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STABILITY AND B-CONVERGENCE OF LINEARLY IMPLICIT RUNGE-KUTTA METHODS

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Abstract. In this paper we study stability and convergence properties of linearly implicit Runge-Kutta methods applied to stiff semi-linear systems of differential equations. The stability analysis includes stability with respect to internal perturbations. All results presented in this paper are independent of the stiffness of the system.

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1. Introduction

We shall be concerned with the numerical solution of stiff nonlinear initial value problems for systems of ordinary differential equations

$$(1.1) \quad U'(t) = f(t, U(t)) \quad (0 \leq t \leq T), \quad U(0) = u_0.$$

The analysis will be restricted to semi-linear problems where

$$(1.2) \quad f(t, u) = Qu + g(t, u) \quad (\text{for all } t \in \mathbb{R} \text{ and } u \in \mathbb{R}^m)$$

with $m \geq 1$, Q an $m \times m$ -matrix and $g : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ such that

$$(1.3) \quad |g(t, \tilde{u}) - g(t, u)| \leq \alpha |\tilde{u} - u| \quad (\text{for all } t \in \mathbb{R} \text{ and } \tilde{u}, u \in \mathbb{R}^m),$$

$$(1.4) \quad \langle u, Qu \rangle \leq \beta |u|^2 \quad (\text{for all } u \in \mathbb{R}^m).$$

Here $\alpha \geq 0$, $\beta \in \mathbb{R}$ are given constants, $\langle \cdot, \cdot \rangle$ is an inner product on \mathbb{R}^m and $|\cdot|$ stands for the corresponding norm on \mathbb{R}^m .

The class of functions $f : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ given by (1.2) with $m \geq 1$ and g, Q satisfying (1.3), (1.4) will be denoted by $S(\alpha, \beta)$. Occasionally the initial value problems (1.1) with $f \in S(\alpha, \beta)$ will also be referred to as the class of problems $S(\alpha, \beta)$. The problems in this class may be arbitrarily stiff since there is no bound on the Lipschitz constant of $f(t, \cdot)$. On the other hand these problems are properly posed because $f(t, \cdot)$ does satisfy a one-sided Lipschitz condition with constant $\alpha + \beta$ (see e.g. [3]).

Let $h > 0$ be a given stepsize and $t_n = nh$ ($n \geq 0$). For the numerical solution of the initial value problem (1.1) with f given by (1.2) we shall deal with *linearly implicit Runge-Kutta methods* which yield approximations u_n to $U(t_n)$ by the scheme

$$(1.5a) \quad u_{n+1} = u_n + \sum_{i=1}^s b_i(hQ) hf(t_n + c_i h, y_i^{(n)}),$$

$$(1.5b) \quad y_i^{(n)} = u_n + \sum_{j=1}^{i-1} a_{ij}(hQ) hf(t_n + c_j h, y_j^{(n)}) \quad (1 \leq i \leq s).$$

The integer $s \geq 1$ is the number of stages, c_i ($1 \leq i \leq s$) are real para-

meters and the b_i ($1 \leq i \leq s$), a_{ij} ($1 \leq j < i \leq s$) are rational functions. These methods are called linearly implicit because only linear systems of algebraic equations have to be solved to compute the approximations u_n . In the literature (e.g. [6], [7], [9]) such methods are also called generalized Runge-Kutta methods or semi-implicit methods. The class of methods (1.5), introduced by van der Houwen [7], contains among others the popular *W-methods* [12] (ROW-methods with inexact Jacobian; cf. example 3.5 and [8]).

The object of this paper is the derivation of stability and convergence results which hold uniformly on the class of problems $S(\alpha, \beta)$. In particular, our results are independent of the stiffness of the problem under consideration and the dimension m (which makes the results also relevant for partial differential equations).

In section 2 we regard some stability questions. We introduce the concepts AS-stability and ASI-stability, used already in [1] for implicit Runge-Kutta methods, which guarantee that one step of the process (1.5) is not too sensitive for perturbations on the internal stages (1.5b). Some results in this direction given in [8] are generalized. Further it will be shown that A-stability together with ASI-stability is sufficient for the integration process to be stable w.r.t. a perturbation on the initial value u_0 .

Next we shall turn our attention to convergence for the linearly implicit Runge-Kutta methods. By the paper of Prothero and Robinson [11] it has become known that stiffness may not only affect the stability of a scheme but also its order of accuracy. For implicit Runge-Kutta methods this phenomenon has been analyzed in the papers of Frank, Schneid and Überhuber ([4], [5]), and, more recently, in [1], [2], [10]. Following [2] (and essentially also [5]) we put

$$\|U\|^{(q)} = \max\{ |U^{(j)}(t)| : 0 \leq t \leq T, 0 \leq j \leq q \}$$

and we give the following definition.

Definition 1.1. Method (1.5) is said to be *B-convergent of order p on $S(\alpha, \beta)$* if there are constants $\gamma_0, h_0 > 0$, $p_0 \in \mathbb{N}$ such that

$$|U(t_n) - u_n| \leq \gamma_0 \|U\|^{(p_0)} h^p \quad (\text{for } 0 < h \leq h_0, n \geq 0, 0 \leq t_n \leq T)$$

whenever $f \in S(\alpha, \beta)$, the u_n satisfy (1.5), and U is a solution of (1.1) with a continuous p_0 -th derivative.

In this definition γ_0, h_0, p_0 may only depend on α, β, T and the coefficients of the method.

In section 3 sufficient conditions on the method (1.5) will be given for having B-convergence with order 1 on $S(\alpha, \beta)$. For the class of linear (nonhomogeneous) problems $S(0, \beta)$ we shall present necessary and sufficient conditions for B-convergence with order p .

2. Stability

2.1. Preliminaries

In order to write the scheme (1.5) in a more compact way we introduce some notations that were also used in [1].

