

ON THE ALGEBRAIC EQUATIONS IN IMPLICIT RUNGE-KUTTA METHODS*

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Abstract. This paper is concerned with the system of (nonlinear) algebraic equations which arise in the application of implicit Runge-Kutta methods to stiff initial value problems. Without making the classical assumption that the stepsize $h > 0$ is small, we derive transparent conditions on the method that guarantee existence and uniqueness of solutions to the equations. Besides, we discuss the sensitivity of the Runge-Kutta procedure with respect to perturbations in the algebraic equations.

Key words. numerical analysis, stiff initial value problems, implicit Runge-Kutta methods, nonlinear algebraic equations, stability

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1. Introduction. We shall deal with the numerical solution of the system of n ordinary differential equations

$$(1.1) \quad \frac{d}{dt} U(t) = f(t, U(t)) \quad (t \geq t_0),$$

under an initial condition $U(t_0) = u_0$. Here $t_0 \in \mathbb{R}$, $u_0 \in \mathbb{K}^n$ and $f: \mathbb{R} \times \mathbb{K}^n \rightarrow \mathbb{K}^n$ is a given continuous function. To cope simultaneously with real and with complex differential equations, the set \mathbb{K} will stand consistently for either \mathbb{R} or \mathbb{C} . Further, $\langle \cdot, \cdot \rangle$ is an arbitrary inner product on \mathbb{K}^n , and $|\xi| = \langle \xi, \xi \rangle^{1/2}$ (for $\xi \in \mathbb{K}^n$).

In order to introduce the problem treated in this article we assume

$$(1.2) \quad \operatorname{Re} \langle f(t, \tilde{\xi}) - f(t, \xi), \tilde{\xi} - \xi \rangle \leq 0 \quad (\text{for all } t \in \mathbb{R} \text{ and } \tilde{\xi}, \xi \in \mathbb{K}^n).$$

This condition implies (cf. e.g. [9]) that for any two solutions U, \tilde{U} to (1.1) the norm $|\tilde{U}(t) - U(t)|$ does not increase when t increases.

Let $h > 0$ denote a stepsize and $t_k = t_{k-1} + h$ ($k = 1, 2, 3, \dots$). Using an implicit Runge-Kutta method, approximations u_k to $U(t_k)$ are computed (for $k \geq 1$) by

$$(1.3a) \quad u_k = u_{k-1} + h \sum_{i=1}^m b_i f(t_{k-1} + c_i h, y_i),$$

$$(1.3b) \quad y_i = u_{k-1} + h \sum_{j=1}^m a_{ij} f(t_{k-1} + c_j h, y_j) \quad (1 \leq i \leq m).$$

Here $m \geq 1$ and a_{ij}, b_j are real parameters, $c_i = a_{i1} + a_{i2} + \dots + a_{im}$. We define the $m \times m$ matrices $A = (a_{ij})$, $B = \operatorname{diag}(b_1, b_2, \dots, b_m)$ and the vector $b = (b_1, b_2, \dots, b_m)^T \in \mathbb{R}^m$.

During these last years *algebraically stable* Runge-Kutta methods have gained much interest. These methods can be characterized by the property that B is positive

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definite while $(BA + A^T B - bb^T)$ is positive semidefinite. In [1], [4] this property was shown to imply the important *contractivity* relation

$$|\tilde{u}_k - u_k| \leq |\tilde{u}_{k-1} - u_{k-1}| \quad (k \geq 1),$$

for any two sequences $\{u_k\}, \{\tilde{u}_k\}$ computed from (1.3) with the same arbitrary stepsize $h > 0$. However, algebraic stability does not guarantee that the system of algebraic equations (1.3b) has a solution for arbitrary $h > 0$ (see [5]).

