

The existence of stepsize-coefficients for boundedness of linear multistep methods

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Abstract. This paper deals with general linear multistep methods (LMMs) for the numerical solution of initial value problems. In the context of semi-discretizations of nonlinear time-dependent partial differential equations, much attention was paid to LMMs fulfilling special stability requirements, indicated by the terms total-variation-diminishing (TVD), strong stability preserving (SSP) and monotonicity. Stepsize restrictions, for the fulfillment of these requirements, were studied by Shu & Osher [J. Comput. Phys., 77 (1988) pp. 439-471 and in numerous subsequent papers.

These special stability requirements imply essential boundedness properties for the numerical methods, among which the property of being total-variation-bounded (TVB). Unfortunately, for many LMMs, the above special requirements are violated, so that one cannot conclude via them that the methods are (total-variation-)bounded.

In this paper, we focus on stepsize restrictions for boundedness directly - rather than via the detour of the above special stability requirements. We present conditions by means of which one can check, for given LMMs, whether or not nontrivial stepsize restrictions exist guaranteeing boundedness.

We illustrate the relevance of the above conditions by applying them to various classes of well-known LMMs, hereby supplementing earlier results, for these classes, given in the literature.

Key words. initial value problem, semi-discretization, ordinary differential equation, nonlinear hyperbolic partial differential equation, linear multistep method (LMM), monotonicity, strong-stability-preserving (SSP), total-variation-diminishing (TVD), boundedness, total-variation-bounded (TVB).

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1 Introduction

1.1 Stepsize-coefficients for monotonicity

In this paper we deal with the numerical solution of initial value problems, for systems of ordinary differential equations which can be written in the form

$$(1.1) \quad \frac{d}{dt}u(t) = F(u(t)) \quad (t \geq 0), \quad u(0) = u_0.$$

Here $F : \mathbb{V} \rightarrow \mathbb{V}$ denotes a given function from a vector space \mathbb{V} into itself, $u_0 \in \mathbb{V}$ is given, and $u(t) \in \mathbb{V}$ is unknown (for $t > 0$).

The general linear multistep method (LMM), for solving initial-value problems, yields approximations $u_n \approx u(n \Delta t)$, where Δt denotes a positive stepsize. The method can be written in the form

$$(1.2) \quad u_n = \sum_{j=1}^k a_j u_{n-j} + \Delta t \sum_{j=0}^k b_j F(u_{n-j}).$$

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Here $k \geq 1$ is a fixed integer – the step-number – and a_j, b_j are coefficients specifying the method. The vectors u_n are computed successively from preceding approximations u_{n-k}, \dots, u_{n-1} using (1.2) for $n \geq k$. The method is called *explicit* if $b_0 = 0$, and *implicit* otherwise.

Throughout the paper, we assume that

$$(1.3) \quad \sum_{j=1}^k a_j = 1, \quad \sum_{j=1}^k j a_j = \sum_{j=0}^k b_j,$$

which amounts to requiring *consistency* of the method, cf. e.g. Butcher [1], Hairer, Nørset & Wanner [5], Henrici [8].

In the following, $\|\cdot\|$ denotes a seminorm on the vector space \mathbb{V} . Much attention has been paid in the literature to situations where the approximations u_n satisfy

$$(1.4) \quad \|u_n\| \leq \max_{1 \leq j < k} \|u_{n-j}\|.$$

This inequality has often been referred to by the term *monotonicity* or *strong stability*. It is of particular importance in situations where the initial value problem (1.1) results from (method of lines) semidiscretizations of time-dependent partial differential equations. Choices for $\|\cdot\|$ which occur in that context, include e.g. the *supremum norm* $\|x\| = \|x\|_\infty = \sup_i |\xi_i|$ and the *total variation seminorm* $\|x\| = \|x\|_{TV} = \sum_i |\xi_{i+1} - \xi_i|$ (for vectors x with components ξ_i). Numerical processes, satisfying $\|u_n\|_{TV} \leq \max\{\|u_{n-1}\|_{TV}, \dots, \|u_{n-k+1}\|_{TV}\}$, play a special role in the solution of hyperbolic conservation laws and are called *total-variation-diminishing* (TVD), cf. e.g. Harten [7], Shu [17], Shu & Osher [18], LeVeque [15], Hundsdorfer & Verwer [13].

In the literature, restrictions on Δt can be found which guarantee the monotonicity property (1.4). In most papers, a condition on F is imposed which essentially amounts to the basic assumption

$$(1.5) \quad \|v + \tau F(v)\| \leq \|v\| \quad (\text{for all } v \in \mathbb{V}),$$

where τ denotes a given positive constant. We will say that γ is a *stepsize-coefficient for monotonicity* of the LMM, if $\gamma > 0$ and the stepsize restriction

$$(1.6) \quad 0 < \Delta t \leq \gamma \cdot \tau$$

implies monotonicity, in the sense of (1.4), whenever \mathbb{V} is a vector space with seminorm $\|\cdot\|$, and $F: \mathbb{V} \rightarrow \mathbb{V}$ satisfies the above basic assumption. A necessary and sufficient condition, for any given $\gamma > 0$ to be such a stepsize-coefficient, is as follows:

$$(1.7) \quad b_0 \geq 0, \quad \text{and } a_j \geq 0, b_j \geq 0, \gamma b_j \leq a_j \quad (\text{for } 1 \leq j \leq k).$$

For the sufficiency of this condition, see e.g. Gottlieb, Ketcheson & Shu [4], Hundsdorfer & Ruuth [11], Shu [17], Shu & Osher [18], and for the necessity, cf. Spijker [19], [20].

It follows from condition (1.7) that there is a stepsize-coefficient for monotonicity, if and only if

$$(1.8) \quad b_0 \geq 0, a_j \geq 0, b_j \geq 0 \quad (\text{for } 1 \leq j \leq k), \quad \text{and } a_i > 0 \quad \text{for all } i \in \{1, 2, \dots, k\} \quad \text{with } b_i > 0.$$

Clearly, using criterion (1.8), it is very easy to check, for any given LMM, whether or not a stepsize-coefficient exists for monotonicity.

1.2 Stepsize-coefficients for boundedness

Condition (1.8) requires evidently that all coefficients of the LMM are non-negative. Unfortunately, many methods of practical interest fail to have this property – notably the well-known Adams-Bashforth and Adams-Moulton methods as well as the backward differentiation methods (for $k > 1$), see e.g. Hairer, Nørsett & Wanner [5], Henrici [8] and Section 5 of the present paper. Moreover, by

Lenferink [14] (Theorem 2.2), a general negative result was proved for explicit methods with order of accuracy $p = k > 1$: none of these methods have a stepsize-coefficient for monotonicity.

These circumstances suggest that there are situations where monotonicity may essentially be too strong a theoretical demand. Accordingly, various authors were led to study, along with monotonicity, the weaker boundedness property

$$(1.9) \quad \|u_N\| \leq \mu \cdot \max_{0 \leq j < k} \|u_j\|,$$

for approximations u_N obtained by the LMM from starting vectors u_0, \dots, u_{k-1} . Here μ is a constant, independent of $N \geq k$, which is allowed to be greater than 1. This property, with $\|\cdot\| = \|\cdot\|_{TV}$, is known as *total variation boundedness* (TVB), which is of crucial importance in the solution of hyperbolic conservation laws, cf. e.g. LeVeque [15], Hundsdorfer & Verwer [13].