The $s \times s$ and $m \times m$ identity matrices will be denoted by I_s, I_m , respectively, or, if no confusion can arise, simply by I . The vector e stands for the vector in \mathbb{R}^s with all components equal to 1. By $L(\mathbb{K}^N, \mathbb{K}^M)$ we denote the space of linear operators (or matrices) from \mathbb{K}^N to \mathbb{K}^M , and $L(\mathbb{K}^N)$ stands for $L(\mathbb{K}^N, \mathbb{K}^N)$. Here \mathbb{K} may be either \mathbb{R} or \mathbb{C} . Further $A(\zeta) = (a_{ij}(\zeta)) \in L(\mathbb{C}^s)$, $b(\zeta) = (b_i(\zeta)) \in \mathbb{C}^s$ for $\zeta \in \mathbb{C}$ with a_{ij}, b_i ($1 \leq i, j \leq s$, $a_{ij} = 0$ for $i \leq j$) the coefficient-functions of the method (1.5), and we put $c = (c_1, c_2, \dots, c_s)^T$, $c^j = (c_1^j, c_2^j, \dots, c_s^j)^T$ for $j \geq 0$. We define $\underline{e} = e \otimes I_m$, $\underline{I} = I_s \otimes I_m$, $\underline{c} = c \otimes I_m$ and $\underline{c}^j = c^j \otimes I_m$, with \otimes standing for the Kronecker product. If $Z \in L(\mathbb{R}^m)$ then $\underline{A}(Z)$ stands for the block-matrix in $L(\mathbb{R}^{sm})$ with blocks $a_{ij}(Z) \in L(\mathbb{R}^m)$. Similarly $\underline{b}(Z)^T = (b_1(Z), b_2(Z), \dots, b_s(Z))^T \in L(\mathbb{R}^{sm}, \mathbb{R}^m)$. On the space \mathbb{R}^{sm} we shall deal with the norm

$$\|y\| = \left(\sum_{i=1}^s |y_i|^2 \right)^{\frac{1}{2}} \quad \text{for } y = (y_1, y_2, \dots, y_s)^T \in \mathbb{R}^{sm}$$

where $|\cdot|$ is the inner product-norm on \mathbb{R}^m . Also the induced operator norms on $L(\mathbb{R}^m)$, $L(\mathbb{R}^{sm})$ will be denoted by $|\cdot|$, $\|\cdot\|$, respectively.

For a given stepsize $h > 0$ and f given by (1.2) we put $Z = hQ$ and we define $F : \mathbb{R} \times \mathbb{R}^{sm} \rightarrow \mathbb{R}^{sm}$ by

$$F(t, y) = (f(t+c_1h, y_1), f(t+c_2h, y_2), \dots, f(t+c_sh, y_s))^T$$

for $t \in \mathbb{R}$ and $y = (y_1, y_2, \dots, y_s)^T \in \mathbb{R}^{sm}$.

With these notations the linearly implicit Runge-Kutta scheme can be written as

$$(2.1a) \quad u_{n+1} = u_n + \underline{b}(Z)^T h F(t_n, y_n),$$

$$(2.1b) \quad y_n = \underline{e} u_n + \underline{A}(Z) h F(t_n, y_n)$$

where $y_n = (y_1^{(n)}, y_2^{(n)}, \dots, y_s^{(n)})^T \in \mathbb{R}^{sm}$. Besides (2.1) we also consider the perturbed scheme

$$(2.2a) \quad \tilde{u}_{n+1} = \tilde{u}_n + \underline{b}(Z)^T h F(t_n, \tilde{y}_n) + v_n,$$

$$(2.2b) \quad \tilde{y}_n = \underline{e} \tilde{u}_n + \underline{A}(Z) h F(t_n, \tilde{y}_n) + w_n$$

with perturbations $v_n \in \mathbb{R}^m$, $w_n = (w_1^{(n)}, w_2^{(n)}, \dots, w_s^{(n)})^T \in \mathbb{R}^{sm}$. These perturbations may stand for local (discretization) errors, but they may also represent round-off errors or errors caused by not solving exactly the linear algebraic systems (e.g. iteratively with only a few iterations).

Let \underline{Z}_n be the block-diagonal matrix $\text{diag}(Z_1^{(n)}, Z_2^{(n)}, \dots, Z_s^{(n)}) \in L(\mathbb{R}^{sm})$ with $Z_i^{(n)} \in L(\mathbb{R}^m)$ such that

$$Z_i^{(n)} (\tilde{y}_i^{(n)} - y_i^{(n)}) = h (f(t_n + c_i h, \tilde{y}_i^{(n)}) - f(t_n + c_i h, y_i^{(n)})).$$

If $f \in S(\alpha, \beta)$ the $Z_i^{(n)}$ can be chosen such that $|Z_i^{(n)} - Z| \leq h\alpha$, and this will always be assumed. Subtraction of (2.1) from (2.2) yields

$$(2.3a) \quad \tilde{u}_{n+1} - u_{n+1} = \tilde{u}_n - u_n + \underline{b}(Z)^T \underline{Z}_n (\tilde{y}_n - y_n) + v_n,$$

$$(2.3b) \quad \tilde{y}_n - y_n = \underline{e} (\tilde{u}_n - u_n) + \underline{A}(Z) \underline{Z}_n (\tilde{y}_n - y_n) + w_n.$$

From (2.3b) we obtain

$$(2.4) \quad \tilde{y}_n - y_n = (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} (\underline{e} (\tilde{u}_n - u_n) + w_n).$$

Insertion of this expression into (2.3a) leads to the following recursion scheme for the $\tilde{u}_n - u_n$,

$$(2.5) \quad \begin{aligned} \tilde{u}_{n+1} - u_{n+1} = & [I + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} \underline{e}] (\tilde{u}_n - u_n) + \\ & + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} w_n + v_n. \end{aligned}$$

The relations (2.4), (2.5) will be basic for the analysis in the subsequent sections. For this analysis we shall sometimes work with complex scalar differential equations. These equations can be easily converted to real equations (with $f \in S(\alpha, \beta)$) by identifying \mathbb{C} with the \mathbb{R}^2 in the usual way.

