xi+1),$$
$$r(z) = 2z, \qquad s(z) = z^2 - 1/3,$$
$$f_0(y,w) = w\,y^2 + 2y + w/3, \qquad f_1(y,w) = 0,$$
$$g(y,w) = 4y^2 - w^2(y^2+1/3)^2,$$
$$h_0(x) = (x + 1/3)^2, \qquad h_1(x) = 4\,x.$$

Choose $c_1=-1/3$ and $h(x)=(x+1/3)$. Then the conditions of LEMMA 3.8 are satisfied; thus $4x - w^2(x+1/3)^2$ does not have a real zero, if $|w|>\tilde{w}_0=\sqrt{3}$, and likewise $g(y,w)$ does not have real zeros for these values of w.
If $|w|<\tilde{w}_0$, then all roots of $g(y,w)$, and also of $f_0(y,w)$ are real, and they are simple if $|w|\neq\tilde{w}_0$. Thus, the Milne-Simpson method is stable for $q\in I$, if $|q|<\sqrt{3}$.

EXAMPLE 3.5: For the trapezoidal rule we have (see also EXAMPLE 3.3)

$$f_0(y,w) = wy + 2,$$

$$g(y,w) = 4 - w^2 y^2,$$

and we may set

$$R(x,w) = x\, g(\sqrt{x},w) = 4x - w^2 x^2.$$

We have to choose $c_1=0$, in order to satisfy (3.9); however, this value is not negative, and we can not apply LEMMA 3.8. Obviously, $g(y,w)$ has two real zeros for all real values of w.

REMARK 3.5: If the conditions of LEMMA 3.8 are satisfied, then the function $w^2 + R(x,w)/\{h(x)\}^2$ has at least one hill, and the top of this hill is at most equal to $\tilde{w}_0^2$. We note that the actual top can be smaller, due to the (possible not sharp) inequalities used in the proof of this lemma.

LEMMA 3.9: *Let* $R(x,w)$ *be a polynomial in* x *of degree* 2m *for* $w\neq0$ *and of degree at most* 2m *for* w=0 *and let the coefficients of* R *be real continuous functions of* w. *Assume*

(i) $R(x,0)$ *has* m-1 *double real zeros,* $c_2,\dots,c_m$*;*
(ii) $R(x,w)$ *does not have zeros in* $c_1,\dots,c_m$, *if* $w\neq0$ *;*
(iii) $R(x,w)$ *has two zeros in each of the intervals* $I_1,\dots,I_m$ *if* $0<|w|\leq\varepsilon$*;*
(iv) $\exists j$, $1\leq j\leq m$, *such that* $R(x,\tilde{w}_0)$ *has no zeros in* I_j.

Then there exists a w_1, $0<w_1\leq\tilde{w}_0$, *such that* $R(x,w_1)$ *has at most* 2m-2 *zeros.*

PROOF: Let $n_j(w)$ denote the number of roots of $R(x,w)$ in the interval I_j, $1\leq j\leq m$, double roots counting double. Define the sets S_H and S_V by

$$S_H = \{\, w>0 \mid \forall j,\ 0<\tilde{w}\leq w,\ n_j(\tilde{w})\geq 2 \,\},$$

$$S_V = \{ w > 0 \mid \exists j, \exists \tilde{w} < w, n_j(\tilde{w}) < n_j(w) \}.$$

We note that both sets are closed, as the roots can not move across the boundaries of the intervals ($R(c_j,w) \neq 0$ if $w > 0$, $\forall j$) and they can not vanish (the degree is 2m for $w > 0$). Moreover, the first set is not empty, because $\varepsilon \in S_H$, and is bounded because $\tilde{w}_0 \notin S_H$. We define the real numbers $w_H = \max\{ x \mid x \in S_H\}$ and $w_V = \min\{ x \mid x \in S_V\}$, if S_V is not empty, and $w_V = 2w_H$ if S_V is empty. We may think of w_H and w_V as the top of the hill and the bottom of the valley of a function like $Q(y)$ in figure 3.1.
From $\sum_{j=1}^{m} n_j(w) = 2m$, $0 < w \leq w_H$, we conclude that $w_H < w_V$; otherwise, there would be a w, $w < w_V \leq w_H$ with $\sum_{j=1}^{m} n_j(w) > 2m$. Thus, the total number of roots in the intervals, $\sum_{j=1}^{m} n_j(w)$ is less than 2m for $w_H < w < w_V$. Moreover, none of the points c_j is a root of $R(x,w)$, and the total number of real roots must be even, so we arrive at the assertion of the lemma. □