We will say that $\gamma > 0$ is a *stepsize-coefficient for boundedness* of the LMM, if a constant μ exists such that the stepsize restriction (1.6) implies the bound (1.9) (for all $N \geq k$), whenever \mathbb{V} is a vector space with seminorm $\|\cdot\|$, and $F : \mathbb{V} \rightarrow \mathbb{V}$ satisfies the basic assumption (1.5).

In the literature, LMMs were identified for which no stepsize-coefficient exists for monotonicity but still for boundedness, notably by Hundsdorfer and co-authors, see [9], [10], [11], [12], [16] – cf. also Section 5 of the present paper.

1.3 Purpose of the paper

The natural question arises of whether criteria (1.7) and (1.8) have simple counterparts which are decisive for boundedness, rather than monotonicity.

A suitable counterpart of criterion (1.7) follows easily from the material in Hundsdorfer, Mozartova & Spijker [9]. But, this variant of criterion (1.7) does *not* lead directly to a corresponding variant of criterion (1.8) – in a similar easy way as criterion (1.7) leads to (1.8). In the literature, no general and simple criterion seems to be available, thus far, for the existence of a stepsize-coefficient for boundedness. In the present paper, we are looking for such a criterion.

Using results of Crouzeix & Raviart [3], Hundsdorfer, Mozartova & Spijker [9], Tjeldeman [21], we shall find simple conditions for the existence of a stepsize-coefficient for boundedness. We shall apply these conditions to well-known classes of LMMs, viz. Adams-Moulton, Adams-Bashforth, Milne-Simpson and Nyström methods as well as backward differentiation formulas and extrapolated versions thereof.

1.4 Outline of the rest of the paper

In Section 2 we give definitions and make basic assumptions, to be used in the rest of the paper. Furthermore, we formulate the Theorems 2.1 and 2.2, which are related to the results mentioned above of Crouzeix & Raviart [3] and Hundsdorfer, Mozartova & Spijker [9], respectively.

In Section 3 we formulate – without proof – our main result, Theorem 3.1. The theorem yields, for a large class of LMMs, a relatively simple condition which is necessary and sufficient for the existence of a stepsize-coefficient for boundedness. Moreover, the theorem leads to Corollary 3.3 which gives two general and still more simple conditions – one being sufficient and one necessary for a stepsize-coefficient to exist.

Section 4 is devoted to proving Theorem 3.1. In Sections 4.2, 4.3 we first derive the two key Lemmas 4.1 and 4.4; Tjeldeman's result, [21], plays a part in proving the latter lemma. Next, in Section 4.4, these two lemmas are used, together with Theorems 2.1, 2.2, in the actual proof of Theorem 3.1.

In Section 5 we illustrate Theorem 3.1 and Corollary 3.3 in an analysis of implicit and explicit Adams methods and backward differentiation formulas, as well as of Milne-Simpson and Nyström methods. The outcome of this analysis supplements earlier results for these methods given in the literature.

2 Some results from the literature

2.1 Definitions and basic assumptions

Any polynomial, with complex coefficients, will be said to satisfy the *root condition* if

- (2.1) All roots ζ of the polynomial have a modulus $|\zeta| \leq 1$, and any roots of modulus 1 are simple.

We adjoin to method (1.2) the following polynomials:

$$(2.2) \quad \begin{aligned} a(z) &= 1 - \sum_1^k a_j z^j, & \rho(\zeta) &= \zeta^k a(1/\zeta) \quad \text{and} \\ b(z) &= \sum_0^k b_j z^j, & \sigma(\zeta) &= \zeta^k b(1/\zeta). \end{aligned}$$

Consider the polynomial $\rho_\delta(\zeta) = \rho(\zeta) - \delta \cdot \sigma(\zeta)$, depending on the parameter $\delta \in \mathbb{C}$. We define the *stability region* \mathcal{S} of the LMM to be the set of all $\delta \in \mathbb{C}$ for which $1 - \delta \cdot b_0 \neq 0$ and $\rho_\delta(\zeta)$ satisfies the root condition. We shall denote the *interior of* \mathcal{S} by $\text{int}(\mathcal{S})$.

Throughout the rest of the paper, it will be assumed that

- (2.3) The polynomial $\rho(\zeta)$ satisfies the root condition,

- (2.4) The polynomials $\rho(\zeta)$ and $\sigma(\zeta)$ have no common root.

These two conditions on the LMM amount to requiring *zero-stability* and *irreducibility*, respectively, which are no practical restrictions, cf. e.g. [1], [5]. Furthermore, it will be assumed throughout that

- (2.5) $b_0 \geq 0$.

This inequality is fulfilled for all well-known implicit LMMs, and trivially for all explicit ones.

2.2 Disks within the stability region

Boundedness of LMMs will be related, in Section 4.4, to the existence of values $\alpha > 0$ with the following geometric property:

- (2.6) The disk $\{z : z \in \mathbb{C} \text{ with } |z + \alpha| \leq \alpha\}$ belongs to \mathcal{S} .

In the present subsection we recall a criterion, given in the literature, for the existence of $\alpha > 0$ satisfying (2.6).

To formulate the criterion, we need some definitions. Similarly as e.g. in [8], we refer to the roots of $\rho(\zeta)$ with modulus equal to 1, say η_1, \dots, η_q , as the *essential roots*; and we adjoin to them the *growth parameters* $\lambda_1, \dots, \lambda_q$, defined by

$$(2.7) \quad \lambda_j = \frac{\sigma(\eta_j)}{\eta_j \cdot \rho'(\eta_j)}.$$

We choose the numbering of the essential roots such that

$$(2.8) \quad \eta_1 = 1.$$

It can easily be seen (cf. e.g. [8]) that, corresponding to each essential root η_j , there is a root $\zeta(\delta)$ of the polynomial $\rho_\delta(\zeta)$ with

$$(2.9) \quad \zeta(\delta) = [1 + \lambda_j \cdot \delta + \mathcal{O}(\delta^2)] \cdot \eta_j \quad (\text{for } \delta \rightarrow 0).$$

Using (2.9), the following theorem can be proved – see [3] (Chapter 1, Theorem 4.5).

Theorem 2.1 (Crouzeix & Raviart, 1980). *There exists a value $\alpha > 0$ with property (2.6), if and only if all growth parameters λ_j are real and positive.*

2.3 A condition for stepsize-coefficients relevant to boundedness

In the literature, results were obtained yielding a condition that is necessary and sufficient in order that a given $\gamma > 0$ is a stepsize-coefficient for boundedness. To formulate the condition, we introduce values μ_n (for $n \in \mathbb{Z}$) by the relations

$$(2.10) \quad \begin{aligned} \mu_n &= 0 \quad (n < 0), & \mu_n &= \sum_{j=1}^k a_j \mu_{n-j} - \gamma \sum_{j=0}^k b_j \mu_{n-j} + b_n \quad (0 \leq n \leq k), \\ \mu_n &= \sum_{j=1}^k a_j \mu_{n-j} - \gamma \sum_{j=0}^k b_j \mu_{n-j} \quad (n > k). \end{aligned}$$

Clearly, the values μ_n depend on γ . For the sake of readability however, we suppress this dependence in our notation.

