IMA Journal of Numerical Analysis (1992) **12**, 487–502

Unified approach to spurious solutions introduced by time discretization Part II: BDF-like methods

A. ISERLES

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge CB3 9EW, UK

AND

A. M. STUART

Program in Scientific Computing and Computational Mathematics, Division of Applied Mechanics, Stanford University, Stanford CA 94305-4040, USA

Dedicated to Professor A. R. Mitchell on the occasion of his 70th birthday

[Received 14 May 1990 and in final revised form 6 December 1991]

It has been proved *inter alia* in part I of the present paper (Iserles *et al.*, 1991) that irreducible multistep methods for ordinary differential equations may possess period-2 solutions as asymptotic states if and only if $\sigma(-1)\neq 0$, where the underlying method is

$$\sum_{k=0}^{m} \rho_k y_{n+k} = h \sum_{k=0}^{m} \sigma_k f(y_{n+k})$$

and $\sigma(z) := \sum_{k=0}^{m} \sigma_k z^k$. We provide an alternative proof of that statement and examine in detail properties of methods that obey $\sigma(-1)=0$. By using a variation of the original proof of the first Dahlquist barrier (Henrici, 1962), we establish an attainable upper bound on the order of zero-stable multistep methods with the aforementioned feature. Moreover, we modify the concept of backward differentiation formulae (BDF) to require that $\sigma(-1)=0$. A zero-stability bound on the ensuing methods is produced by extending the method of proof in (Hairer & Wanner, 1983).

Introduction

This paper returns to the theme already investigated in (Iserles, 1990; Iserles *et al.*, 1991; Stuart, 1990), namely the asymptotic behaviour of multistep methods for ordinary differential equations. The objective is to characterise and study methods which correctly reproduce the asymptotic behaviour of the underlying differential equation. The numerical method is considered as a map, parameterised by the (constant) step length $h>0$. It is known from the general theory of multistep methods (Henrici, 1962) that, as $h\to 0$ and subject to consistency and zero-stability, the numerical trajectories on finite time-intervals converge to the trajectories of the differential system. Furthermore, recent analysis has shown that as $h\to 0$, many of the asymptotic states (ω and α limit sets) of differential equations are faithfully reproduced by multistep methods (Beyn, 1987; Eirola, 1988; Hale *et al.*, 1988; Kloeden and Lorenz, 1986). However, for fixed values of

h, the numerical solution trajectory may behave in a qualitatively different way from the true solution trajectory as the number of steps becomes unbounded. This occurs for instance when the numerical method has spurious asymptotic states (possibly including infinity) which are not close to the asymptotic states of the differential equations (Griffiths and Mitchell, 1988; Iserles, 1990; Stuart and Peplow, 1989). For this reason it is interesting to examine the asymptotic states of multistep methods for fixed values of h so that methods can be constructed which do not have spurious asymptotic states.

There are three classes of spurious asymptotic states which are of particular importance. Their existence can be motivated by a simple bifurcation argument detailed in (Iserles *et al.*, 1991): as h varies, a numerical method can undergo spurious bifurcations from a genuine fixed point inherited from the differential equation. These bifurcations occur when the eigenvalues of the Jacobian of the variational equation at the fixed point cross the unit circle (Guckenheimer & Holmes, 1983) with varying h. The three main bifurcations of this kind occur when an eigenvalue crosses $+1$ (giving rise to a *steady bifurcation* of a spurious fixed point), when it crosses -1 (leading to a *flip bifurcation* of a period 2, or sawtooth, solution) or when a complex conjugate pair of eigenvalues crosses the unit disc away from the real axis (a *Hopf bifurcation* of a spurious invariant curve.) Although these bifurcations typically occur at values of h above those used in practice (for example, bifurcation occurs at the linear stability limit of the method), the branches of spurious solutions can extend back to values of h used in practice. Hence it may be important to avoid the existence of spurious solutions introduced by discretization.

Consider the multistep method

$$\sum_{k=0}^{m} \rho_k y_{n+k} = h \sum_{k=0}^{m} \sigma_k f(y_{n+k}), \qquad \rho_m \neq 0, \tag{1.1}$$

for the numerical solution of the autonomous differential system

$$y' = f(y). \tag{1.2}$$

The polynomials ρ and σ are defined by

$$\rho(z) := \sum_{k=0}^{m} \rho_k z^k, \qquad \sigma(z) := \sum_{k=0}^{m} \sigma_k z^k.$$

It is proved in (Iserles, 1990) that the multistep metod (1.1) cannot possess spurious steady solutions, assuming exact solution of the nonlinear equations in the presence of implicitness. This property is not shared by most Runge–Kutta methods (Hairer *et al.*, 1990) and confers an important advantage on multistep schemes. Moreover it is demonstrated *inter alia* in (Iserles *et al.*, 1991) that the multistep method (1.1) cannot possess period 2 solutions in n if and only if $\rho(-1) \neq 0$, $\sigma(-1) = 0$. The concern of the present paper is in investigating the ramifications of the condition $\rho(-1) \neq 0$, $\sigma(-1) = 0$ on various features of the underlying multistep method (1.1), in particular stability.

In Section 2 we prove that a period 2 solution of an irreducible multistep method may exist if and only if $\sigma(-1) \neq 0$. This result has already been proved in (Iserles *et al.*, 1991) as the corollary of result concerning spurious bifurcations of period 2 solutions; here we present a direct, and hence substantially shorter, proof of the result. We employ classical techniques of numerical analysis, rather than bifurcation theory.

A multistep method should be zero-stable since, by a celebrated theorem of Dahlquist, zero-stability and consistency are equivalent to convergence on a finite time-interval (Hairer *et al.*, 1987; Henrici, 1962). The so-called *first Dahlquist barrier* establishes the maximal order of a zero-stable multistep method as $2[m/2]+2$ (Henrici, 1962; Iserles & Nørsett, 1984). Under the additional condition that $\sigma(-1)=0$ this bound is too generous: in Section 3 we derive $2[(m+1)/2]$ as the order barrier for zero-stable multistep methods satisfying $\sigma(-1)=0$.