It was proved by Crouzeix (cf. [6], [5], [10]) that, whenever (1.2) is fulfilled and

(1.4) there is a positive definite diagonal matrix D such that $DA + A^T D$ is positive definite,

then the system (1.3b) does have a unique solution (for arbitrary $h > 0$). Some well-known algebraically stable methods satisfy (1.4) (the Gauss methods, the Radau IA and IIA methods, the 2-stage Lobatto IIC method—see [13]). But, e.g., the 3-stage Lobatto IIC method is known to violate (1.4) (see [13], [10], [11], [12]).

The theory in the present paper provides a simple condition on A which is less restrictive than (1.4) and which still implies the existence of a unique solution to (1.3b) (for arbitrary $h > 0$). The 3-stage Lobatto IIC method fulfills this new condition.

In [2], [8], [3] contractivity (and stability) relations were derived under assumptions on f that are more general than assumption (1.2). Our main theorem on the existence of solutions to (1.3b) will also cope with f satisfying such generalized assumptions.

An important tool in obtaining our existence and unicity results consists in a study of the sensitivity of the solution of the algebraic equations with respect to (so-called internal) perturbations. As a by-product we thus shall obtain generalizations of results on this sensitivity already given in [13], [10], [12].

In § 2 we shall state and discuss our main result (Theorem 2.1) on the existence and uniqueness of solutions to (1.3b). In § 3 we derive the material that is basic for the proof of Theorem 2.1. We also apply this material in a study of the sensitivity of u_k (see (1.3)) with respect to internal perturbations. The final § 4 contains the proof of Theorem 2.1.

Remark 1.1. The Runge-Kutta step (1.3) is often written in the form

$$(1.5a) \quad u_k = u_{k-1} + \sum_{i=1}^m b_i x_i,$$

$$(1.5b) \quad x_i = hf \left(t_{k-1} + c_i h, u_{k-1} + \sum_{j=1}^m a_{ij} x_j \right) \quad (i \leq i \leq m).$$

Our results on the existence of solutions to (1.3b) are also relevant to (1.5b), since (1.5b) has a unique solution iff (1.3b) has such a solution (see Lemma 4.1).

Remark 1.2. The results of this paper are also applicable to *general linear methods* (cf. [2]). The systems of algebraic equations arising in such methods are essentially of type (1.3b) (or (1.5b)).

2. Existence and uniqueness.

2.1. Formulation of the main theorem. Let α, β be given real constants. We consider the following three conditions on f, A and h .

(2.1) The function $f: \mathbb{R} \times \mathbb{K}^n \rightarrow \mathbb{K}^n$ is continuous, and
 $\operatorname{Re} \langle f(t, \tilde{\xi}) - f(t, \xi), \tilde{\xi} - \xi \rangle \leq \alpha |f(t, \tilde{\xi}) - f(t, \xi)|^2 + \beta |\tilde{\xi} - \xi|^2$
 (for all $t \in \mathbb{R}$ and $\xi, \tilde{\xi} \in \mathbb{K}^n$).

(2.2) There are real diagonal matrices $D = \operatorname{diag}(\delta_1, \delta_2, \dots, \delta_m)$,

$S = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_m)$ and $T = \text{diag}(\tau_1, \tau_2, \dots, \tau_m)$ such that the matrix $DA + A^T D - S - A^T T A$ is positive semidefinite

- (2.3) \mathcal{M}_1 and \mathcal{M}_2 are disjoint index sets with $\mathcal{M}_1 \cup \mathcal{M}_2 = \{1, 2, \dots, m\}$;
 $\delta_i \geq 0, \sigma_i - 2h^{-1}\alpha\delta_i \geq 0, \tau_i - 2h\beta\delta_i \geq 0$ (if $1 \leq i \leq m$);
 $\sigma_i - 2h^{-1}\alpha\delta_i > 0$ if either $i \in \mathcal{M}_1$ or ($i \in \mathcal{M}_2$ and $\alpha\delta_i \neq 0$);
 $\tau_i - 2h\beta\delta_i > 0$ if either $i \in \mathcal{M}_2$ or ($i \in \mathcal{M}_1$ and $\beta\delta_i \neq 0$).