From [9] (Theorem 4.1 and Lemma 4.3), one arrives easily at

Theorem 2.2. *Any given $\gamma > 0$ is a stepsize-coefficient for boundedness if and only if*

$$(2.11) \quad -\gamma \in \text{int}(\mathcal{S}) \quad \text{and} \quad \mu_n \geq 0 \quad (\text{for all } n \geq 1).$$

This theorem might – in principle – be used to check, numerically, whether for a given LMM there exists any stepsize-coefficient for boundedness. But, because the μ_n depend on γ , an obvious difficulty with this approach would lie in the formal necessity to check the inequalities $\mu_n \geq 0$ – not only for all $n \geq 1$ but possibly also – for *infinitely many values* $\gamma > 0$.

In the present paper, the above theorem will be used differently. It will play a part in deriving a relatively simple condition which is *sufficient* for the existence of a stepsize-coefficient for boundedness – cf. below Theorem 3.1 (I) and Section 4.4. Moreover, Theorem 2.2 will play a part in obtaining a slightly weaker condition which is *necessary* for the existence of a stepsize-coefficient – cf. Theorem 3.1 (II) and again Section 4.4.

3 The main theorem and a corollary

To formulate our main result, Theorem 3.1, we introduce the values τ_n which are generated by the above relations (2.10), if the factor γ in front of the sum $\sum_{j=0}^k b_j \mu_{n-j}$ is replaced by 0, i.e.

$$(3.1) \quad \begin{aligned} \tau_n &= 0 \quad (n < 0), & \tau_n &= \sum_{j=1}^k a_j \tau_{n-j} + b_n \quad (0 \leq n \leq k), \\ \tau_n &= \sum_{j=1}^k a_j \tau_{n-j} \quad (n > k). \end{aligned}$$

In the theorem, we will refer to the following condition:

$$(3.2.a) \quad \tau_n \geq 0 \quad (\text{whenever } n \geq 1),$$

$$(3.2.b) \quad \tau_j \tau_{n-j} = 0 \quad (\text{for } 1 \leq j \leq n-1) \quad \text{whenever } \tau_n = 0.$$

Theorem 3.1. (I) *Assume that $\zeta = 1$ is the only essential root. Then condition (3.2) implies the existence of a stepsize-coefficient for boundedness.*

(II) *Conversely, assume there exists a stepsize-coefficient for boundedness. Then condition (3.2) is fulfilled, and all growth parameters λ_j are equal to 1.*

The theorem will be proved in Section 4.

Clearly, Theorem 3.1 doesn't give – for the full class of LMMs – a single condition that is at the same time necessary *and* sufficient, for the existence of a stepsize-coefficient. But, the theorem does yield such a condition, e.g. within the – slightly restricted – class of LMMs for which

$$(3.3) \quad \zeta = 1 \text{ is the only essential root with growth parameter } \lambda_j = 1.$$

For such LMMs, the theorem evidently shows that *a stepsize-coefficient for boundedness exists if and only if*

$$(3.4) \quad \zeta = 1 \text{ is the only essential root, and (3.2) holds.}$$

Remark 3.2. *Without the restriction (3.3), condition (3.4) would no longer be a sufficiently general criterion for the existence of a stepsize-coefficient. This can be seen from a counterexample, e.g. (5.8) or (5.9) in Section 5.5.*

Using consistency and zero-stability of the LMM, it can be seen that there is an index n with $1 \leq n \leq k$ and $\tau_n \neq 0$. The smallest of such indices will be denoted by n_0 , i. e.:

$$n_0 = \min \{ n : 1 \leq n \leq k \text{ and } \tau_n \neq 0 \}.$$

The following corollary, to the above theorem, involves the simple conditions

$$(3.5) \quad \tau_n > 0 \quad (\text{for all } n \geq n_0)$$

and

$$(3.6) \quad \tau_n \leq 0 \quad (\text{for some index } n \geq n_0 \text{ which is a multiple of } n_0).$$

Clearly, (3.5) \implies (3.2). Furthermore, it is not difficult to see that property (3.6) violates (3.2). We thus have the following consequence of Theorem 3.1:

Corollary 3.3. *If (3.5) holds and $\zeta = 1$ is the only essential root, then there exists a stepsize-coefficient for boundedness. On the other hand, if (3.6) holds, then no such coefficient exists.*

Condition (3.5) does, of course, not cover *all* situations where condition (3.2) is fulfilled. But, when $n_0 = 1$, either condition (3.5) or (3.6) must be fulfilled – so that: (3.5) \iff (3.2). Checking condition (3.2) is thus particularly simple in case $n_0 = 1$. For all LMMs to be studied in Sections 5.1 - 5.4, the last equality will turn out to be in force.

Many methods of practical interest have a ρ -polynomial that has no essential roots different from $\zeta = 1$, cf. e.g. [5], [8]. Theorem 3.1 shows that, for all of these methods, criterion (3.2) is decisive for the existence of a stepsize-coefficient for boundedness. Moreover, Corollary 3.3 shows that, for such methods with $n_0 = 1$, a stepsize-coefficient for boundedness exists if and only if the simple condition (3.5) is fulfilled.

4 Proof of the main theorem

4.1 Preliminaries

We consider an arbitrary consistent, zero-stable and irreducible LMM, with $b_0 \geq 0$. We shall prove below Parts (I) and (II) of Theorem 3.1. We have split up our proof in three steps, to be described in the Sections 4.2, 4.3, 4.4, respectively.

With an eye to the condition on μ_n occurring in Theorem 2.2, we shall relate, in Section 4.2, condition (3.2) to the non-negativity of μ_n for bounded n . Next, we shall analyse, in Section 4.3, the non-negativity of μ_n for $n \rightarrow \infty$. In Section 4.4, we shall complete the proof of Theorem 3.1, using the conclusions of Sections 4.2, 4.3 and the material of Section 2.

4.2 Non-negativity of μ_n – for $1 \leq n \leq m$

For given integer $m \geq 1$, we shall denote by I the identity matrix of order $m + 1$ and by $E = (e_{ij})$ the square matrix, of order $m + 1$, with $e_{ij} = 1$ for $i = j + 1$ and $e_{ij} = 0$ otherwise.

The values μ_n and τ_n (for $0 \leq n \leq m$), defined by (2.10), (3.1), can conveniently be related to each other by introducing the following lower triangular Toeplitz matrices (of order $m + 1$):

$$(4.1) \quad M = \sum_{j=0}^m \mu_j E^j, \quad T = \sum_{j=0}^m \tau_j E^j.$$

Using the polynomials $a(z)$, $b(z)$, introduced in Section 2, we can rewrite the relations defining μ_n and τ_n ($0 \leq n \leq m$) as $[a(E) + \gamma b(E)]M = b(E)$ and $a(E)T = b(E)$, respectively. From the last two equalities, one finds the expression

$$(4.2) \quad M = T(I + \gamma T)^{-1}.$$

In Lemma 4.1 below, the restrictions imposed on τ_n by condition (3.2) will be related to the following non-negativity property of μ_n :

$$(4.3) \quad \text{For each } m \geq 1, \text{ a value } \gamma^{[m]} > 0 \text{ exists such that: } \mu_n \geq 0 \text{ for all } \gamma \in (0, \gamma^{[m]}] \text{ and } 1 \leq n \leq m.$$

Note that this property can be viewed as a variant of the property of μ_n occurring in Theorem 2.2 – the latter property being that $\mu_n \geq 0$ for *fixed* $\gamma > 0$ and *all* $n \geq 1$.

Lemma 4.1. *Property (4.3) is present if and only if the values τ_n satisfy (3.2).*

Proof.