The methods of choice for the integration of stiff equations are the *backward differentiation formulae* (*BDF*), becaue of their superior damping at infinity. For such methods $\sigma(z)=Cz^m$ for some $C\neq 0$; thus $\sigma(-1)\neq 0$ and period 2 solutions in n may occur. The obvious remedy is to consider methods with $\sigma(z)=Cz^{m-1}(z+1)$. Schemes of this form are investigated in Section 3, where coefficients of maximal-order schemes are presented for $m=1, 2, \ldots, 10$.

It has been first observed by Mitchell and Craggs (1953) that BDF schemes are zero-stable if and only if $m\leqslant 6$. This has been subsequently proved by Cryer (1971, 1972). Of course, zero-stability is the *sine qua non* for the applicability of a multistep method. Thus, it is central to our analysis to characterise all the zero-stable methods with $\sigma(z)=Cz^{m-1}(z+1)$. The very elegant approach applied to the BDF in (Hairer & Wanner, 1983) is extended in Section 4 to investigate the methods from Section 3. For greater generality (and no extra difficulty!) we let $\sigma(z)=Cz^{m-1}(z+\alpha)$ for any $\alpha\in(-1, 1]$ (we term these *BDF-like methods*) and prove that zero-stability, in unison with order m, implies that $m\leqslant 15$, $m\neq 14$. In particular, the inspection of the finite number of outstanding cases when $\alpha=1$ implies that the bound $m\leqslant 6$ is valid within this framework.

Further in Section 4 we sketch and examine linear stability domains of BDF-like methods for relevant values of m. It transpires that $\alpha=1$ leads to similar linear stability properties as the classical BDF. However, for example, the value $\alpha=-\frac{1}{2}$ (which, of course, cannot be justified by the dynamical considerations of Section 2) produces zero-stability and non-trivial linear stability domains for all $m\leqslant 7$.

Implementation of multistep methods involves in practice techniques for error control and step-variation. Our framework excludes these phenomena, hence the impact of our results is limited. Initial analysis of asymptotic behaviour of numerical methods for ordinary differential equations that incorporates error control strategies has been presented by (Griffiths, 1987).

2. Multistep methods with $\sigma(-1)=0$

Let the method (1.1) be irreducible (thus, ρ and σ do not share zeros), zero-stable and of order $p\geqslant 1$. If we assume that a period 2 solution $\{\hat{\boldsymbol{v}}, \hat{\boldsymbol{u}}\}$, $\hat{\boldsymbol{v}}\neq\hat{\boldsymbol{u}}$, exists then we may take

$$y_{2n}=\hat{\boldsymbol{u}} \quad\text{and}\quad y_{2n+1}=\hat{\boldsymbol{v}}.$$

Substituting in (1.1) for even n gives

$$\sum_{k=0}^{[m/2]} \rho_{2k}\hat{v} + \sum_{k=0}^{[(m-1)/2]} \rho_{2k+1}\hat{u} = h\left\{\sum_{k=0}^{[m/2]} \sigma_{2k}f(\hat{v}) + \sum_{k=0}^{([m-1)/2]} \sigma_{2k+1}f(\hat{u})\right\}. \quad (2.1)$$

Likewise, odd values of n yield

$$\sum_{k=0}^{[(m-1)/2]} \rho_{2k+1}\hat{v} + \sum_{k=0}^{[m/2]} \rho_{2k}\hat{u} = h\left\{\sum_{k=0}^{[(m-1)/2]} \sigma_{2k+1}f(\hat{v}) + \sum_{k=0}^{[m/2]} \sigma_{2k}f(\hat{u})\right\}. \quad (2.2)$$

But

$$\sum_{k=0}^{[m/2]} \rho_{2k} = \tfrac{1}{2}(\rho(1)+\rho(-1)), \qquad \sum_{k=0}^{[(m-1)/2]} \rho_{2k+1} = \tfrac{1}{2}(\rho(1)-\rho(-1))$$

and similarly for the σ_k. Moreover, $p \geq 1$ implies that $\rho(1)=0$. Thus, addition and subtraction of (2.1) and (2.2) yield

$$\rho(-1)(\hat{v}-\hat{u}) = h\sigma(-1)\{f(\hat{v})-f(\hat{u})\} \quad (2.3)$$

and

$$0 = h\sigma(1)\{f(\hat{v})+f(\hat{u})\} \quad (2.4)$$

respectively. Now, suppose that $\sigma(-1)=0$. Thus, by irreducibility, $\rho(-1)\neq 0$ and (2.3) implies that $\hat{v}=\hat{u}$, in contradiction to our assumption. Thus, no period 2 solution is possible if $\sigma(-1)=0$.

THEOREM 2.1 A period 2 solution of an irreducible multistep method (1.1) may occur for some differential system (1.2) if and only if $\sigma(-1)\neq 0$.

Proof. The 'only if' part is proved above. It remains to prove that $\sigma(-1)\neq 0$ implies the existence of a period 2 solution for some ordinary differential equation (1.2). In the case of $\rho(-1)=0$ we choose $f(y)=1-y^2$ and arbitrary $h>0$, if $\rho(-1)\sigma(-1)>0$ we take $f(y)=y$, $h=\rho(-1)/\sigma(-1)>0$ and, finally, if $\rho(-1)\sigma(-1)<0$ then $f(y)=-y$, $h=-\rho(-1)/\sigma(-1)>0$. Moreover, we let $\hat{v}=1$, $\hat{u}=-1$. It follows at once that both (2.3) and (2.4) are satisfied. Thus, letting $y_0=\hat{v}$, $y_1=\hat{u}$ generates a period two solution. □

Note that in all three cases it suffices to take a simple specific scalar equation to prove the existence of a period 2 solution. In (Iserles *et al.*, 1991) the existence of spurious period 2 solutions for arbitrary nonlinearities is examined. In addition, the rôle of period 2 solutions in stability breakdown is highlighted in (Iserles *et al.*, 1991). Clearly, a numerical algorithm is safer when such solutions are forbidden and Theorem 2.1 provides us with a handy and easy means to implement a criterion to that end.

3. Zero-stability barrier

We assume again that the method (1.1) is irreducible, zero-stable and of order $p \geq 1$. We bound the order p for the method, subject to the constraint $\sigma(-1)=0$, to obtain the following theorem, which is proved as a succession of propositions and corollaries.