2.2. Stability per step w.r.t. internal perturbations

In order to introduce some stability concepts we consider one step of (2.1), (2.2) for the simple testproblem (the A-stability model problem)

$$(2.6) \quad U'(t) = \lambda U(t) \quad \text{with } \lambda \in \mathbb{C}^-$$

where $\mathbb{C}^- = \{\zeta: \zeta \in \mathbb{C}, \operatorname{Re} \zeta \leq 0\}$. Let $z = h\lambda$, $n \geq 0$ and assume for convenience $\tilde{u}_n = u_n$. From (2.4), (2.5) we then obtain

$$(2.7) \quad \tilde{y}_n - y_n = (I - A(z)z)^{-1} w_n,$$

$$(2.8) \quad \tilde{u}_{n+1} - u_{n+1} = b(z)^T z (I - A(z)z)^{-1} w_n + v_n.$$

Therefore, if we want $\|\tilde{y}_n - y_n\|$ and $|\tilde{u}_n - u_n|$ to be small if $\|w_n\|$ and $|v_n|$ are so, we need bounds for (all the entries of) $(I - A(z)z)^{-1} \in L(\mathbb{C}^m)$ and $b(z)^T z (I - A(z)z)^{-1} \in L(\mathbb{C}^m, \mathbb{C})$.

Definition 2.1. The method (1.5) is said to be *ASI-stable* if $(I - A(\zeta)\zeta)^{-1}$ is uniformly bounded for $\zeta \in \mathbb{C}^-$.

Definition 2.2. The method (1.5) is called *AS-stable* if $b(\zeta)^T \zeta (I - A(\zeta)\zeta)^{-1}$ is uniformly bounded for $\zeta \in \mathbb{C}^-$.

These definitions are similar to the ones given in [1] for implicit Runge-Kutta methods. For the linearly implicit methods (1.5) such stability concepts were considered in [8; sect.3.3.2] and there a result closely related to the following lemma 2.3 was proved. In all of the following it is tacitly assumed that the coefficient-functions a_{ij} and b_i do not have a pole at the origin.

Lemma 2.3. Method (1.5) is AS-stable and ASI-stable iff all a_{ij} , b_i are regular on \mathbb{C}^- and $a_{ij}(\infty) = b_i(\infty) = 0$ ($1 \leq i, j \leq s$).

Proof. In the proof of lemma 2.4.11 in [8] the sufficiency has been demonstrated and it was shown that AS- and ASI-stability imply that $a_{ij}(\zeta)\zeta, b_i(\zeta)\zeta$ remain bounded for $\zeta \rightarrow \infty$. This proof can be extended in a straightforward way to show that all $a_{ij}(\zeta)\zeta, b_i(\zeta)\zeta$ must be uniformly bounded for $\zeta \in \mathbb{C}^-$ in order to have AS- and ASI-stability. \square

We note that the conditions in this lemma on the coefficient-functions a_{ij}, b_i were already used in [13] to formulate sufficient conditions for S-stability. Lemma 2.3 shows that most well-known linearly-implicit Runge-Kutta methods are AS- and ASI-stable. In particular it can be easily seen that any W-method whose stability function is regular on \mathbb{C}^- has these stability properties.

The names AS- and ASI-stability are derived from BS- and BSI-stability. These concepts, introduced in [4], are designed for the B-stability model problem (problem (1.1) with f dissipative). Our definitions arise from considerations on the A-stability model problem (2.6). The following theorem shows that our concepts for linear, scalar problems are also relevant for nonlinear, nonscalar problems in $S(\alpha, \beta)$.

Theorem 2.4. Let (2.1), (2.2) hold with $\tilde{u}_n = u_n$ and $f \in S(\alpha, \beta)$. Suppose the method (1.5) is AS- stable and ASI-stable. Then there are positive constants γ_i, h_i ($i=1,2$), which only depend on α, β and the coefficients of the method, such that $\|\tilde{y}_n - y_n\| \leq \gamma_1 \|w_n\|$ (for $0 < h \leq h_1$) and $|\tilde{u}_{n+1} - u_{n+1}| \leq |v_n| + \gamma_2 \|w_n\|$ (for $0 < h \leq h_2$).

Proof. We note that if $h\beta \leq \omega$ with $\omega > 0$ such that all a_{ij}, b_i are regular on $\{\zeta: \zeta \in \mathbb{C}, \operatorname{Re} \zeta \leq \omega\}$, then the matrices $a_{ij}(Z), b_i(Z)$ are well defined. In the same way as in [1; lemmas 3.5-3.7] one can prove the existence of $\gamma_i, h_i > 0$ such that

$$(2.9) \quad \|(\underline{I} - \underline{A}(Z)\underline{Z}_n)^{-1}\| \leq \gamma_1 \quad (\text{for } 0 < h \leq h_1),$$

$$(2.10) \quad |\underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z)\underline{Z}_n)^{-1} w| \leq \gamma_2 \|w\| \quad (\text{for } 0 < h \leq h_2, w \in \mathbb{R}^{sm}).$$

The proof of the theorem now follows immediately from (2.4), (2.5). \square

From our considerations on the model problem (2.6) it can be seen that AS-stability, ASI-stability are necessary for having bounds as in theorem 2.4 for $|\tilde{u}_{n+1} - u_{n+1}|$, $\|\tilde{y}_n - y_n\|$, respectively. However, also if we are only interested in a bound for $|\tilde{u}_{n+1} - u_{n+1}|$ on $S(\alpha, \beta)$ with $\alpha > 0$, then ASI-stability is essential. This will be shown by means of the following example.