1. For any fixed $m \geq 1$ and sufficiently small $\gamma > 0$, we see from the expression (4.2) that $M = T[I - (\gamma T)^2]^{-1}(I - \gamma T) = [I + (\gamma T)^2 + (\gamma T)^4 + \dots](T - \gamma T^2)$, which implies

$$(4.4) \quad M = [I + (\gamma T)^2 + (\gamma T)^4 + \dots] \sum_{n=0}^m (\tau_n - \gamma \sigma_n) E^n, \quad \text{where} \quad \sigma_n = \sum_{j=0}^n \tau_j \tau_{n-j}.$$

It follows that (3.2) implies property (4.3).

2. Conversely, assume (4.3). Consider any $m \geq 1$ and let $\gamma \in (0, \gamma^{[m]})$. All entries of the $m \times m$ matrix M , corresponding to this γ , are non-negative.

By letting $\gamma \rightarrow 0$ in the expression (4.4), we find (for $1 \leq n \leq m$) that $\tau_n \geq 0$, and $\sigma_n = 0$ as soon as $\tau_n = 0$. Hence, (3.2) is in force. \square

4.3 Non-negativity of μ_n – for $n > m$

In this section we focus on another variant of the property of μ_n occurring in Theorem 2.2, viz.:

$$(4.5) \quad \gamma_0 > 0 \text{ and } m \geq 1 \text{ exist such that: } \mu_n \geq 0 \text{ for all } \gamma \in (0, \gamma_0] \text{ and all } n > m.$$

To study this property, it is convenient to analyse first the values v_n defined by

$$(4.6) \quad v_n = 0 \quad (n < 0), \quad v_0 = 1, \quad v_n = \sum_{j=1}^k a_j v_{n-j} - \gamma \sum_{j=0}^k b_j v_{n-j} \quad (n \geq 1);$$

because the solution μ_n of (2.10) can be represented as

$$(4.7) \quad \mu_n = (1 + \gamma b_0)^{-1} \sum_{j=0}^k b_j v_{n-j}.$$

Defining $u_n = v_{n-k+1}$, we see that u_n satisfies the LMM-relations (1.2) (for $n \geq k$), with $F(v) = -\gamma v$, $\Delta t = 1$ and $u_{k-1} = 1$, $u_i = 0$ ($0 \leq i \leq k-2$). The values v_n may thus be viewed as LMM approximations arising in solving the test equation $u'(t) = -\gamma u(t)$. An analysis of such approximations was given earlier in the literature, notably in [8], Section 5.3.1. Our analysis below will differ from from the one in that reference; we will study the behavior of v_n when γ and n tend (independently of each other) to 0 and ∞ , respectively, by using contour integration in the complex plane.

The behavior of v_n (for $n \rightarrow \infty$) is governed by the roots of the equation $\rho(\zeta) + \gamma \sigma(\zeta) = 0$, which we denote by $\zeta_j(\gamma)$ ($1 \leq j \leq k$). Indicating by η_j the essential roots, as in Section 2.2, we (can) choose the numbering of the roots $\zeta_j(\gamma)$ such that

$$\lim_{\gamma \rightarrow 0} \zeta_j(\gamma) = \zeta_j(0), \quad \text{with} \quad \zeta_j(0) = \eta_j \quad (1 \leq j \leq q), \quad |\zeta_j(0)| < 1 \quad (q < j \leq k).$$

We define $\xi_j(\gamma) = 1/\zeta_j(\gamma)$ for $\zeta_j(\gamma) \neq 0$, and choose positive $\varepsilon, \theta_0, \theta_1, \gamma_0$ with $\theta_0 < \theta_1 < 1$ such that, for all $\gamma \in (0, \gamma_0]$,

$$|1 - \zeta_j(\gamma) \xi_i(\gamma)| \geq \varepsilon, \quad (\text{for } 1 \leq i \leq q, 1 \leq j \leq q, i \neq j),$$

$$\theta_1 \leq |\zeta_j(\gamma)| \leq 1/\theta_1 \quad (\text{for } 1 \leq j \leq q) \quad \text{and} \quad |\zeta_j(\gamma)| \leq \theta_0 \quad (\text{for } q < j \leq k).$$

For such γ , the function $f(z) = \sum_0^\infty v_n z^n$ is analytic on the disk $|z| < \theta_1$, and because of the definition of v_n , we have $(1 + \gamma b_0)^{-1} [a(z) + \gamma b(z)] f(z) = 1$, which implies

$$f(z) = \sum_0^\infty v_n z^n = (1 + \gamma b_0) [a(z) + \gamma b(z)]^{-1} = \prod_1^k [1 - \zeta_j(\gamma) z]^{-1} \quad (\text{for } |z| < \theta_1).$$

We shall obtain a useful expression for v_n , by combining the formula

$$(4.8) \quad v_n = \frac{1}{2\pi i} \oint_{|z|=\theta_0} z^{-n-1} f(z) dz$$

with the partial fraction decomposition $f(z) = g(z) + h(z)$, where $g(z), h(z)$ are defined by

$$g(z) = \sum_{i=1}^q \left\{ [1 - \zeta_i(\gamma) z]^{-1} \prod_{\substack{j=1 \\ j \neq i}}^k [1 - \zeta_j(\gamma) \xi_i(\gamma)]^{-1} \right\}, \quad h(z) = f(z) - g(z).$$

It can be seen that

$$h(z) = H(z; \zeta_1(\gamma), \dots, \zeta_k(\gamma)) \prod_{j=q+1}^k [1 - \zeta_j(\gamma) z]^{-1},$$

where $H(z; z_1, \dots, z_k)$ is a polynomial with respect to the variable z , as well as a continuous function of $(z; z_1, \dots, z_k)$ on the set specified by the inequalities

$$(4.9) \quad \begin{aligned} |1 - z_j/z_i| &\geq \varepsilon \quad (\text{for } 1 \leq i \leq q, 1 \leq j \leq q, i \neq j), \\ \theta_1 \leq |z_j| &\leq 1/\theta_1 \quad (\text{for } 1 \leq j \leq q), \quad \text{and} \quad |z_j| \leq \theta_0 \quad (\text{for } q < j \leq k). \end{aligned}$$

Because $h(z)$ is holomorphic for $|z| < 1/\theta_0$, we find, by inserting the decomposition $f(z) = g(z) + h(z)$ into (4.8), that

$$(4.10) \quad \begin{aligned} v_n &= J_0 + J_1, \quad \text{with} \quad J_0 = \frac{1}{2\pi i} \oint_{|z|=\theta_0} z^{-n-1} g(z) dz \quad \text{and} \\ J_1 &= \frac{1}{2\pi i} \oint_{|z|=\varrho} z^{-n-1} h(z) dz, \quad \text{where} \quad \varrho = \frac{1/\theta_0 + 1/\theta_1}{2} > 1. \end{aligned}$$

We have the expression

$$(4.11) \quad \begin{aligned} J_0 &= \sum_{i=1}^q \alpha_i(\gamma) \zeta_i(\gamma)^n \quad \text{where, for } \gamma \rightarrow 0, \\ \alpha_i(\gamma) &= \prod_{\substack{j=1 \\ j \neq i}}^k [1 - \zeta_j(\gamma) \xi_i(\gamma)]^{-1} = \frac{(1 + \gamma b_0) \zeta_i(\gamma)^{k-1}}{\varrho'(\zeta_i(\gamma)) + \gamma \cdot \sigma'(\zeta_i(\gamma))} \sim \frac{(1 + \gamma b_0) \zeta_i(\gamma)^{k-1}}{\varrho'(\zeta_i(\gamma))}. \end{aligned}$$