THEOREM 3.1 The highest order attainable by a zero-stable multistep method with $\sigma(-1)=0$ is $2[(m+1)/2]$. □

Following (Henrici, 1962) we define

$$r(\zeta):=\left(\frac{1-\zeta}{2}\right)^m \rho\left(\frac{1+\zeta}{1-\zeta}\right)=\sum_{k=0}^{m} a_k\zeta^k;$$

$$s(\zeta):=\left(\frac{1-\zeta}{2}\right)^m \sigma\left(\frac{1+\zeta}{1-\zeta}\right)=\sum_{k=0}^{m} b_k\zeta^k$$

and let

$$\frac{\zeta}{\log\frac{1+\zeta}{1-\zeta}}=\sum_{k=0}^{\infty} c_k\zeta^k.$$

The following points are true:

(a) $a_0=0$;

(b) $c_{2k-1}=0,\ c_{2k}<0$ for all $k=1,2,\ldots$;

(c) $a_k\geqslant 0,\ k=1,2,\ldots,m$;

(d)

$$\frac{\zeta}{\log\frac{1+\zeta}{1-\zeta}}\frac{r(\zeta)}{\zeta}-s(\zeta)=\mathcal{O}(\zeta^p);$$

(e) $b_m=0$.

(a) is implied by $\rho(1)=0$, (b) follows by the Cauchy theorem, (c) comes from zero-stability and (d) is a consequence of order p—all these are classical observations, originally due to Dahlquist (Henrici, 1962). (e) is true since $\sigma(-1)=0$, because the mapping $z\mapsto(1-z)/(1+z)$ takes -1 to ∞.

We assume that $p\geqslant m+1$. First we let m be even, $m=2M$. Thus, (a), (d) and (e) imply that

$$0=b_{2M}=c_2a_{2M-1}+c_4a_{2M-3}+\cdots+c_{2M}a_1.$$

This, in unison with (b) and (c), yields $a_1=a_3=\cdots=a_{2M-1}=0$, hence r is an even polynomial. Zero-stability implies that all the zeros of ρ are in the closed complex unit disc, hence all the zeros of r must reside in the closed left half-plane. The only even, real polynomial that possesses this feature is a polynomial with all its zeros on $i\mathbb{R}$.

Likewise, if $m=2M+1$ then

$$0=b_{2M+1}=c_2a_{2M}+c_4a_{2M-2}+\cdots+c_{2M}a_2=0$$

implies that $a_2=a_4=\cdots=a_{2M}=0$. Thus, r is odd and, again, all its zeros are on $i\mathbb{R}$.

Since the inverse map takes $i\mathbb{R}$ to $|z|=1$, we have

PROPOSITION 3.1 If $p\geqslant m+1$ then all the zeros of ρ are on the unit circle. □

COROLLARY If m is even then $p\leqslant m$.

Proof. If $p \geq m+1$ then all the zeros of ρ are on $|z|=1$. But $\rho(1)=0$, $\rho'(1)\neq 0$, m is even, hence $\rho(-1)=0$. This contradicts irreducibility. □

The remaining option is m odd, $p \geq m+1$. Since the first Dahlquist barrier is valid independently of the constraint on $\sigma(-1)$, we need only consider $p=m+1$.

PROPOSITION 3.2 If $p=m+1$ then all the zeros of σ are symmetric with respect to $|z|=1$.

Proof. Let $\rho^*(z):=z^m\rho(z^{-1})$, $\sigma^*(z):=-z^m\sigma(z^{-1})$. Thus,

$$\rho(z)=\sigma(z)\log z+\mathcal{O}((z-1)^{m+2}),$$
$$\rho^*(z)=\sigma^*(z)\log z+\mathcal{O}((z-1)^{m+2}), \qquad z\to 1.$$

Since all the zeros of ρ reside on $|z|=1$, we have $\rho^*\equiv\pm\rho$. The number of steps m being odd, irreducibility implies that $\rho^*=-\rho$. Thus, adding, we have

$$(\sigma(z)+\sigma^*(z))\log z=\mathcal{O}((z-1)^{m+2}).$$

But $\log z=z+1+\mathcal{O}((z-1)^2)$, thus

$$\sigma(z)+\sigma^*(z)=\mathcal{O}((z-1)^{m+1})$$

and, since σ, σ^* are mth degree polynomials,

$$\sigma^*\equiv-\sigma.$$

The proposition follows. □

Note that m odd, symmetry of σ with respect to $|z|=1$ and irreducibility of the underlying multistep method imply $\sigma(-1)=0$, since σ must have an even number of zeros in $\mathbb{C}\backslash\{+1,-1\}$ and $\sigma(1)\neq 0$ by irreducibility.

Let us now fix ρ and set

$$\tilde{\sigma}(z):=\frac{\sigma(z)}{1+z}.$$

Thus,

$$\tilde{\sigma}(z)=\frac{\rho(z)}{(1+z)\log z}+\mathcal{O}((z-1)^p).$$

Since the degree of $\tilde{\sigma}$ is $(m-1)$, it follows that $p=m$ is always attainable. This, together with Proposition 3.1, establishes Theorem 3.1 for m even.

Let m be odd and ρ have all its zeros on $|z|=1$, while the zeros of σ are symmetric with respect to the unit circle. Thus, r is odd and s is even. Therefore, all the terms on the left of

$$\frac{z}{\log\dfrac{z-1}{z+1}}\frac{r(z)}{z}-s(z)=\mathcal{O}(z^p)$$

are even, implying that so is p. Provided that we choose σ so that $p\geq m$ (which we can always do for a given ρ), it follows that $p=m+1$. This establishes Theorem 3.1 for m odd. □

BDF methods attain maximal damping at infinity by letting $\sigma(z) = Cz^m$ for some constant $C \neq 0$. Thus, $\sigma(-1) \neq 0$ and these methods might display spurious oscillations. An alternative, that trades off superior damping for enhanced dynamics, is to impose $\sigma(-1) = 0$ and to exploit the remaining degrees of freedom in σ to damp at infinity $m-1$ components of the linear stability function. We do not claim that this is necessarily better than standard BDF for stiff *linear* problems, but that the situation for nonlinear problems is far from clear and so we are suggesting a tentative alternative method which may be superior in certain situations. Hence we choose

$$\sigma(z) = Cz^{m-1}(z+1), \qquad C \neq 0. \tag{3.1}$$

We stipulate order $p = m$ (as is the case with BDF methods). Note that, for odd m, this order falls short of the upper bound of Theorem 3.1. This, however, is illusory: by Proposition 3.1 order $m+1$, zero-stability and $\sigma(-1) = 0$ imply that all the zeros of ρ reside on the unit circle, hence, subject to $m \geqslant 2$, the scheme is only marginally zero-stable. Our definition means that ρ is the mth degree polynomial that matches the expansion of

$$z^{m-1}(1+z)\log z$$

at $z = 1$ up to $\mathcal{O}(|z-1|^{m+1})$, scaled so that $\rho_m = 1$. For $m = 1$ we recover the trapezoidal rule, $\rho(z) = z - 1$, $\sigma(z) = \frac{1}{2}(z+1)$. The case $m = 2$ leads to reducibility and, eventually, to the trapezoidal rule. Herewith we list the schemes (3.1) for $m = 3, \ldots, 10$:

$m = 3$:

$$\rho(z) = z^3 - \frac{15}{13}z^2 + \frac{3}{13}z - \frac{1}{13}, \qquad \sigma(z) = \frac{6}{13}z^2(z+1).$$

$m = 4$:

$$\rho(z) = z^4 - \frac{19}{14}z^3 + \frac{9}{14}z^2 - \frac{5}{14}z + \frac{1}{14},$$

$$\sigma(z) = \frac{3}{7}z^3(z+1).$$

$m = 5$:

$$\rho(z) = z^5 - \frac{235}{149}z^4 + \frac{180}{149}z^3 - \frac{140}{149}z^2 + \frac{55}{149}z - \frac{9}{149},$$

$$\sigma(z) = \frac{60}{149}z^4(z+1).$$

$m = 6$:

$$\rho(z) = z^6 - \frac{283}{157}z^5 + \frac{300}{157}z^4 - \frac{300}{157}z^3 + \frac{175}{157}z^2 - \frac{57}{157}z + \frac{8}{157}$$

$$\sigma(z) = \frac{60}{157}z^5(z+1).$$

$m=7$:

$$\rho(z)=z^7-\frac{777}{383}z^6+\frac{1050}{383}z^5-\frac{3850}{1149}z^4+\frac{2975}{1149}z^3-\frac{483}{383}z^2+\frac{406}{1149}z-\frac{50}{1149},$$

$$\sigma(z)=\frac{140}{383}z^6(z+1).$$

$m=8$:

$$\rho(z)=z^8-\frac{897}{398}z^7+\frac{735}{199}z^6-\frac{3185}{597}z^5+\frac{6125}{1194}z^4-\frac{1323}{298}z^3+\frac{833}{597}z^2-\frac{205}{597}z$$
$$+\frac{15}{398},$$

$$\sigma(z)=\frac{70}{199}z^7(z+1).$$

$m=9$:

$$\rho(z)=z^9-\frac{18351}{7409}z^8+\frac{35280}{7409}z^7-\frac{58800}{7409}z^6+\frac{67620}{7409}z^5-\frac{1764}{239}z^4+\frac{30576}{7409}z^3$$
$$-\frac{11280}{7409}z^2+\frac{2475}{7409}z-\frac{245}{7409},$$

$$\sigma(z)=\frac{2520}{7409}z^8(z+1).$$

$m=10$:

$$\rho(z)=z^{10}-\frac{20591}{7633}z^9+\frac{45360}{7633}z^8-\frac{5040}{449}z^7+\frac{114660}{7633}z^6-\frac{111132}{7633}z^5+\frac{77616}{7633}z^4$$
$$-\frac{38160}{7633}z^3+\frac{12555}{7633}z^2-\frac{2485}{7633}z+\frac{224}{7633},$$

$$\sigma(z)=\frac{2520}{7633}z^9(z+1).$$

Examination of the zeros of ρ for different values of m demonstrates that $m\leqslant 6$ yields zero-stability, whereas schemes (3.1) with $7\leqslant m\leqslant 10$ are not zero-stable. There is but a short step from this observation to the conjecture that, like the conventional BDF methods, the methods (3.1) are zero-stable if and only if $m\leqslant 6$. This will be proved in the next section.

4. Zero-stability of BDF-like methods

In the last section we introduced order-m methods with $\sigma(z)=Cz^{m-1}(z+1)$. In this section we analyze the zero-stability properties of BDF-like methods; the analysis remains valid upon the introduction of an extra free parameter into such methods. As this requires very little effort and brings about new results that are interesting on their own merit, we extend our framework accordingly.

DEFINITION 4.1 We say that an m-step method of order m is *BDF-like* if $\sigma(z) = Cz^{m-1}(z+\alpha)$, where C and α are real constants.

The order condition is equivalent to

$$\sum_{k=0}^{m} \rho_k z^k = Cz^{m-1}(\alpha + z)\log z + E(z-1)^{m+1} + \mathcal{O}(|z-1|^{m+2}), \qquad E \neq 0. \quad (4.1)$$

Changing the variable $z \mapsto z^{-1}$ in (4.1) and multiplying by z^m yields

$$\sum_{k=0}^{m} \rho_k z^{m-k} = -C(1+\alpha z)\log z + E(1-z)^{m+1} + \mathcal{O}(|z-1|^{m+2}).$$

Since $\rho(1) = 0$, there exist real numbers $p_1, \ldots, p_m$ such that

$$\sum_{k=1}^{m} p_k(1-z)^k = \frac{1}{C}\sum_{k=0}^{m} \rho_k z^{m-k}.$$

We obtain the order condition

$$\sum_{k=1}^{m} p_k(1-z)^k = -(1+\alpha z)\log z + \frac{E}{C}(1-z)^{m+1} + \mathcal{O}(|z-1|^{m+2}). \quad (4.2)$$