Example 2.5. Consider the method (1.5) with $s=2$, c_i arbitrary,

$$a_{21}(\zeta) \equiv \frac{1}{2}, \quad b_i(\zeta) = \frac{1}{2}(1-\zeta)^i \quad (i=1,2).$$

This method is AS-stable (and A-stable), but, since $a_{21}(\infty) \neq 0$, it is not ASI-stable.

Let $\alpha > 0$, $\beta \in \mathbb{R}$, and let f be given by (1.2) with $m=2$,

$$Q = \begin{pmatrix} \beta & 0 \\ 0 & \lambda \end{pmatrix}, \quad g(t, u) = v(t) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} u \quad (\text{for } t \in \mathbb{R}, u \in \mathbb{R}^2),$$

where $\lambda \in \mathbb{R}$, $\lambda \leq \beta$ and $v: \mathbb{R} \rightarrow \mathbb{R}$, $|v(t)| \leq \alpha$. Clearly $f \in S(\alpha, \beta)$. Further we take $\tilde{u}_n = u_n$, $v_n = w_2^{(n)} = 0$ and $w_1^{(n)} = (0, \varepsilon)^T$. Then we get in view of (2.5), with $Z_i^{(n)}$ equal to $Z + hg(t_n + c_i h, \cdot)$,

$$\begin{aligned} \tilde{u}_{n+1} - u_{n+1} &= [b_1(Z)Z_1^{(n)} + b_2^{(n)}(Z)Z_2^{(n)}a_{21}Z_1^{(n)}]w_1^{(n)} = \\ &= [b_1(Z)Z + b_1(Z)(Z_1^{(n)} - Z) + a_{21}b_2(Z)Z^2 + a_{21}b_2(Z)Z(Z_1^{(n)} - Z) + \\ &\quad + a_{21}b_2(Z)(Z_2^{(n)} - Z)Z + a_{21}b_2(Z)(Z_2^{(n)} - Z)(Z_1^{(n)} - Z)]w_1^{(n)} = \\ &= \varepsilon b_1(h\lambda)h\lambda e_2 + \varepsilon v_1 b_1(h\beta)e_1 + \varepsilon a_{21}b_2(h\lambda)h^2\lambda^2 e_2 + \varepsilon v_1 a_{21}b_2(h\beta)h\beta e_1 + \\ &\quad + \varepsilon v_2 a_{21}b_2(h\beta)h\lambda e_1 \end{aligned}$$

where $v_i = h v(t_n + c_i h)$, $e_1 = (1, 0)^T$, $e_2 = (0, 1)^T$. All terms on the right-hand side except the last one are uniformly bounded for $\lambda \leq \beta$. For any $h > 0$ such that $v(t_n + c_2 h) \neq 0$ this last term $\varepsilon v_2 a_{21} b_2(h\beta) h \lambda e_1$ does not stay bounded if $\lambda \rightarrow -\infty$, and thus we have $\lim_{\lambda \rightarrow -\infty} |\tilde{u}_{n+1} - u_{n+1}| = \infty$.

2.3. Stability on the integration interval

In this section we study the stability of the entire integration process (1.5) with t_n ranging from 0 to T . First we consider the effect of an error in the initial value u_0 on the unperturbed scheme.

Theorem 2.6. Consider (2.1), (2.2) with $v_n = 0$, $w_n = 0$ (for all n), and $f \in S(\alpha, \beta)$. Suppose the method (1.5) is A-stable and ASI-stable. Then there are constants $\gamma_3 \geq 0$, $h_3 > 0$, which only depend on α , β and the coefficients of the method, such that

$$|\tilde{u}_n - u_n| \leq e^{\gamma_3 t_n} |\tilde{u}_0 - u_0| \quad (\text{for } 0 < h \leq h_3, n \geq 0, 0 \leq t_n \leq T).$$

Proof. In the same way as in [1; lemma 3.6] it can be shown that there exist $\gamma_3 \geq 0$, $h_3 > 0$ such that

$$(2.11) \quad |I + b(Z)^T Z_n (I - A(Z) Z_n)^{-1} e| \leq 1 + \gamma_3 h \quad (\text{for } 0 < h \leq h_3).$$

The recursion (2.5) thus yields $|\tilde{u}_{n+1} - u_{n+1}| \leq (1 + \gamma_3 h) |\tilde{u}_n - u_n|$ (for $0 < h \leq h_3$), from which the theorem can be easily proved. \square

Remark 2.7. For any W-method which is A-stable theorem 2.6 provides a stability result on the class of problems $S(\alpha, \beta)$. In [6] (cf. also [8]) additional conditions on these methods are given which ensure *contractivity* of the scheme, i.e. $|\tilde{u}_{n+1} - u_{n+1}| \leq |\tilde{u}_n - u_n|$ (for $0 < h \leq h_3$), for given constants α, β with $\alpha + \beta \leq 0$. Such a stronger stability property may be quite useful if the integration interval $[0, T]$ is very long, but in most practical situations one will not encounter numerical instabilities if only a stability result as in theorem 2.6 holds.

Remark 2.8. If $\alpha = 0$ the condition that the method should be ASI-stable can be removed from the assumptions in theorem 2.6; for the linear problems $S(0, \beta)$ A-stability is sufficient (and necessary). However, if $\alpha > 0$ this condition cannot be removed. This can be seen by considering the 2-stage method and the function f of example 2.5 with $\tilde{u}_n - u_n = (0, \varepsilon)^T$ and $v_n = 0$, $w_n = 0$. As in example 2.5 we then get $|\tilde{u}_{n+1} - u_{n+1}| \rightarrow \infty$ if $\lambda \rightarrow -\infty$.

By combining (2.5) with the upper bounds (2.10), (2.11) we obtain the following result.