THEOREM 2.1. *Assume (2.1), (2.2), (2.3). Then the system (1.3b) has a unique solution $y_1, y_2, \dots, y_m \in \mathbb{K}^n$.*

We note that the index sets occurring in condition (2.3) are allowed to be empty. Condition (2.1) on f is a generalization of the well-known one-sided Lipschitz condition (where $\alpha = 0$, see e.g. [1], [7], [13]) and of the circle condition in [9] (where $\beta = 0$). It was also used in [17], [8].

If $\alpha \geq 0$, then there exist functions f satisfying (2.1) with arbitrarily large Lipschitz constants. It follows that initial value problems (1.1) are covered that can be arbitrarily stiff.

We conclude this section with a lemma which gives some more insight into condition (2.1) and which simplifies the application of the main Theorem 2.1. For given $\alpha, \beta \in \mathbb{R}$ we denote the class of functions f satisfying (2.1) by $\mathcal{F}(\alpha, \beta)$.

LEMMA 2.2. *Let $\alpha, \beta \in \mathbb{R}$.*

(a) *Suppose $\beta_1 \in \mathbb{R}, \beta_1 > \beta$ and $\alpha \neq 0$. Then there exists a number $\alpha_1 < \alpha$ such that $\mathcal{F}(\alpha, \beta) \subset \mathcal{F}(\alpha_1, \beta_1)$.*

(b) *Suppose $\alpha_1 \in \mathbb{R}, \alpha_1 > \alpha$ and $\beta \neq 0$. Then there exists a number $\beta_1 < \beta$ such that $\mathcal{F}(\alpha, \beta) \subset \mathcal{F}(\alpha_1, \beta_1)$.*

Proof. We shall only prove part (a) of this lemma. A proof of part (b) can be given along the same lines. Suppose first $\alpha < 0$ and $\beta_1 > \beta$. Let $f \in \mathcal{F}(\alpha, \beta)$, and let $t \in \mathbb{R}, \tilde{\xi}, \xi \in \mathbb{K}^n$ be arbitrary. Put $v = \tilde{\xi} - \xi, w = f(t, \tilde{\xi}) - f(t, \xi)$. We have

$$\text{Re} \langle v, w \rangle \leq \alpha |w|^2 + \beta |v|^2.$$

Using the Schwarz inequality it follows that

$$\alpha |w|^2 + \beta |v|^2 + |w||v| \geq 0.$$

Hence there is a $\gamma_0 > 0$ (only depending on α and β) such that

$$|w|^2 \leq \gamma_0 |v|^2.$$

Take $\alpha_1 < \alpha$ such that $(\beta_1 - \beta) / (\alpha - \alpha_1) \geq \gamma_0$. We then have

$$\alpha |w|^2 + \beta |v|^2 \leq \alpha_1 |w|^2 + \beta_1 |v|^2,$$

from which it is easily seen that $f \in \mathcal{F}(\alpha_1, \beta_1)$.

We now consider the case where $\alpha > 0, \beta_1 > \beta$. For any $\alpha_1 \in (\frac{1}{2}\alpha, \alpha)$ and $v, w \in \mathbb{K}^n$ satisfying

$$\text{Re} \langle v, w \rangle > \alpha_1 |w|^2 + \beta_1 |v|^2,$$

we have

$$|v||w| > \frac{1}{2}\alpha |w|^2 + \beta_1 |v|^2.$$

It follows that there is a constant $\gamma_1 > 0$ (only depending on α and β_1) such that

$$|w|^2 \leq \gamma_1 |v|^2.$$

Take $\alpha_1 \in (\frac{1}{2}\alpha, \alpha)$ such that $(\beta_1 - \beta) / (\alpha - \alpha_1) \geq \gamma_1$. Assume $f \in \mathcal{F}(\alpha, \beta)$ but $f \notin \mathcal{F}(\alpha_1, \beta_1)$. Then we know there are $t \in \mathbb{R}$ and $\tilde{\xi}, \xi \in \mathbb{K}^n$ such that

$$\alpha_1 |w|^2 + \beta_1 |v|^2 < \text{Re} \langle v, w \rangle \leq \alpha |w|^2 + \beta |v|^2,$$

and

$$|w|^2 \leq [(\beta_1 - \beta)/(\alpha - \alpha_1)]|v|^2$$

with $v = \tilde{\xi} - \xi$, $w = f(t, \tilde{\xi}) - f(t, \xi)$. This yields a contradiction. \square