PROPOSITION 4.1 The coefficients $p_1, \ldots, p_m$ obey (4.2) if and only if $p_1 = 1 + \alpha$ and

$$p_k = \frac{k-1-\alpha}{(k-1)k}, \qquad k = 2, 3, \ldots, m.$$

Proof. It is a consequence of equation 4.2 that

$$\begin{aligned}\sum_{k=1}^{m} p_k(1-z)^k &= (1+\alpha-\alpha(1-z))\sum_{k=1}^{\infty}\frac{1}{k}(1-z)^k + \mathcal{O}(|z-1|^{m+1})\\ &= (1+\alpha)\sum_{k=1}^{m}\frac{1}{k}(1-z)^k - \alpha\sum_{k=2}^{m}\frac{1}{k-1}(1-z)^k + \mathcal{O}(|z-1|^{m+1}), \qquad z \to 1,\end{aligned}$$

and the statement of the lemma follows at once by comparison of coefficients. □

Herewith we assume that $\alpha \geq 0$, $p_1, \ldots, p_m$ are chosen to conform with Proposition 4.1, and set

$$\begin{aligned}P_m(z;\alpha) := \sum_{k=1}^{m} p_k z^k &= (1+\alpha)\sum_{k=1}^{m}\frac{1}{k}z^k - \alpha z\sum_{k=1}^{m-1}\frac{1}{k}z^k\\ &= (1+\alpha)P_m(z;0) - \alpha z P_{m-1}(z;0).\end{aligned}$$

Thus, the underlying method is zero-stable if and only if all the zeros of $P_m(\cdot;\alpha)$ are in $\{z \in \mathscr{C} : |z-1| \geq 1\}$, with only simple zeros on the boundary.

Following Hairer and Wanner (1983), we express $P_m(\cdot;0)$ in an integral form,

$$P_m(re^{i\theta};0) = \int_0^r (1 - e^{im\theta}s^m)\frac{e^{i\theta}}{1-se^{i\theta}}\,ds.$$

Given $m \geqslant 10$, we let

$$\mathcal{S} := \left\{ re^{i\theta} : |\theta| \leqslant \frac{5\pi}{m},\ R_- < |z| < R_+ \right\},$$

where $0 < R_- \ll 1 \ll R_+$. Let $\theta^* = \pm\frac{5\pi}{m}$ be the argument along the straight-line portion of $\mathcal{S}$. Then $e^{im\theta^*} = -1$, hence

$$P_m(re^{i\theta^*}; \alpha) = \int_0^r ((1+\alpha)(1+s^m) - \alpha r(e^{i\theta^*} + s^{m-1})) \frac{e^{i\theta^*} - s}{|1 - se^{i\theta^*}|^2} ds.$$

We deduce that

$$\operatorname{Im} P_m(re^{i\theta^*}; \alpha) = \sin\theta^* \int_0^r U_m(s) \frac{ds}{|1 - se^{i\theta^*}|^2},$$

where

$$U_m(s) := (1+\alpha)s^m - \alpha r s^{m-1} + \alpha r s + (1 + \alpha - 2\alpha r \cos\theta^*).$$

Since $\alpha \geqslant 0$ and $\cos\theta^* > 0$ (because $m \geqslant 10$), it follows from the Descartes rule of signs (Pólya and Szegő, 1976; Vol. II, Problem V-36) that for $r \gg 1$ U_m has at most three positive zeros.

We let

$$V_m(r) := \int_0^r U_m(s) \frac{ds}{|1 - se^{i\theta^*}|^2},$$

hence $\operatorname{Im} P(re^{i\theta^*}; \alpha) = \sin\theta^* V_m(r)$. Since the integrand changes sign only at zeros of U_m, it follows that the line segment (R_-, R_+) can be decomposed into at most 4 intervals where V_m is monotone. In particular, V_m has at most 3 zeros there.

PROPOSITION 4.2 Given $\alpha \geqslant 0$, $m \geqslant 10$ and $R_- \downarrow 0$, $R_+ \uparrow \infty$, the set $\mathcal{S}$ includes a zero of $P_m(\cdot; \alpha)$.

Proof. The boundary of $\mathcal{S}$ is composed of four portions: the two straight lines where the argument is θ^*, as well as the small (radius R_-) and the large (radius R_+) circular sections. If a zero of P_m lies on the straight lines then it is in $\mathcal{S}$ and there is nothing to prove. Hence we may assume that no zero of P_m lies there.

We measure the variation of the argument along the positively oriented boundary of $\mathcal{S}$, by extending the reasoning in (Hairer & Wanner, 1983). As $R_+ \to \infty$, $R_- \to 0$, the outer circular portion contributes $10\pi + o(1)$, since P_m has an m-fold pole at infinity, whereas the inner circular section adds $o(1)$, because of a simple zero at the origin. Finally, since $\operatorname{Im} P_m$ has at most 6 zeros along the two straight-line portions of the boundary, the argument there cannot decrease by more than 7π. Thus, totally, the argument along $\partial\mathcal{S}$ increases by at least 2π and it follows from the argument principle that there is at least one zero of P_m in $\mathcal{S}$. □

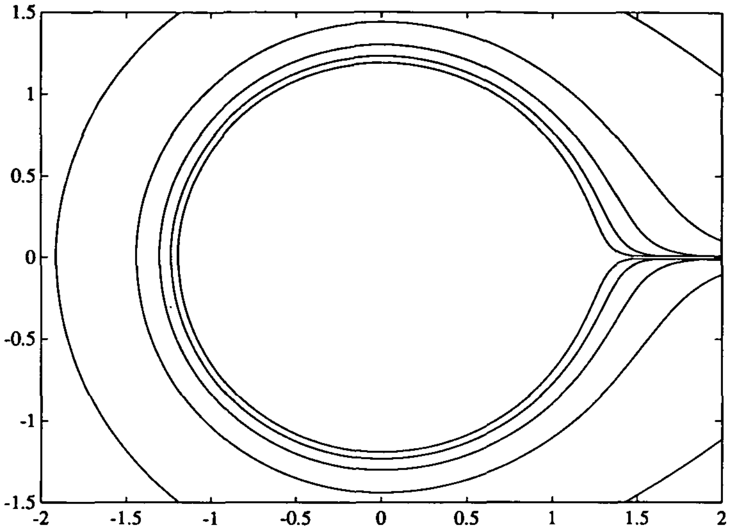

FIG. 4.1. The curves $\omega_m^{[1]}$ for $m \in \{5, 10, 15, 20, 25\}$.