LEMMA 3.10: *Let* $c_2,\ldots,c_m$ *be positive constants,* $h(x)$ *a real polynomial satisfying (3.9) and* c_1 *be negative. Then, for all* $\varepsilon > 0$, *there exists a* w_1, $0 < w_1 < (-c_1)^{-\frac{1}{2}} + \varepsilon$, *such that the polynomial* $R(x,w_1)$, *as defined by (3.]]) has at most 2m-2 real zeros.*

PROOF: We may assume without loss of generality that $h(x)$ does not have roots in common with $\prod_{j=2}^{m}(x-c_j)^2$. If there are common roots, we divide both polynomials by the common factors, and apply the proof to the resulting polynomials. We verify that R satisfies the assumptions of LEMMA 3.9:

(i) The real constants $c_2, \ldots, c_m$ are double roots of $R(x,0)$;

(ii) $R(c_j,w) \neq 0$, $j=2,\ldots,m$, if $w \neq 0$ and $R(c_1,w) < 0$, as c_1 is negative;

(iii) For small values of w, $R(x,w)$ has 2m-2 zeros in the neighbourhood of the points c_j, $j=2,\ldots,m$, one on each side of each point, and two zeros in the neighbourhood of the points $x=0$ and $x=\infty$. Thus, $R(x,w)$ has two zeros in I_j, $j=1,\ldots,m$, if $0 < |w| < \varepsilon$. (In I_1 because $c_1 < 0 < c_2$)

(iv) According to LEMMA 3.8, $R(x,w)$ has no zeros in I_j for some j, if $|w| > (-c_1)^{-\frac{1}{2}}$. Thus, for all $\varepsilon > 0$, $R(x,w)$ has no zeros in I_j, if $w = (-c_1)^{-\frac{1}{2}} + \varepsilon$.

Application of LEMMA 3.9 yields the statement of this lemma. □

By virtue of this lemma we arrive at the main result of this paper:

THEOREM 3.11: *The imaginary stability boundary of a linear k-step method of order at least two, is at most* $(\frac{1}{2}\tilde{C}_3 + 1/3)^{-\frac{1}{2}}$*, where* $\tilde{C}_3$ *is the modified error constant of the third order term, defined by (2.4).*

PROOF: Let $f(z,q)$ be the polynomial in z of degree k, associated with the k-step method, according to (3.1). Assume that $f(z,q)$ is stable, for $q \in I$, $|q| < \beta$. Then, according to LEMMA 3.6, all roots of $g(y,w)$, defined by (3.5) and (3.6), are real if $|w| < \beta$.

LEMMA 3.4 states that all roots of h_1 are non-negative, and according to REMARK 3.2, the positive roots are double. Denote these roots by $c_2,\dots,c_m$, and consider the polynomial $R(x,w)$ as defined by (3.11). We distinguish two cases:

(i) k is even. Then, we choose $h(x) = \sqrt{h_0(x)}$; the coefficient of the second term of $h(x)$ is $-b_{k-2}$. Because $\sum_{j=2}^{m} c_j = -\frac{1}{2}a_{k-3}$, we have to take $c_1 = b_{k-2} - \frac{1}{2}a_{k-3} = -(\frac{1}{2}\tilde{C}_3 + 1/3)$ in order to satisfy (3.9).

(ii) k is odd. Then, we choose $h(x) = \sqrt{x\, h_0(x)}$, and again $c_1 = -(\frac{1}{2}\tilde{C}_3 + 1/3)^{-\frac{1}{2}}$.

In both cases, the conditions of LEMMA 3.10 are satisfied, if $c_1 < 0$; thus, $R(x,w_1)$ has at most $2m-2$ real zeros, for a $w_1 \le (-c_1)^{-\frac{1}{2}} + \varepsilon$.
However, $R(y^2,w)$ is equal to $g(y,w)$ if k is even, and equal to $y^2 g(y,w)$ if k is odd. Thus, if k is even, $g(y,w_1)$ has at most $2(2m-2)=2k-4$ real zeros; likewise, if k is odd, $g(y,w_1)$ has at most $2(2m-2)-2=2k-4$ real zeros. Hence, $g(y,w_1)$ has complex zeros; however, all roots of $g(y,w)$ are real if $|w| < \beta$. Thus, for all ε, $\beta < (-c_1)^{-\frac{1}{2}} + \varepsilon$, and we conclude that $\le (-c_1)^{-\frac{1}{2}}$. □

COROLLARY 3.3: *The imaginary stability boundary of a linear k-step method of order higher than two, is at most* $\sqrt{3}$.

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