Furthermore, defining $\mu = \max |H(z; z_1, \dots, z_k)|$, where the maximum is over the set specified by the equality $|z| = \varrho$ and the inequalities (4.9), there follows $|\mathcal{J}_1| \leq \mu \cdot \varrho^{-n}$. Combining the last inequality with (4.10), (4.11), we see that there is a $\gamma_0 > 0$ such that, for $0 < \gamma \leq \gamma_0$ and $n \geq 0$,

$$v_n = (1 + \gamma b_0) \sum_{i=1}^q [1 + \varepsilon_i(\gamma, n)] \frac{\zeta_i(\gamma)^{n+k-1}}{\varrho'(\zeta_i(\gamma))} \quad \text{where} \quad \lim_{n \rightarrow \infty} \varepsilon_i(\gamma, n) = 0.$$

By inserting this expression for v_n into (4.7) and applying the definition of the growth parameters, (2.7), it can be seen that

$$\mu_n = \sum_{i=1}^q [1 + E_i(\gamma, n)] \lambda_i \zeta_i(\gamma)^n \quad \text{where} \quad \lim_{n \rightarrow \infty} E_i(\gamma, n) = 0.$$

From the expression (2.9) we have $\zeta_i(\gamma) = [1 - \lambda_i \gamma + \mathcal{O}(\gamma^2)] \cdot \eta_i$ (for $\gamma \rightarrow 0$), which leads to

Lemma 4.2. *There is a $\gamma_0 > 0$ such that, for $0 < \gamma \leq \gamma_0$, the values μ_n ($n \geq 1$), defined by (2.10), satisfy*

$$(4.12) \quad \mu_n = \sum_{i=1}^q [1 + E_i(\gamma, n)] \lambda_i \cdot \eta_i^n \cdot \exp\{-\lambda_i \gamma n [1 + D_i(\gamma)]\},$$

where $\lim_{n \rightarrow \infty} E_i(\gamma, n) = 0$ and $D_i(\gamma) = \mathcal{O}(\gamma)$ (for $\gamma \rightarrow 0$).

When applying the above lemma for studying the non-negativity property (4.5), the following theorem, given in [21], will be helpful:

Theorem 4.3 (Tijdeman, 2011). *Let real values w_j and distinct complex z_j (for $1 \leq j \leq p$) be given, with all $|z_j| = 1$, $z_j \neq 1$. Assume for each index j there is an index i such that $w_i = w_j$, $z_i z_j = 1$. Define $s_n = \sum_{j=1}^p w_j z_j^n$. Then*

$$(4.13) \quad \liminf_{n \rightarrow \infty} s_n \leq -(|w_1| + \dots + |w_p|)/p.$$

Using Lemma 4.2 in combination with the last theorem, we shall prove the following key lemma:

Lemma 4.4. (I) *Assume there are no essential roots different from $\zeta = 1$. Then the non-negativity property (4.5) is present.*

(II) *Conversely, assume (4.5), and let all growth parameters λ_j be real. Then there are no growth parameters different from 1.*

Proof.

Part (I). Assume there are no essential roots different from $\zeta = 1$.

Because $q = 1$, we see from the expression for μ_n , given in Lemma 4.2, that $\mu_n \geq 0$ as soon as $1 + E_1(\gamma, n) \geq 0$. Hence, $\mu_n \geq 0$ for all sufficiently small $\gamma > 0$ and sufficiently large $n \geq 1$, i.e. property (4.5) is present.

Part (II). Assume (4.5) is valid.

Suppose first that $c = \min_j \lambda_j < 1$. We choose $\gamma = n^{-3/4}$ and let $n \rightarrow \infty$. The exponential expressions in (4.12) then satisfy

$$\exp\{-\lambda_i \gamma n [1 + D_i(\gamma)]\} = \exp\{-\lambda_i n^{1/4} + \mathcal{O}(n^{-1/2})\} \sim \exp\{-\lambda_i n^{1/4}\}.$$

Assume, without loss of generality, that $\lambda_{q-p+1} = \dots = \lambda_q$ are the (only) growth parameters equal to c . We split the expression in the right-hand member of (4.12) up into partial sums μ_n^0 and μ_n^1 ; the former sum containing the terms with $1 \leq i \leq q-p$, and the latter containing those with $q-p+1 \leq i \leq q$. For the first partial sum, we have

$$\exp\{c n^{1/4}\} \cdot \mu_n^0 \longrightarrow 0 \quad (\text{for } n \rightarrow \infty),$$

and for the second one

$$\exp\{c n^{1/4}\} \cdot \mu_n^1 - s_n \longrightarrow 0 \quad (\text{for } n \rightarrow \infty), \quad \text{where } s_n = c \cdot \sum_{i=q-p+1}^q \eta_i^n.$$

It can be seen that the conditions of Tijdeman's theorem are fulfilled with $z_j = \eta_{q-p+j}$, $w_j = c$. Hence,

$$\limsup_{n \rightarrow \infty} s_n \leq -|c|.$$

Because the LMM is irreducible, cf. (2.4), all growth parameters must be different from zero, so that $|c| \neq 0$. Therefore, the above implies: $\exp\{c n^{1/4}\} \cdot \mu_n = \exp\{c n^{1/4}\} \cdot (\mu_n^0 + \mu_n^1) < 0$ for $\gamma = n^{-3/4}$ and infinitely many $n \geq 1$ – which contradicts property (4.5). Hence, there are no $\lambda_j < 1$.

Next suppose all $\lambda_j \geq 1$ and some $\lambda_j > 1$. We shall compare the values μ_n with the values $\tilde{\mu}_n = \sum_{i=1}^q \lambda_i \eta_i^n = 1 + \sum_{i=2}^q \lambda_i \eta_i^n$. It can be seen that the conditions of Tijdeman's theorem are fulfilled with $p = q - 1$, $w_j = \lambda_{1+j}$, $z_j = \eta_{1+j}$. Therefore, for each $\varepsilon > 0$, there are infinitely many $n \geq 1$ with $\tilde{\mu}_n \leq 1 + \varepsilon - (\lambda_2 + \dots + \lambda_q)/(q - 1) = \varepsilon + \alpha$, where $\alpha = 1 - (\lambda_2 + \dots + \lambda_q)/(q - 1) < 0$. Hence, $\tilde{\mu}_n \leq \alpha/2 < 0$ for infinitely many $n \geq 1$.