2.2. Application of the main theorem. From Theorem 2.1 one easily obtains

COROLLARY 2.3. *Assume $f: \mathbb{R} \times \mathbb{K}^n \rightarrow \mathbb{K}^n$ is continuous and satisfies (1.2). Suppose (2.2) holds with*

$$\delta_i \geq 0, \quad \sigma_i \geq 0, \quad \tau_i \geq 0, \quad \sigma_i + \tau_i > 0 \quad (\text{for } 1 \leq i \leq m).$$

Then (1.3b) has a unique solution.

When $\tau_i = 0$ ($1 \leq i \leq m$), the corollary is proved by applying Theorem 2.1 with $\mathcal{M}_1 = \{1, 2, \dots, m\}$, $\mathcal{M}_2 = \emptyset$, and when $\sigma_i = 0$ ($1 \leq i \leq m$) it is proved with $\mathcal{M}_1 = \emptyset$, $\mathcal{M}_2 = \{1, 2, \dots, m\}$. In the general case one can choose $\mathcal{M}_1 = \{i \mid \sigma_i > 0\}$, $\mathcal{M}_2 = \{i \mid \sigma_i = 0 \text{ and } \tau_i > 0\}$.

The above corollary is a generalization of [6, Thm. 5.4], [5, Thm. 1] and [10, Lem. 4.2], where (1.4) was required. Condition (1.4) implies that the assumption on (2.2) in the corollary is fulfilled (with $\tau_i = 0$). On the other hand, (2.2) can be fulfilled with $\delta_i \geq 0$, $\sigma_i \geq 0$, $\tau_i \geq 0$, $\sigma_i + \tau_i > 0$ while (1.4) is violated. An example of this situation is provided by the 3-stage Lobatto IIIC method referred to in the Introduction (see also § 2.3).

COROLLARY 2.4. *Let $h > 0$ and $\alpha, \beta \in \mathbb{R}$ be given. Suppose $\kappa, \lambda \in \mathbb{R}$ and $D = \text{diag}(\delta_1, \delta_2, \dots, \delta_m)$ are such that the matrix*

$$DA + A^T D - \kappa D - \lambda A^T DA$$

is positive semidefinite. Assume further $\delta_i > 0$ ($1 \leq i \leq m$), $2\alpha h^{-1} \leq \kappa$, $2\beta h \leq \lambda$ and $2\alpha h^{-1} + 2\beta h < \kappa + \lambda$. Then (1.3b) has a unique solution whenever f satisfies (2.1).

Proof. For the cases [$2\alpha h^{-1} \leq \kappa$, $2\beta h < \lambda$, $\alpha \neq 0$] and [$2\alpha h^{-1} < \kappa$, $2\beta h \leq \lambda$, $\beta \neq 0$] the proof easily follows by combining Theorem 2.1 and Lemma 2.2. If [$2\alpha h^{-1} \leq \kappa$, $2\beta h < \lambda$, $\alpha = 0$], Theorem 2.1 can be applied directly with $\mathcal{M}_1 = \emptyset$, and if [$2\alpha h^{-1} < \kappa$, $2\beta h \leq \lambda$, $\beta = 0$], we take $\mathcal{M}_2 = \emptyset$ in Theorem 2.1. \square

We note that if $\alpha = \kappa = 0$, the content of the above corollary reduces to a theorem formulated in [15, Thm. 4.3.1]. The latter theorem in its turn generalizes results on the system (1.3b) formulated in [12, Thms. 5.3.9, 5.3.12].