The next stage of our analysis parallels closely the work of Hairer and Wanner. When $m \geq 20$, it follows from the last proposition that there are zeros of P_m in the wedge $\left\{z \in \mathscr{C} : |\arg z| \leq \frac{\pi}{4}\right\}$, and our purpose is to show that, subject to m being sufficiently large, these zeros lie sufficiently near to the origin to belong to $|z-1|<1$ and infringe zero-stability. Let

$$\phi(s) := \frac{e^{i\theta}}{1 - se^{i\theta}}.$$

The integral representation from (Hairer & Wanner, 1983) gives

$$P_m(z;\alpha) = (1+\alpha)\int_0^r (1 - e^{im\theta}s^m)\phi(s)\,ds - \alpha r e^{i\theta}\int_0^r (1 - e^{i(m-1)\theta}s^{m-1})\phi(s)\,ds$$
$$:= K_1 - K_2,$$

where

$$K_2 := e^{im\theta}\left\{(1+\alpha)\int_1^r s^m\phi(s)\,ds - \alpha r\int_1^r s^{m-1}\phi(s)\,ds\right\}$$

and

$$K_1 := P_m(z;\alpha) + K_2.$$

Both K_1 and K_2 can be estimated identically to the quantities

$$I_1 := \int_0^r \phi(s)\,ds - \int_0^1 e^{im\theta}s^m\phi(s)\,ds,$$

$$I_2 := e^{im\theta}\int_1^r s^m\phi(s)\,ds$$

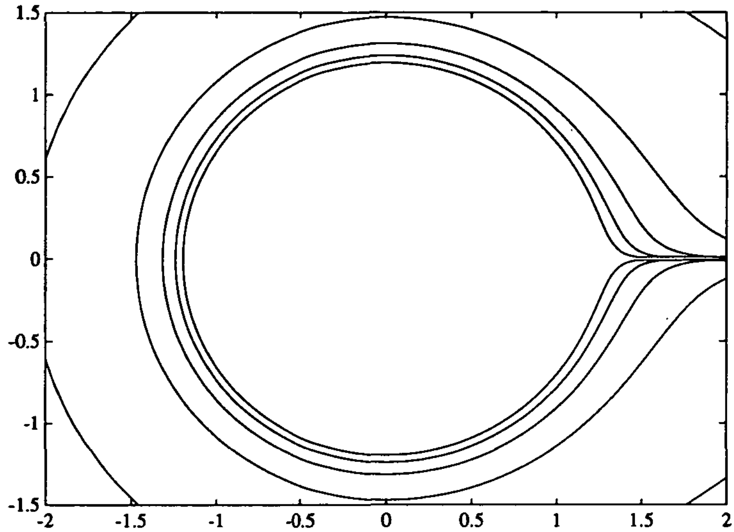

FIG. 4.2. The curves $\omega_m^{[2]}$ for $m \in \{5, 10, 15, 20, 25\}$.

in (Hairer & Wanner, 1983), since they can be expressed easily in terms of I_1 and I_2. Let

$$B(\theta)=\begin{cases} \dfrac{1}{\sin\theta} & : 0<\theta\leqslant\dfrac{\pi}{2}, \\ 1 & : \dfrac{\pi}{2}\leqslant\theta\leqslant\pi \end{cases}$$

Then, given $\alpha\geqslant 0$,

$$|K_1|\leqslant\left((1+\alpha)\frac{m+2}{m+1}+\alpha r\frac{m+1}{m}\right)B(\theta)r \tag{4.3}$$

and

$$|K_2|>(1+\alpha)r\frac{r^{m-1}-1}{2m+2}+\alpha r^2\frac{r^{m-2}-1}{2m}. \tag{4.4}$$

We wish to explore conditions that ensure $P_m\neq 0$. To that end, it is sufficient to establish that $|K_2|>|K_1|$. Comparing (4.3) with (4.4),

$$\begin{aligned}|K_2|>|K_1| &\Leftarrow (1+\alpha)\frac{r^{m-1}-1}{2m+2}+\alpha r\frac{r^{m-2}-1}{2m}\geqslant\left((1+\alpha)\frac{m+2}{m+1}+\alpha r\frac{m+1}{m}\right)B(\theta)\\ &\Leftrightarrow \big(m+(2m+1)\alpha\big)r^{m-1}-(m+1)\alpha\big(1+2(m+1)B(\theta)\big)r\\ &\quad -m(1+\alpha)\big(1+2(m+2)B(\theta)\big)\geqslant 0.\end{aligned} \tag{4.5}$$

But, for sufficiently large m, it is true that

$$r\geqslant\left((\alpha r+1+\alpha)\frac{2mB(\theta)}{1+2\alpha}\right)^{1/(m-1)}.$$

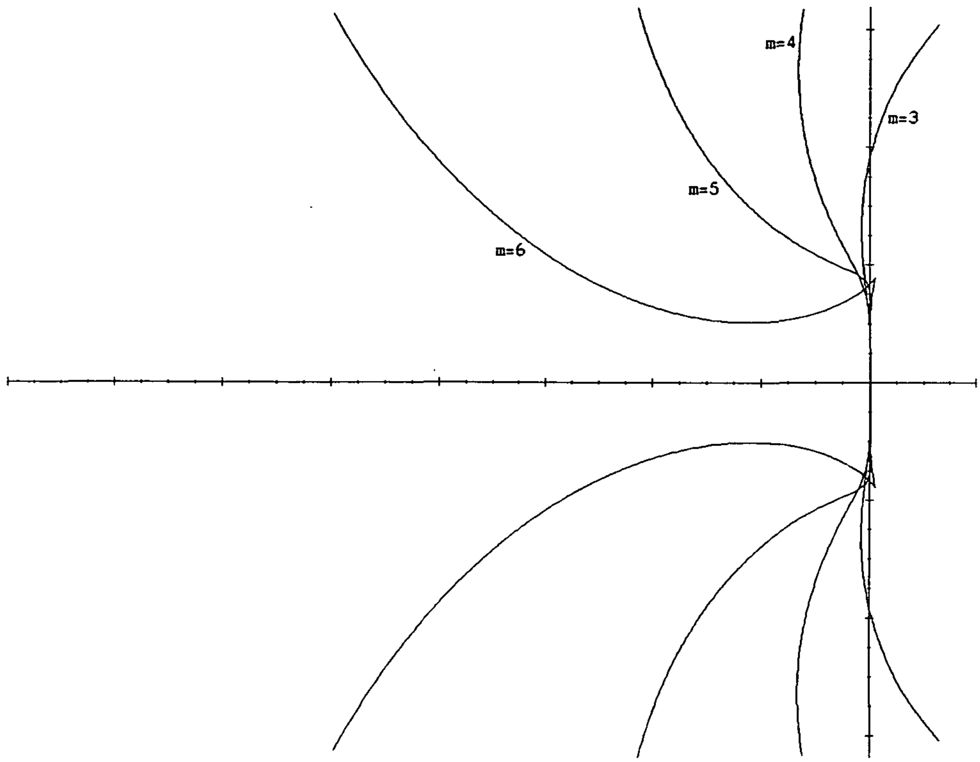

FIG. 4.3. Linear stability domains for $\alpha = 0$.