For $\gamma = n^{-2}$, $n \rightarrow \infty$, we have $\mu_n - \tilde{\mu}_n \rightarrow 0$ so that also $\mu_n < 0$ for infinitely many $n \geq 1$. This contradicts property (4.5), so that there can be no $\lambda_j > 1$. \square

4.4 Actual proof of Theorem 3.1

1. Proving Part (I) of Theorem 3.1.

We assume that (3.2) holds, and there are no essential roots different from $\zeta = 1$. By Lemma 4.4, Part (I), there are $\gamma_0 > 0$, $m \geq 1$ with

$$\mu_n \geq 0 \quad (\text{whenever } 0 < \gamma \leq \gamma_0 \text{ and } n > m).$$

Corresponding to this m , there exists – by Lemma 4.1 – a value $\gamma_1 > 0$ such that

$$\mu_n \geq 0 \quad (\text{whenever } 0 < \gamma \leq \gamma_1 \text{ and } 1 \leq n \leq m).$$

Theorem 2.1 implies the existence of a value $\gamma_2 > 0$ such that

$$-\gamma \in \text{int}(\mathcal{S}) \quad (\text{for all } \gamma \text{ with } 0 < \gamma \leq \gamma_2).$$

We define $\gamma = \min\{\gamma_0, \gamma_1, \gamma_2\}$. Because this γ satisfies condition (2.11), we can apply Theorem 2.2, so as to conclude that it is a stepsize-coefficient for boundedness. \square

2. Proving Part (II) of Theorem 3.1.

We assume $\gamma_0 > 0$ is a stepsize-coefficient for boundedness. Because also any γ with $0 < \gamma \leq \gamma_0$ is a stepsize-coefficient for boundedness, we see from Theorem 2.2, that $\mu_n \geq 0$ for all $\gamma \in (0, \gamma_0]$ and $n \geq 1$.

Property (4.3) is, of course, in force, so that, by Lemma 4.1, condition (3.2) is fulfilled.

To study the growth parameters λ_j , we first note that any application of method (1.2) to the scalar, complex test equation $u'(t) = z \cdot u(t)$, with $z = \alpha + i\beta$ and real α, β , can be reformulated as an application of the method to $u'(t) = F(u(t))$ in $\mathbb{V} = \mathbb{R}^2$, with $F(v) = F_z(v) = (\alpha v_1 - \beta v_2, \beta v_1 + \alpha v_2)$ for $v = (v_1, v_2) \in \mathbb{V}$.

We choose any z in the disk $\mathcal{D} = \{\zeta : \zeta \in \mathbb{C}, |\zeta + 1| \leq 1\}$. The corresponding function F_z satisfies the basic condition (1.5) with $\tau = 1$, $\mathbb{V} = \mathbb{R}^2$ and $\|\cdot\|$ equal to the Euclidean norm.

Because $\gamma_0 > 0$ is a stepsize-coefficient for boundedness, all vectors $u_n \in \mathbb{V} = \mathbb{R}^2$ generated by the LMM, with $F = F_z$ and $\Delta t = \gamma_0 \cdot \tau = \gamma_0$, stay bounded when $n \rightarrow \infty$. Hence, the polynomial $\rho_\delta(\zeta)$, with $\delta = \gamma_0 z$, satisfies the root condition. It follows that $\gamma_0 z \in \mathcal{S}$. Consequently, the disk $\{\zeta : \zeta \in \mathbb{C} \text{ with } |\zeta + \gamma_0| \leq \gamma_0\} = \gamma_0 \cdot \mathcal{D}$ is contained in the stability region \mathcal{S} . Theorem 2.1 thus implies that all growth parameters λ_j lie on the positive real axis.

Next, we note that property (4.5) is – trivially – in force, so that we can conclude via Lemma 4.4, Part (II), that all λ_j are equal to 1. This completes the proof. \square

5 Applications

5.1 Adams-Moulton methods

The well-known k -step Adams-Moulton methods – also called implicit Adams methods – have order of accuracy $k + 1$, and are of the form

$$u_n = u_{n-1} + \Delta t \cdot [b_0 F(u_n) + \cdots + b_k F(u_{n-k})].$$

The coefficients $b_j = b_{k,j}$ are specified e.g. in [5] (Section III-1), [8] (p. 194-199). From (3.1), the corresponding values $\tau_n = \tau_{k,n}$ are seen to satisfy

$$\tau_n = b_0 + \cdots + b_n \quad (\text{for } 0 \leq n \leq k), \quad \tau_n = b_0 + \cdots + b_k \quad (\text{for } n > k).$$

Because, for given k , the values τ_n are constant for $n \geq k$, the conditions (3.5), (3.6) can be checked in a finite number of steps.

Using the material in the literature just mentioned, it can be seen for all $k \geq 1$ that $b_0 > 0$, $b_1 > 0$, so that the value n_0 , defined in Section 3, equals $n_0 = 1$. Furthermore, it can be seen that

$$b_2 < 0 \quad (\text{for } k \geq 2), \quad \tau_n > 0 \quad (\text{for all } n \geq 1 \text{ and } 1 \leq k \leq 8).$$

A direct computation shows that $\tau_{k,4} = -\frac{797}{5670}$ for $k = 9$; whereas it can be proved that $\tau_{k+1,4} < \tau_{k,4}$ (for all $k \geq 9$). Hence,

$$\tau_4 \leq 0 \quad (\text{for } k \geq 9).$$

Combining these results with criterion (1.8) and Corollary 3.3 (with $n_0 = 1$) there follows

Theorem 5.1. (I) For $k = 1$, there exists a stepsize-coefficient for monotonicity;

(II) For $2 \leq k \leq 8$, there exists no such coefficient, but there is a stepsize-coefficient for boundedness;

(III) For all $k \geq 9$, there doesn't even exist a stepsize-coefficient for boundedness.

The result for $k = 2$, given in the theorem, is related to earlier results obtained in [11] (Section 5.3.1) and [12] (Section 3.3). The author is not aware of related results in the literature for $k \geq 3$.

5.2 Adams-Bashforth methods

The well-known k -step Adams-Bashforth methods – also called explicit Adams methods – have order of accuracy k , and are of the form

$$u_n = u_{n-1} + \Delta t \cdot [b_1 F(u_{n-1}) + \cdots + b_k F(u_{n-k})].$$

The coefficients $b_j = b_{k,j}$ are specified e.g. in [5] (Section III-1), [8] (p. 192-194). From (3.1), the corresponding values $\tau_n = \tau_{k,n}$ are seen to satisfy

$$\tau_0 = 0, \quad \tau_n = b_1 + \cdots + b_n \quad (\text{for } 1 \leq n \leq k), \quad \tau_n = b_1 + \cdots + b_k \quad (\text{for } n > k).$$

We can again check conditions (3.5), (3.6) in a finite number of steps.

Using the material in the literature just mentioned, one easily sees for all $k \geq 1$ that $b_1 > 0$, so that again $n_0 = 1$. Furthermore,

$$b_2 < 0 \quad (\text{for } k \geq 2), \quad \tau_n > 0 \quad (\text{for all } n \geq 1 \text{ and } k = 1, 2, 3).$$

In [12], p. 617, it was proved that $b_1 + b_2 < 0$ for all $k \geq 4$, so that

$$\tau_2 \leq 0 \quad (\text{for } k \geq 4).$$

The following theorem summarizes the conclusions obtainable from these results, by applying criterion (1.8) and Corollary 3.3 (with $n_0 = 1$):

Theorem 5.2. (I) For $k = 1$, there exists a stepsize-coefficient for monotonicity;

(II) For $k = 2, 3$, there exists no such coefficient, but there is a stepsize-coefficient for boundedness;

(III) For all $k \geq 4$, there doesn't even exist a stepsize-coefficient for boundedness.

Part (II) is related to earlier results for $k = 2, 3$ obtained in [9] (Section 6.3), [10] (Section 4.2) and [12] (Theorems 3.3, 4.2). Part (III) amounts to a stronger version of a result for $k \geq 4$ in [12] (Theorem 4.2) – where it was shown that a specific *sufficient* condition, for the existence of a stepsize-coefficient, is violated.