2.3. Examples.

Example 2.5. The algebraically stable, 3-stage Lobatto IIIC method is given by

$$A = \begin{pmatrix} 1/6 & -1/3 & 1/6 \\ 1/6 & 5/12 & -1/12 \\ 1/6 & 2/3 & 1/6 \end{pmatrix}, \quad b = \begin{pmatrix} 1/6 \\ 2/3 \\ 1/6 \end{pmatrix}.$$

Condition (1.4) is not fulfilled (see e.g. [13]). However, with the choice $\delta_1 = 1$, $\delta_2 = 4$, $\delta_3 = 1$, $\tau_1 = 2$, $\sigma_2 = 2$, $\tau_3 = 2$ and the other τ_i, σ_i equal to zero, condition (2.2) is fulfilled. From Corollary 2.3 we thus see that (1.3b) always has a unique solution when f is continuous and satisfies (1.2).

We note that this Runge-Kutta method does not satisfy (2.2) with any $\delta_i \geq 0$, $\sigma_i > 0$, $\tau_i = 0$ ($1 \leq i \leq m$) or with $\delta_i \geq 0$, $\sigma_i = 0$, $\tau_i > 0$ ($1 \leq i \leq m$).

Example 2.6. Consider an arbitrary method that is algebraically stable. Applying Corollary 2.4 with $\kappa = \lambda = 0$, it follows that (1.3b) has a unique solution whenever f satisfies (2.1) with some $\alpha \leq 0$, $\beta \leq 0$, $\alpha + \beta < 0$ (which is a bit stronger than (1.2)). This result provides an extension of [6, Remark 5.7], [5, Cor. and Remark 3, p. 90].

Example 2.7. Consider a method satisfying (1.4). From Corollary 2.4 it can be seen that there exist $\kappa_0, \lambda_0 > 0$ such that (1.3b) has a unique solution for any $h > 0$ and f satisfying (2.1) with $\alpha h^{-1} \leq \kappa_0$ and $\beta h \leq \lambda_0$. This generalizes a related result on the system (1.3b) formulated in [12, Thms. 5.3.9, 5.3.12] where $\alpha = 0$ is assumed.

3. Stability with respect to internal perturbations.

3.1. Notation. For given column vectors $x_1, x_2, \dots, x_m \in \mathbb{K}^n$ we denote the column vector $(x_1^T, x_2^T, \dots, x_m^T)^T \in \mathbb{K}^{nm}$ by $[x_i]$. On the space \mathbb{K}^{nm} we deal with the norm

$$\|x\| = (|x_1|^2 + |x_2|^2 + \dots + |x_m|^2)^{1/2}$$

for $x = [x_i] \in \mathbb{K}^{nm}$, where $|\cdot|$ denotes the norm of § 1. For any linear mapping L from \mathbb{K}^{nm} into \mathbb{K}^{nm} we define $\|L\| = \sup \{\|Lx\| : x \in \mathbb{K}^{nm} \text{ with } \|x\| = 1\}$.

\mathcal{M}_1 and \mathcal{M}_2 are disjoint sets with $\mathcal{M}_1 \cup \mathcal{M}_2 = \{1, 2, \dots, m\}$, and the projections $I_j : \mathbb{K}^{nm} \rightarrow \mathbb{K}^{nm}$ (for $j = 1, 2$) are defined by $I_j x = y$ for $x = [x_i]$ with $y = [y_i]$ given by

$$y_i = x_i \quad (\text{when } i \in \mathcal{M}_j), \quad y_i = 0 \quad (\text{when } i \notin \mathcal{M}_j).$$