Theorem 2.9. Consider (2.1), (2.1) with $f \in S(\alpha, \beta)$. Suppose the method (1.5) is A-stable, AS-stable and ASI-stable. Then we have

$$|\tilde{u}_n - u_n| \leq e^{\gamma_3 t_n} |\tilde{u}_0 - u_0| + (e^{\gamma_3 t_n} - 1) \frac{1}{\gamma_3 h} \max_{0 \leq k \leq n-1} \{ |v_k| + \gamma_2 \|w_k\| \}$$

for $0 < h \leq \min\{h_2, h_3\}$, $n \geq 0$, $0 \leq t_n \leq T$, with γ_i, h_i ($i=2,3$) as in the theorems 2.4, 2.6.

If the v_n, w_n represent local errors and $|v_k|, \|w_k\| = O(h^{q+1})$ uniformly in k , the above theorem can be used to prove convergence of order q . In the following section we shall use a more refined technique which shows that these local and the global errors often have the same order.

3. B-convergence

3.1. *B-convergence on $S(\alpha, \beta)$*

Let U be the solution of the initial value problem (1.1). We define $Y_i^{(n)} = U(t_n + c_i h)$, $Y_n = (Y_1^{(n)}, Y_2^{(n)}, \dots, Y_s^{(n)})^T$. Then

$$(3.1a) \quad U(t_{n+1}) = U(t_n) + \underline{b}(Z)^T h F(t_n, Y_n) + \rho_n,$$

$$(3.1b) \quad Y_n = \underline{c} U(t_n) + \underline{A}(Z) h F(t_n, Y_n) + r_n$$

where $\rho_n \in \mathbb{R}^m$, $r_n \in \mathbb{R}^{sm}$ are the residual errors. By a Taylor series expansion we get

$$\rho_n = [I - \underline{b}(Z)^T \underline{c}] h U'(t_n) + [\frac{1}{2} I - \underline{b}(Z)^T \underline{c}] h^2 U''(t_n) + \dots,$$

$$r_n = [\underline{c} - \underline{A}(Z) \underline{c}] h U'(t_n) + [\frac{1}{2} \underline{c}^2 - \underline{A}(Z) \underline{c}] h^2 U''(t_n) + \dots$$

Thus, unless $\underline{b}(Z)^T \underline{c} \equiv 1$, $\underline{A}(Z) \underline{c} \equiv \underline{c}$, which is impossible if the method is AS- and ASI-stable, we only have $\rho_n = O(h^{q+1})$, $r_n = O(h^{q+1})$ ($h \downarrow 0$, uniformly on $S(\alpha, \beta)$) with $q = 0$. Therefore theorem 2.9 cannot be applied to prove B-convergence on $S(\alpha, \beta)$. Yet we can prove such convergence for a large class of linearly implicit Runge-Kutta methods. This will be done along the same lines as in [1], by employing a technique introduced by Kraaijevanger [10] for some simple implicit Runge-Kutta methods.

Let ϕ stand for the stability function of the method (1.5)

$$(3.2) \quad \phi(\zeta) = 1 + b(\zeta)^T \zeta (I - A(\zeta)\zeta)^{-1} e \quad (\text{for } \zeta \in \mathbb{C}),$$

and define the rational function ψ by

$$(3.3) \quad \psi(\zeta) = [1 - \phi(\zeta)]^{-1} [1 + b(\zeta)^T (I - A(\zeta)\zeta)^{-1} (c\zeta - e)] \quad (\text{for } \zeta \in \mathbb{C})$$

Theorem 3.1. Assume method (1.5) is A-stable, AS-stable and ASI-stable, and ψ is bounded on \mathbb{C}^- . Then the method (1.5) is B-convergent on $S(\alpha, \beta)$ (with order ≥ 1).

The proof of this theorem will be given in the next section. The following corollary shows that the B-convergence result is valid for many well-known linearly implicit Runge-Kutta methods which are A-stable.

Corollary 3.2. Assume method (1.5) is A-stable, all a_{ij}, b_i are regular on \mathbb{C}^- and have a zero at infinity, $b(0)^T e = 1$, and $\phi(\zeta) \neq 1$ for $\zeta \in \mathbb{C}^- \cup \{\infty\}, \zeta \neq 0$. Then the method is B-convergent on $S(\alpha, \beta)$.

Proof. From lemma 2.3 we know the method is AS- and ASI-stable, and thus we only have to show that ψ is bounded on \mathbb{C}^- . From the AS-stability it follows that $1 + b(\zeta)^T (I - A(\zeta)\zeta)^{-1} (c\zeta - e)$ is uniformly bounded for $\zeta \in \mathbb{C}^-$ and since $\phi(\zeta) \neq 1$ for $\zeta \in \mathbb{C}^- - \{0\}$ we only have to make sure that ψ is bounded near $\zeta = 0$. This is so if $b(0)^T e = 1$, because then $\phi'(0) = 1$ and $\lim_{\zeta \rightarrow 0} \{1 + b(\zeta)^T (I - A(\zeta)\zeta)^{-1} (c\zeta - e)\} = 0$. \square

The condition $b(0)^T e = 1$ in this corollary is simply the requirement for having order 1 for nonstiff problems (see e.g. [7]). Results on the condition $\phi(\zeta) \neq 1$ for $\zeta \in \mathbb{C}^- - \{0\}$ can be found in [1],[2] for some interesting stability functions ϕ .

The necessity of the requirement that ψ is bounded on \mathbb{C}^- will be demonstrated in section 3.3 where the linear problems $S(0, \beta)$ are considered. For such problems Q is the exact Jacobian $\frac{\partial}{\partial u} f(t, u)$, and also higher order results will be obtained. It is not clear whether B-convergence on $S(\alpha, \beta)$ with order $p > 1$ is possible for a method (1.5) in case $\alpha > 0$.