5.3 Backward differentiation formulas

The well-known k -step backward differentiation formulas (BDFs), with order of accuracy k , are of the form

$$(5.1) \quad u_n = a_1 u_{n-1} + \cdots + a_k u_{n-k} + \Delta t \cdot b_0 F(u_n).$$

The coefficients $b_0 = b_{k,0}$ and $a_j = a_{k,j}$ are specified e.g. in [2] (Section 7), [5] (Section III-1), [8] (p. 206-208). When $k = 1$, we have $a_1 = b_0 = 1$ so that a stepsize-coefficient for monotonicity exists; whereas, when $k \geq 2$, we have $a_{k,2} < 0$ so that no such stepsize-coefficient exists – see (1.8).

We study the methods below for $2 \leq k \leq 6$, because, for these values the methods are zero-stable, without essential roots different from $\zeta = 1$, whereas, for $k \geq 7$, the methods fail to be zero-stable.

By (3.1), the values $\tau_n = \tau_{k,n}$ satisfy

$$\tau_n = 0 \quad (\text{for } n < 0), \quad \tau_0 = b_0, \quad \tau_n = a_1 \tau_{n-1} + \cdots + a_k \tau_{n-k} \quad (\text{for } n \geq 1).$$

Checking conditions (3.5), (3.6) is now less simple than for the Adams methods, because the τ_n are not constant from some index on. But, we have $\lim_{n \rightarrow \infty} \tau_n = 1$ – this is obvious from the representation (4.12), with $q = 1$ and $\gamma \rightarrow 0$.

From the material in the above references, one sees that $\tau_1 = a_1 b_0 \neq 0$, so that $n_0 = 1$ (for $2 \leq k \leq 6$). Furthermore, one sees that (3.5) holds for $k = 2$. For $k = 3, 4, 5, 6$ we used Matlab and found, also for these values, that condition (3.5) is fulfilled.

It is fair to say that for the last four values of k we have no formal proof of (3.5). But, we have conclusive numerical evidence: we computed exact values $\tau_{k,n}$ with the Symbolic Math Toolbox software of Matlab and found for $3 \leq k \leq 6$ that $\tau_{k,n}$, rounded to 16 decimal digits, equals precisely 1 (for $250 \leq n \leq 500$), while

$$\min_{1 \leq n < 250} \tau_{k,n} \geq 237\,416\,500/282\,475\,249.$$

Corollary 3.3 thus leads to the following result – which we call a conclusion rather than a theorem, because for $3 \leq k \leq 6$ we have no formal proof of (3.5), but convincing numerical evidence instead.

Conclusion 5.3. (I) For $k = 1$ there exists a stepsize-coefficient for monotonicity;

(II) For $2 \leq k \leq 6$ there exists no such coefficient, but there is a stepsize-coefficient for boundedness.

For $k = 2$, the statement in Part (II) is related to results in [11] (Section 5.3.1) and [12] (Section 3.3). The author is not aware of related results in the literature for $k \geq 3$.

5.4 Extrapolated backward differentiation formulas

The k -step extrapolated backward differentiation formula (EBDF) has the same order of accuracy and coefficients a_j as the corresponding BDF, but it is explicit. It is obtained by replacing, in the BDF, the value $F(u_n)$ with the value at the grid point $t_n = n \Delta t$ of the Lagrange interpolating polynomial which takes on the values $F(u_{n-1}), \dots, F(u_{n-k})$ at the grid points t_{n-1}, \dots, t_{n-k} , cf. e.g. [13].

For the EBDFs it can be seen, similarly as for the BDFs, that a stepsize-coefficient for monotonicity exists only for $k = 1$ – and that the values $\tau_n = \tau_{k,n}$ satisfy again $\lim_{n \rightarrow \infty} \tau_n = 1$ (for $2 \leq k \leq 6$).

One easily sees that $n_0 = 1$ for $2 \leq k \leq 6$. Furthermore, it can be seen that condition (3.5) is fulfilled for $k = 2$, and that $\tau_2 < 0$ for $k = 6$. For $k = 3, 4, 5$ we used again Matlab, obtaining conclusive numerical evidence – similarly as for the BDFs – that condition (3.5) is fulfilled. We thus arrive at

Conclusion 5.4. (I) For $k = 1$ there exists a stepsize-coefficient for monotonicity;

(II) For $2 \leq k \leq 5$ there exists no such coefficient, but there is a stepsize-coefficient for boundedness;

(III) For $k = 6$ there exists not even a stepsize-coefficient for boundedness.

Part (II) is related to results in [9] (Section 6), [11] (Section 3.2), [12] (Sections 3.2, 4.2) and [16] (Section 3). Part (III) amounts to a stronger version of a result for $k = 6$ in [16] (Theorem 3.1) – where it was shown that a specific *sufficient* condition, for the existence of a stepsize-coefficient, is violated.

5.5 Classes of linear multistep methods with two essential roots

We consider general LMMs of the form

$$(5.2) \quad u_n = u_{n-2} + \Delta t \cdot [b_0 F(u_n) + b_1 F(u_{n-1}) + \cdots + b_k F(u_{n-k})],$$

where $k \geq 2$ and

$$(5.3) \quad b_0 \geq 0, \quad \sum_{j=0}^k b_j = 2, \quad \sum_{j \text{ is odd}} b_j \neq 1, \quad b_k \neq 0 \quad (\text{when } k > 2).$$

The last three of these assumptions guarantee consistency and avoid reducibility.

The growth parameters corresponding to the essential roots $\zeta_1 = 1$ and $\zeta_2 = -1$, respectively, are

$$\lambda_1 = 1 \quad \text{and} \quad \lambda_2 = 1 - \sum_{j \text{ is odd}} b_j$$

– cf. definition (2.7). By Theorem 3.1, (II), the following condition is thus *necessary* for the existence of a stepsize-coefficient for boundedness:

$$(5.4) \quad \sum_{j \text{ is odd}} b_j = 0.$$

Below we analyse three special cases of the above general method.

Case 1. Milne-Simpson methods

The Milne-Simpson methods are implicit, with order of accuracy p equal to $p = 4$ (for $k = 2$) and $p = k + 1$ (for $k > 2$), cf. e.g. [5] (p. 310-311), [8] (p. 201-202). For $k = 2$, we have $b_0 = \frac{1}{3}$, $b_1 = \frac{4}{3}$, $b_2 = \frac{1}{3}$ – the so-called Milne method.

From the material in the last references, one easily sees that (5.4) is violated, for all $k \geq 2$, so that there is *no* stepsize-coefficient for boundedness.

Case 2. Nyström methods

The well-known k -step Nyström methods are of the form (5.2), with $b_0 = 0$ and order of accuracy equal to k , cf. e.g. [5] (p. 309), [8] (p. 199-201). For $k = 2$, we have $b_1 = 2$, $b_2 = 0$ – the so-called explicit mid-point rule.

From the material in the last references, one easily sees that (5.4) is again violated, for all $k \geq 2$, so that there is once more *no* stepsize-coefficient for boundedness.

Case 3. The general two-step method of type (5.2)

For $k = 2$, the above general method reads

$$(5.5) \quad u_n = u_{n-2} + \Delta t \cdot [b_0 F(u_n) + b_1 F(u_{n-1}) + b_2 F(u_{n-2})],$$

and assumption (5.3) reduces to

$$(5.6) \quad b_0 \geq 0, \quad b_0 + b_1 + b_2 = 2, \quad b_1 \neq 1.$$

In view of condition (5.4), a stepsize-coefficient for boundedness may thus exist only when $b_1 = 0$.