Given that $r \leq 2$, this is valid if

$$r \geq \omega_m^{[1]} := \left((3\alpha + 1)\frac{2mB(\theta)}{1+2\alpha}\right)^{1/(m-1)}. \tag{4.6}$$

Thus,

$$(1+2\alpha)r^{m-1} - 2\alpha mB(\theta)r - 2m(1+\alpha)B(\theta) \geq 0$$

and (4.5) is implied by

$$r \geq \left(\frac{(m+1)\alpha\big(1+2(m+1)B(\theta)r\big) + m(1+\alpha)\big(1+2(m+2)B(\theta)\big)}{m+(2m+1)\alpha}\right)^{1/(m-1)}.$$

Stipulating again that $r \leq 2$, this is in turn implied by

$$r \geq \omega_m^{[2]} := \left(\frac{m + (3m+2)\alpha + 2\big(m(m+2) + (3m^2+6m+2)\alpha\big)B(\theta)}{m+(2m+1)\alpha}\right)^{1/(m-1)}. \tag{4.7}$$

Note that for $\alpha = 0$ (4.6) is always true for $r > 1$, whereas (4.7) reduces to an inequality in (Hairer & Wanner, 1983).

Clearly, as $m \to \infty$, both $\omega_m^{[1]}$ and $\omega_m^{[2]}$ tend to 1. More importantly, as can be seen in Figures 4.1–2 and can be verified by simple calculation, the curve $\omega_{m+1}^{[i]}$ lies nested inside $\omega_m^{[i]}$, $i = 1, 2$. Thus, if for certain m_0 the curves constrain a

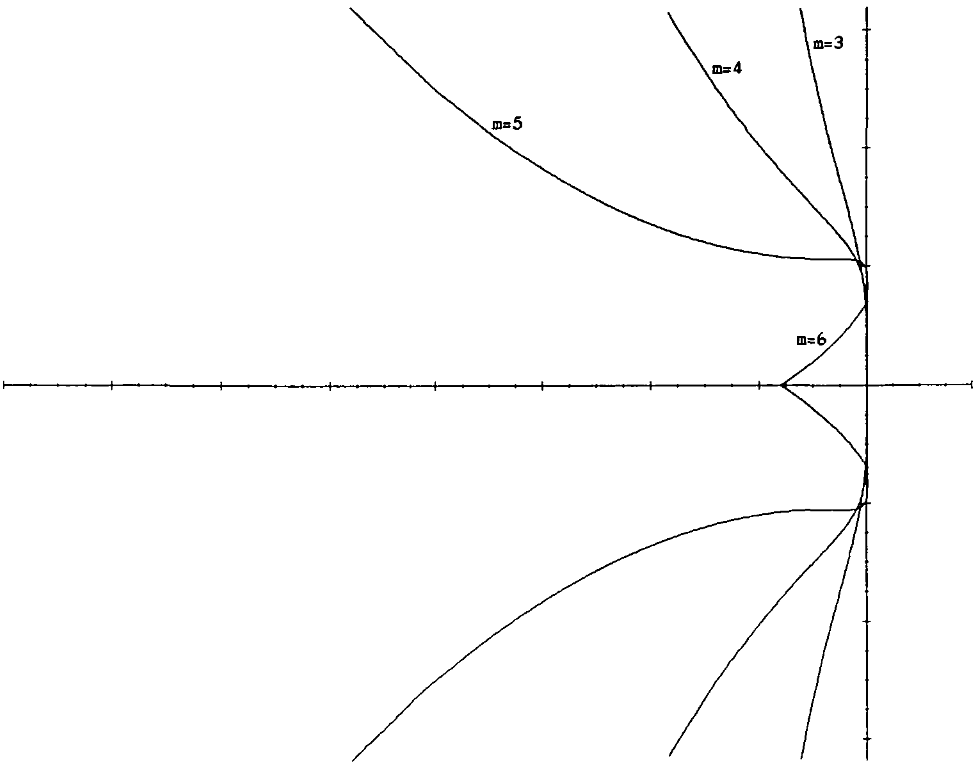

FIG. 4.4. Linear stability domains for $\alpha = 1$.

sector $\mathcal{S}_j$ to have a zero in $\{z \in \mathbb{C} : |z-1| < 1\}$, then so will be the case for all $m \geq m_0$. Simple calculation affirms that $m_0 = 12$ is a valid choice for $\alpha = 1$. Bearing in mind that we have already stipulated $m \geq 20$, zero-instability follows. Since direct calculation affirms zero-stability for $m \leq 6$ and rules it out for $7 \leq m \leq 19$, we obtain a characterisation of zero-stable BDF-like methods with $\sigma(-1) = 0$.

THEOREM 4.3 The m-step BDF-like method with $\alpha = 1$ is zero-stable if and only if $m \leq 6$. □

A similar statement can be deduced for other values of $\alpha \geq 0$, although the bound may exceed 6. For example, $\alpha = \frac{9}{2}$, $m = 7$, are consistent with zero-stability. Other examples of the barrier of Theorem 4.3 being exceeded occur for $\alpha < 0$. A simple example is $\alpha = -\frac{1}{2}$, where $1 \leq m \leq 7$ produces zero-stability.

Figures 4.3–5 display linear stability domains for the 'classical' BDF methods ($\alpha = 0$), the methods with $\sigma(-1) = 0$ ($\alpha = 1$) and, finally, the methods with $\alpha = -\frac{1}{2}$, for all relevant values of m.

Acknowledgements

The authors are grateful to the referees for their helpful comments and for exposing a crucial gap in the original proof of Theorem 4.3.