3.2. The proof of theorem 3.1

Let $\omega > 0$ be a number such that ψ and all a_{ij}, b_i are bounded on $\{\zeta: \zeta \in \mathbb{C}, \operatorname{Re} \zeta \leq \omega\}$, and assume $h_4 > 0$, $h_4 \beta \leq \omega$, and $|\psi(\zeta)| \leq \gamma_4$ for $\zeta \in \mathbb{C}, \operatorname{Re} \zeta \leq \omega$. By a result of von Neumann (see e.g. [6; theorem 4]) it follows that $|\psi(Z)| \leq \gamma_4$, and similar bounds hold for $|a_{ij}(Z)|, |b_i(Z)|$. Further we shall use in this proof the inequalities (2.9)–(2.11), and we assume that $0 < h \leq h_0 = \min\{h_1, h_2, h_3, h_4\}$.

Let $\varepsilon_n = U(t_n) - u_n$. Application of (2.5) with $\tilde{u}_n = U(t_n)$, $v_n = \rho_n$ and $w_n = r_n$ gives

$$\varepsilon_{n+1} = (I + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} \underline{e}) \varepsilon_n + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} r_n + \rho_n.$$

For $\hat{\varepsilon}_n = \varepsilon_n - \psi(Z) h U'(t_n)$ we then obtain the relation

$$\hat{\varepsilon}_{n+1} = (I + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} \underline{e}) \hat{\varepsilon}_n + \hat{\rho}_n$$

where

$$\begin{aligned} \hat{\rho}_n &= \rho_n + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} (r_n + \underline{e} \psi(Z) h U'(t_n)) + \psi(Z) h \{U'(t_n) - U'(t_{n+1})\} \\ &= \{I - \underline{b}(Z)^T \underline{e} + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} (\underline{c} - \underline{A}(Z) \underline{e} + \underline{e} \psi(Z))\} h U'(t_n) + \\ &\quad + \{\rho_n - (I - \underline{b}(Z)^T \underline{e}) h U'(t_n)\} + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} \{r_n - \\ &\quad - (\underline{c} - \underline{A}(Z) \underline{e}) h U'(t_n)\} + \psi(Z) h \{U'(t_n) - U'(t_{n+1})\} \end{aligned}$$

We have

$$\begin{aligned} 1 - \underline{b}(\zeta)^T \underline{e} + \underline{b}(\zeta)^T \underline{\zeta} (\underline{I} - \underline{A}(\zeta) \underline{\zeta})^{-1} (\underline{c} - \underline{A}(\zeta) \underline{e} + \underline{e} \psi(\zeta)) &= 0 \quad (\text{for all } \zeta \in \mathbb{C}), \\ \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} &= \underline{Z} (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} + (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} (\underline{Z}_n - \underline{Z}) (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} \end{aligned}$$

where $\underline{Z} = I_s \otimes Z$. By using these relations it can be seen that

$$\begin{aligned} I - \underline{b}(Z)^T \underline{e} + \underline{b}(Z)^T \underline{Z}_n (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} (\underline{c} - \underline{A}(Z) \underline{e} + \underline{e} \psi(Z)) &= \\ = \underline{b}(Z)^T (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} (\underline{Z}_n - \underline{Z}) (\underline{I} - \underline{A}(Z) \underline{Z}_n)^{-1} (\underline{c} - \underline{A}(Z) \underline{e} + \underline{e} \psi(Z)). \end{aligned}$$

Further we know that $|Z_i^{(n)} - Z| \leq h \alpha$ ($1 \leq i \leq s$), and this implies $\|\underline{Z}_n - \underline{Z}\| \leq h \alpha$. From (2.9), (2.10) and a Taylor series expansion of ρ_n, r_n it can now be seen that there exist a $\gamma_5 > 0$ (only depending on α, β and the coefficients of the method) such that

$$|\hat{\rho}_n| \leq \gamma_5 \|U\|^{(2)} h^2$$

and with (2.11) we thus get

$$|\hat{\varepsilon}_{n+1}| \leq (1 + \gamma_3 h) |\hat{\varepsilon}_n| + \gamma_5 \|U\|^{(2)} h^2.$$

It follows that

$$|\hat{\varepsilon}_n| \leq e^{\gamma_3 t_n} |\hat{\varepsilon}_0| + (e^{\gamma_3 t_n} - 1) \frac{1}{\gamma_3} \gamma_5 \|U\|^{(2)} h$$

for any $n \geq 0$ with $0 \leq t_n \leq T$, and since $|\hat{\varepsilon}_n - \varepsilon_n| \leq \gamma_4 \|U\|^{(1)} h$, the B-convergence result is now easily obtained. \square

3.3. B-convergence on $S(0, \beta)$

In this section we consider the initial value problems in the class $S(0, \beta)$, i.e. problems of the type

$$U'(t) = QU(t) + g(t) \quad (0 \leq t \leq T), \quad U(0) = u_0$$

with $u_0 \in \mathbb{R}^m$, $m \geq 1$, $Q \in L(\mathbb{R}^m)$ satisfying (1.4), and $g: \mathbb{R} \rightarrow \mathbb{R}^m$ arbitrary.

Let the rational functions ψ_j ($j=1, 2, \dots$) be defined by

$$(3.4) \quad \psi_j(\zeta) = l_j(\zeta) + b(\zeta)^T \zeta (I - A(\zeta) \zeta)^{-1} k_j(\zeta) \quad (\text{for } \zeta \in \mathbb{C})$$

where $l_j: \mathbb{C} \rightarrow \mathbb{C}$ and $k_j: \mathbb{C} \rightarrow \mathbb{C}^s$ are given by

$$l_j(\zeta) = \frac{1}{(j-1)!} \left[\frac{1}{j} - b(\zeta)^T c^{j-1} \right], \quad k_j(\zeta) = \frac{1}{(j-1)!} \left[\frac{1}{j} c^j - A(\zeta) c^{j-1} \right]$$

(for $\zeta \in \mathbb{C}$). Note that $\psi(\zeta)$, defined by (3.3), equals $(1 - \phi(\zeta))^{-1} \psi_1(\zeta)$.