For $b_1 = 0$, method (5.5) reduces to $u_n = u_{n-2} + \Delta t \cdot [b_0 F(u_n) + b_2 F(u_{n-2})]$, which is essentially the same as the one-step method

$$(5.7) \quad u_n = u_{n-1} + \Delta t \cdot \left[\frac{b_0}{2} F(u_n) + \frac{b_2}{2} F(u_{n-1}) \right],$$

carried out with twice the original stepsize. There exists a stepsize-coefficient for boundedness, corresponding to the original two-step method (5.5), if and only if such stepsize-coefficient exists for the one-step method (5.7). According to Corollary 3.3, the latter method has certainly a stepsize-coefficient for boundedness when $\tau_n > 0$ (for all $n \geq 1$). One easily sees that the values τ_n of method (5.7) satisfy

$$\tau_n = \frac{b_0 + b_2}{2} = 1 \quad (\text{for } n \geq 1),$$

so that a stepsize-coefficient for boundedness exists.

In view of the above, we have

Theorem 5.5.

- (I) For all Milne-Simpson methods with $k \geq 2$, there is no stepsize-coefficient for boundedness.
- (II) For all Nyström methods with $k \geq 2$, there is no stepsize-coefficient for boundedness.
- (III) For method (5.5), with coefficients satisfying (5.6), there exists a stepsize-coefficient for boundedness if and only if: $b_1 = 0$.

We note that Part (I) amounts to a stronger version of a result in [12] (Remark 4.3) – where it was stated that a specific *sufficient* condition, for the existence of a stepsize-coefficient, is violated.

We illustrate Part (III) of the theorem with three typical examples, viz

$$(5.8) \quad u_n = u_{n-2} + \Delta t \cdot [F(u_n) + F(u_{n-2})],$$

$$(5.9) \quad u_n = u_{n-2} + \Delta t \cdot [3F(u_n) - F(u_{n-2})],$$

$$(5.10) \quad u_n = u_{n-2} + \Delta t \cdot \left[\frac{2}{3} F(u_n) + \frac{2}{3} F(u_{n-1}) + \frac{2}{3} F(u_{n-2}) \right].$$

For the first of these methods there exists a stepsize-coefficient for monotonicity, cf. criterion (1.8).

For the second method, condition (1.8) is violated, so that no stepsize-coefficient exists for monotonicity; but by Theorem 5.5 there exists still a stepsize-coefficient for boundedness.

For method (5.10), there doesn't even exist a stepsize-coefficient for boundedness. It is worth noting that this method has still the property of being A-stable (i.e. all $z \in \mathbb{C}$ with $\text{Re } z \leq 0$ belong to the stability region S), cf. e.g. [6].

6 Conclusions

In this paper, we have analysed under what conditions general linear multistep methods can have a stepsize-coefficient for boundedness. For methods, with just one growth parameter equal to 1, this analysis has led to a simple condition that is necessary and sufficient for the existence of a such a stepsize-coefficient.

Moreover, we have obtained two, still more simple, conditions – one being sufficient and one necessary for a stepsize-coefficient to exist.

We have applied the conditions, found in the paper, in a systematic study of stepsize-coefficients for the following six classes of linear k -step methods: Adams-Moulton, Adams-Bashforth, Backward Differentiation (BD), Extrapolated Backward Differentiation (EBD), Milne-Simpson and Nyström methods. In the table below, the restrictions on k are displayed which have turned out to be necessary and sufficient for the existence of a stepsize-coefficient for boundedness. The table supplements earlier results, for these methods, given in the literature.

Adams-Moulton	Adams-Bashforth	BD	EBD	Milne-Simpson	Nyström
$k \leq 8$	$k \leq 3$	$k \leq 6$	$k \leq 5$	none	none

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References

- [1] Butcher J.C. (2003): *Numerical methods for ordinary differential equations*. Wiley.
- [2] Crouzeix M, Mignot A.-L, (1984): *Analyse numérique des équations différentielles*. Masson, Paris.
- [3] Crouzeix M, Raviart P.-A, (1980): *Approximation des problèmes d'évolution*. Lecture Notes, University Rennes.
- [4] S. Gottlieb, D.I. Ketcheson, C.-W. Shu, *High order strong stability preserving high-order time discretizations*, J. Sci. Comput. **38** (2009), 251–289.
- [5] Hairer E, Nørsett S.P, Wanner G. (1993): *Solving ordinary differential equations I – Nonstiff problems*. Second edition, Springer Series Comput. Math. 8, Springer.
- [6] Hairer E., Wanner G. (1996), *Solving ordinary differential equations II – Stiff and differential-algebraic problems*. Second edition, Springer Series in Comput. Math. 14, Springer.
- [7] Harten A. (1983): *High resolution schemes for hyperbolic conservation laws*, J. Comput. Phys. **49**, 357-393.
- [8] Henrici P. (1962): *Discrete variable methods in ordinary differential equations*, John Wiley & Sons, New York.
- [9] Hundsdorfer W, Mozartova A, Spijker M.N. (2011): *Stepsize restrictions for boundedness and monotonicity of multistep methods*. To appear in J. Sci. Comp. (DOI: 10.1007/s10915-011-9487-1).
- [10] Hundsdorfer W, Mozartova A, Spijker M.N. (2011): *Special boundedness properties in numerical initial value problems*. BIT Numerical Mathematics **51**, 909-936.

- [11] Hundsdorfer W, Ruuth S.J. (2006): *On monotonicity and boundedness properties of linear multistep methods*, Math. Comp. **75** (2006), 655–672.
- [12] Hundsdorfer W, Ruuth S.J, Spiteri R.J. (2003): *Monotonicity-preserving linear multistep methods*, SIAM J. Numer. Anal. **41** (2003), 605–623.
- [13] Hundsdorfer W, Verwer J.G. (2003): *Numerical solution of time-dependent advection-diffusion-reaction equations*. Springer Series in Comput. Math. **33**, Springer.
- [14] Lenferink H.W.J. (1989): *Contractivity preserving explicit linear multistep methods*, Numer. Math. **55** , 213–223.
- [15] LeVeque R.J. (2002): *Finite volume methods for hyperbolic problems*. Cambridge Texts in Applied Mathematics, Cambridge University Press.
- [16] Ruuth S.J, Hundsdorfer W. (2005): *High-order linear multistep methods with general monotonicity and boundedness properties*, J. Comput. Phys. **209** (2005), 226–248.
- [17] Shu C.-W. (1988): *Total-variation-diminishing time discretizations*, SIAM J. Sci. Statist. Comput. **9**, 1073-1084.
- [18] Shu C.-W, Osher S. (1988): *Efficient implementation of essentially nonoscillatory shock-capturing schemes*, J. Comput. Phys. **77**, 439-471.
- [19] Spijker M.N. (1983): *Contractivity in the numerical solution of initial value problems*, Numer. Math. **42** (1983), 271–290.
- [20] Spijker M.N. (2007): *Stepsize conditions for general monotonicity in numerical initial value problems*, SIAM J. Numer. Anal. **45**, 1226-1245.
- [21] Tijdeman R. (2011): *A one-sided power sum inequality*, Submitted to Indagationes Mathematicae (arXiv:1107.5495v1 [math.NT]).