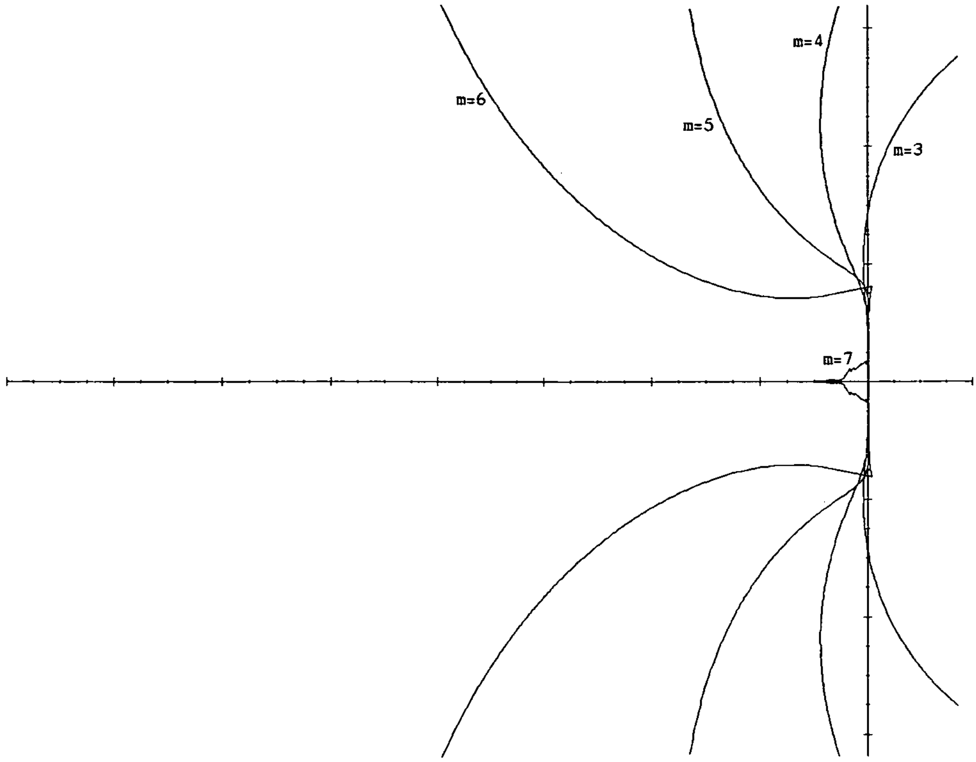

FIG. 4.5. Linear stability domains for $\alpha = -\frac{1}{2}$.

This paper is dedicated to Ron Mitchell on the occasion of his 70th birthday and in appreciation of his pioneering contribution to the development of numerical analysis—not least, by techniques from the theory of nonlinear dynamical systems—and as a tribute to his leadership, inspiration and encouragement.

References

BEYN, W.-J. 1987 "On the numerical approximation of phase portraits near stationary points", *SIAM J. Num. Anal.* **24,** 1095–1113.

CREEDON, D. M., & MILLER, J. J. H. 1975 The stability properties of q-step backward-difference schemes, *BIT* **15,** 244–249.

CRYER, C. W. 1971 *A proof of the instability of backward-difference methods for the numerical integration of ordinary differential equations,* Univ. of Wisconsin at Madison Tech. Rep. 117.

CRYER, C. W. 1972 On the instability of high order backward-difference multistep methods, *BIT* **12,** 17–25.

EIROLA, T. 1988, Invariant curves of one-step methods, *BIT* **28,** 113–122.

GRIFFITHS, D. F. 1987 The dynamics of some linear multistep methods with step-size control, in *Numerical Analysis* (Griffiths, D. F. and Watson, G. A., eds), Longman, Harlow, 115–134.

GRIFFITHS, D. F., & MITCHELL, A. R. 1988 Stable periodic bifurcations of an explicit discretisation of a nonlinear partial differential equation in reaction-diffusion", *IMA J. Num. Anal.* **8,** 435–454.

GUCKENHEIMER, J., & HOLMES, P. 1983 *Nonlinear Oscillations, Dynamical Systems and Bifurcations of Vector Fields, Applied Mathematical Sciences* **42**. Springer-Verlag (New York).

HAIRER, E., ISERLES, A., & SANZ-SERNA, J. M. 1990 Equilibria of Runge–Kutta methods, *Numer. Math.* **58**, 243–254.

HAIRER, E., NØRSETT, S. P., & WANNER, G. 1987 Solving Ordinary Differential Equations I. Nonstiff Problems, Springer-Verlag, Berlin.

HAIRER, E., & WANNER, G. 1983 On the instability of the BDF formulas, *SIAM J. Num. Anal.* **20**, 1206–1209.

HALE, J., LIN, X.-B., & RAUGEL, G. 1988 Upper semicontinuity of attractors for approximations of semigroups and partial differential equations, *Math. Comp.* **50**, 89–123.

HENRICI, P. 1962 Discrete Variable Methods in Ordinary Differential Equations, Wiley, New York.

ISERLES, A. 1990 Stability and dynamics of numerical methods for nonlinear ordinary differential equations, *IMA J. Num. Anal.* **10**, 1–30.

ISERLES, A., & NØRSETT, S. P. 1984 A proof of the first Dahlquist barrier by order stars, *BIT* **24**, 529–537.

ISERLES, A., PEPLOW, A. T., & STUART, A. M. 1991 A unified approach to spurious solutions introduced by time discretisation. Part I: Basic theory, *SIAM J. Num. Anal.* **28**, 1723–1751.

KLOEDEN, P. E., & LORENZ, J. 1986 Stable attracting sets in dynamical systems and in their one-step discretisations, *SIAM J. Num. Anal.* **23**, 986–995.

MITCHELL, A. R., & CRAGGS, J. W. 1953, Stability of difference relations in the solution of ordinary differential equations, *MTAC* **7**, 127–129.

PÓLYA, G., & SZEGŐ, G. 1976 Problems and Theorems in Analysis, Springer-Verlag, Berlin.

SAND, J., & ØSTERBY, O. 1979 *Regions of absolute stability,* Univ. of Århus Tech. Rep. DAIMI PB-102.

STUART, A. M. 1990 The global attractor under discretisation, in *Continuation and Bifurcations: Numerical Techniques and Applications* (D. Roose, B. De Dier and A. Spence, eds), Kluwer, Dordrecht.

STUART, A. M., & PEPLOW, A. T. 1991 The dynamics of the theta method, *SIAM J. Sci. Stat. Comp.* **12**, 1351–1372.