Theorem 3.3. Let $p \geq 1$. Suppose method (1.5) is A-stable and AS-stable. Then the method is B-convergent of order p on $S(0, \beta)$ iff $\psi_j \equiv 0$ ($1 \leq j \leq p-1$) and $(1 - \phi(\zeta))^{-1} \psi_p(\zeta)$ is uniformly bounded for $\zeta \in \mathbb{C}^-$.

Proof. If U is a solution of (1.1) with a continuous $p+1$ -th derivative it follows by a Taylor series expansion that

$$\rho_n = \sum_{j=1}^p l_j(Z) h^j U^{(j)}(t_n) + h^{p+1} \{ \xi_0^{(n)} - \underline{b}(Z)^T \eta_n \},$$

$$r_n = \sum_{j=1}^p k_j(Z) h^j U^{(j)}(t_n) + h^{p+1} \{ \xi_n - \underline{A}(Z) \eta_n \}$$

where $\xi_n = (\xi_1^{(n)}, \xi_2^{(n)}, \dots, \xi_s^{(n)})^T \in \mathbb{R}^{sm}$, $\eta_n = (\eta_1^{(n)}, \eta_2^{(n)}, \dots, \eta_s^{(n)})^T \in \mathbb{R}^{sm}$, $\xi_i^{(n)} = c_i^{p+1} U^{(p+1)}(t_n + \theta_i h) / (p+1)!$ with $\theta_i \in (0, c_i)$ ($0 \leq i \leq s$; $c_0 := 1$), and $\eta_i^{(n)} = c_i^p U^{(p+1)}(t_n + \theta_i' h) / p!$ with $\theta_i' \in (0, c_i)$ ($1 \leq i \leq s$). Defining

$\underline{Z} = I_s \otimes Z$ we obtain

$$(3.5) \quad \underline{b}(Z)^T \underline{Z} (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} r_n + \rho_n = \sum_{j=1}^p \psi_j(Z) h^j U^{(j)}(t_n) + \\ + h^{p+1} \{ \xi_0^{(n)} + \underline{b}(Z)^T \underline{Z} (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} \xi_n - \underline{b}(Z)^T (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} \eta_n \}.$$

We now prove the sufficiency of the conditions. It will be assumed that, if $\beta > 0$, $h\beta$ is small enough for the arising rational functions to be bounded on $\{\zeta: \zeta \in \mathbb{C}, \operatorname{Re} \zeta \leq h\beta\}$. Define $\Psi(\zeta) = (1 - \phi(\zeta))^{-1} \psi_p(\zeta)$ ($\zeta \in \mathbb{C}$), $\varepsilon_n = U(t_n) - u_n$ and $\hat{\varepsilon}_n = \varepsilon_n - \Psi(Z) h^p U^{(p)}(t_n)$ (for $n \geq 0$, $0 \leq t_n \leq T$). From (2.5) it can be seen that the $\hat{\varepsilon}_n$ satisfy

$$\hat{\varepsilon}_{n+1} = \phi(Z) \hat{\varepsilon}_n + \hat{\rho}_n$$

with

$$\hat{\rho}_n = \rho_n + \underline{b}(Z)^T \underline{Z} (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} r_n + \phi(Z) \Psi(Z) h^p U^{(p)}(t_n) - \Psi(Z) h^p U^{(p)}(t_{n+1}).$$

Since $\psi_j \equiv 0$ ($0 \leq j \leq p-1$) we get in view of (3.5)

$$\hat{\rho}_n = \Psi(Z) h^p \{U^{(p)}(t_n) - U^{(p)}(t_{n+1})\} + \\ + h^{p+1} \{ \xi_0^{(n)} + \underline{b}(Z)^T \underline{Z} (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} \xi_n - \underline{b}(Z)^T (\underline{I} - \underline{A}(Z) \underline{Z})^{-1} \eta_n \},$$

from which it can be seen that

$$|\hat{\rho}_n| \leq \gamma_6 \|U\|^{(p+1)} h^{p+1}$$

for some $\gamma_6 > 0$ which only depends on β and the coefficients of the method. Proceeding as in section 3.2 the order p convergence result now easily follows.

In order to prove the necessity of the conditions on the ψ_j we consider the scalar, complex testproblem of Prothero and Robinson [11]

$$U'(t) = \lambda(U(t) - g(t)) + g'(t), \quad U(0) = g(0)$$

with $\lambda \in \mathbb{C}$, $\operatorname{Re} \lambda \leq \beta$ and $g(t) = (1+t)^p/p!$; its solution is $U(t) = g(t)$. The same problem was used in [2] for determining upper bounds for the order of B-convergence of implicit Runge-Kutta methods.

From (2.5) and (3.5) we obtain

$$\varepsilon_1 = \sum_{j=1}^p \psi_j(z) h^j U^{(j)}(0)$$

where $z = h\lambda$. Thus we have $\varepsilon_1 = O(h^p)$ ($h \rightarrow 0$, uniformly for $\lambda \in \mathbb{C}$, $\operatorname{Re} \lambda \leq \beta$) only if $\psi_j \equiv 0$ ($1 \leq j \leq p-1$).

Now assume $\psi_j \equiv 0$ ($1 \leq j \leq p-1$) but $\sup\{|\Psi(\zeta)| : \zeta \in \mathbb{C}\} = \infty$. For the global error we then have, in view of (2.5), (3.5), the recursion

$$\varepsilon_{n+1} = \phi(z)\varepsilon_n + \psi_p(z)h^p$$

and thus we get, for all $n \geq 0$ with $0 \leq t_n \leq T$,

$$\varepsilon_n = (\phi(z)^{n-1} + \dots + \phi(z) + 1)\psi_p(z)h^p,$$

$$\varepsilon_n = (1 - \phi(z)^n)^{-1}\psi_p(z)h^p \quad - \text{ provided } \phi(z) \neq 1.$$

For any $C > 0$ and sufficiently small $h > 0$ we can take $z = h\lambda$ with $\operatorname{Re} \lambda \leq \beta$ such that $|\phi(z)| < 1$, $|\Psi(z)| > C$. For $h \downarrow 0$, $nh = t \in [0, T]$ fixed we get with this choice of λ

$$|\varepsilon_n| \rightarrow |\Psi(z)|h^p > Ch^p.$$

Since C can be chosen arbitrarily large, we see that we do not have convergence of order p uniformly for all $\lambda \in \mathbb{C}$ with $\operatorname{Re} \lambda \leq \beta$. \square

Example 3.4. Consider the linearly implicit Runge-Kutta method (1.5) with $s = 1$, $c_1 \in \mathbb{R}$ and $b_1(\zeta) = 1/(1 - \theta\zeta)$ ($\zeta \in \mathbb{C}$). This method is A-stable for $\theta \geq \frac{1}{2}$, and it is AS- and ASI-stable for $\theta > 0$. We have

$$\phi(\zeta) = (1 - \theta\zeta)^{-1}[1 + (1 - \theta)\zeta],$$

$$\psi_1(\zeta) = (1 - \theta\zeta)^{-1}(c_1 - \theta)\zeta,$$

$$\psi_2(\zeta) = (1 - \theta\zeta)^{-1}[(\frac{1}{2} - c_1) + (\frac{1}{2}c_1^2 - \frac{1}{2}\theta)\zeta].$$

Application of theorem 3.3 shows that for $\theta \geq \frac{1}{2}$ this method is B-convergent of order $p \geq 1$ on $S(0, \beta)$, and

$$p = 2 \quad \text{iff} \quad c_1 = \theta = \frac{1}{2}.$$

This order 2 result does not hold on $S(\alpha, \beta)$ if $\alpha > 0$. For such nonlinear problems Q may differ from the exact Jacobian $\frac{\partial}{\partial u}f(t, u)$, and a simple counter-example can be constructed by considering the problem with $m = 1$, $Q = \beta$ and $g(t, u) = \alpha u$ (for $t, u \in \mathbb{R}$). Then

$$u_{n+1} = u_n + (1 - \frac{1}{2}h\beta)^{-1}(h\alpha + h\beta)u_n = (1 - \tilde{\theta}h\nu)^{-1}(1 + (1 - \tilde{\theta})h\nu)u_n$$

with $\nu = \alpha + \beta$, $\tilde{\theta} = \beta/2\nu$, and we see that the u_n approximate $U(t_n) = e^{\nu t_n} u_0$ up to order 2, uniformly for $t_n \in [0, T]$, only if $\tilde{\theta} = \frac{1}{2}$, i.e. $\alpha = 0$. For the method with $\theta = \frac{1}{2}$ which uses instead of Q the exact Jacobian, a B-convergence result for a class of nonlinear stiff problems can be found in [8].

Example 3.5. Consider the 2-stage W-method

$$\begin{aligned} u_{n+1} &= u_n + \beta_1 x_1^{(n)} + \beta_2 x_2^{(n)}, \\ (I - h\gamma Q)x_1^{(n)} &= hf(t_n + c_1 h, u_n), \\ (I - h\gamma Q)x_2^{(n)} &= hf(t_n + c_2 h, u_n + \alpha_{21} x_1^{(n)}) + \gamma_{21} h Q x_1^{(n)} \end{aligned}$$

with the coefficients satisfying $\beta_1 + \beta_2 = 1$, $\beta_2 \alpha_{21} = \frac{1}{2}$, $\beta_2 \gamma_{21} = -\gamma$ and $\beta_1 c_1 + \beta_2 c_2 = \frac{1}{2}$. This method has order 2 for nonstiff problems (cf. [12]), and it is A-stable for $\gamma \geq \frac{1}{4}$, AS- and ASI-stable for $\gamma > 0$. It can be written in the form (1.5) with

$$a_{21}(\zeta) = (1-\gamma\zeta)^{-1} \alpha_{21}, \quad b_1(\zeta) = (1-\gamma\zeta)^{-2} (\beta_1 + (\beta_2 \gamma_{21} - \beta_1 \gamma) \zeta), \quad b_2(\zeta) = (1-\gamma\zeta)^{-1} \beta_2.$$

This form is only convenient for the analysis, not for actual computations. We have

$$\begin{aligned} \phi(\zeta) &= (1-\gamma\zeta)^{-2} [1 + (1-2\gamma)\zeta + (\frac{1}{2} - 2\gamma + \gamma^2)\zeta^2], \\ \psi_1(\zeta) &= (1-\gamma\zeta)^{-2} [(\gamma - \frac{1}{2})(\gamma - c_1)\zeta^2], \\ \psi_2(\zeta) &= (1-\gamma\zeta)^{-2} [\frac{1}{2}(2\gamma c_1 - \gamma - c_1 + \beta_1 c_1^2 + \beta_2 c_2^2)\zeta + \\ &\quad + \frac{1}{2}(\gamma^2 - \gamma c_1^2 + \frac{1}{2}c_1^2 - \gamma\beta_1 c_1^2 - \gamma\beta_2 c_2^2)\zeta^2], \\ \psi_3(0) &= -\frac{1}{2}(\beta_1 c_1^2 + \beta_2 c_2^2) + 1/6. \end{aligned}$$

From the theorems 3.1, 3.3 it can be seen by some calculations that this method is B-convergent on $S(0, \beta)$ with order

$$\begin{aligned} p \geq 1 \quad \text{iff} \quad & \gamma > \frac{1}{4} \quad \text{or} \quad \gamma = c_1 = \frac{1}{4}, \\ p = 2 \quad \text{iff} \quad & \{\gamma > \frac{1}{4}, (\gamma - \frac{1}{2})(\gamma - c_1) = 0\} \quad \text{or} \\ & \{\gamma = c_1 = \frac{1}{4}, \beta_1 c_1^2 + \beta_2 c_2^2 = 5/16\}, \end{aligned}$$

and that the order 1 result also holds on $S(\alpha, \beta)$ with $\alpha > 0$.

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