Let $u_{k-1} \in \mathbb{K}^n$, $h > 0$ and t_{k-1} be given. We define the functions $f_i : \mathbb{K}^n \rightarrow \mathbb{K}^n$ ($1 \leq i \leq m$) and $F : \mathbb{K}^{nm} \rightarrow \mathbb{K}^{nm}$ by

$$f_i(\xi) = hf(t_{k-1} + c_i h, u_{k-1} + \xi) \quad (\text{for } \xi \in \mathbb{K}^n),$$

$$Fx = [f_i(x_i)] \quad (\text{for } x = [x_i] \in \mathbb{K}^{nm}).$$

Further we define $H : \mathbb{K}^{nm} \rightarrow \mathbb{K}^{nm}$ by $Hx = [h_i(z)]$ (for $z = [z_i] \in \mathbb{K}^{nm}$) with

$$h_i(z) = z_i - \sum_{j \in \mathcal{M}_1} a_{ij} f_j(z_j) - \sum_{j \in \mathcal{M}_2} a_{ij} z_j \quad (\text{if } i \in \mathcal{M}_1),$$

$$h_i(z) = z_i - f_i \left(\sum_{j \in \mathcal{M}_1} a_{ij} f_j(z_j) + \sum_{j \in \mathcal{M}_2} a_{ij} z_j \right) \quad (\text{if } i \in \mathcal{M}_2).$$

The $n \times n$ identity matrix is denoted by $I^{(n)}$ and the Kronecker product by \otimes . We define

$$\mathbf{b} = b \otimes I^{(n)}, \quad \mathbf{A} = A \otimes I^{(n)}, \quad \mathbf{a}_i = a_i \otimes I^{(n)}.$$

Here b, A are as in § 1, and a_i^T denotes the i th row of the matrix A (for $1 \leq i \leq m$).

We define the mappings (from \mathbb{K}^{nm} to \mathbb{K}^{nm})

$$F_j = I_j F, \quad H_j = I_j H, \quad A_j = I_j A \quad (\text{for } j = 1, 2).$$

Remark that, with $I = I_1 + I_2$ denoting the $nm \times nm$ identity mapping, we have

$$(3.1) \quad H = I - (I_1 + F_2)A(F_1 + I_2).$$

3.2. Runge-Kutta methods with internal perturbations. The main purpose of this subsection is a discussion of the following four equalities and of their relations to the Runge-Kutta method (1.3).

$$(3.2) \quad y - \mathbf{A}Fy = p,$$

$$(3.3) \quad x - \mathbf{F}Ax = q,$$

$$(3.4) \quad Hz = r,$$

$$(3.5) \quad y - \mathbf{A}x = s, \quad x - Fy = t.$$

LEMMA 3.1.

(a) (3.2) implies (3.4) with

$$z = (I_1 + F_2)y, \quad r = I_1 p + (F_2 y - F_2(y - p));$$

(3.4) implies (3.2) with

$$y = [I_1 + \mathbf{A}_2(F_1 + I_2)]z, \quad p = (I_1 + \mathbf{A}I_2)r.$$

(b) (3.3) implies (3.4) with

$$z = (\mathbf{A}_1 + I_2)x, \quad r = (\mathbf{A}_1I_1 + I_2)q + (F_2\mathbf{A}x - F_2\mathbf{A}(x - I_1q));$$

(3.4) implies (3.3) with

$$x = (F_1 + I_2)z, \quad q = (F_1z - F_1(z - r)) + I_2r.$$

(c) (3.5) implies (3.4) with

$$z = I_1y + I_2x, \quad r = I_1s + (\mathbf{A}_1I_1 + I_2)t + (F_2y - F_2(y - s - \mathbf{A}I_1t));$$

(3.4) implies (3.5) with

$$x = (F_1 + I_2)z, \quad y = I_1z + \mathbf{A}_2x, \quad s = I_1r, \quad t = I_2r.$$

Using (3.1) the proof of this lemma is straightforward, and we omit it.

With the notation of § 3.1 we can rewrite the Runge-Kutta step (1.3) as

$$(3.6) \quad u_k = u_{k-1} + \mathbf{b}^T Fy, \quad y - \mathbf{A}Fy = 0,$$

and (1.5) can be written in the form

$$(3.7) \quad u_k = u_{k-1} + \mathbf{b}^T x, \quad x - \mathbf{F}\mathbf{A}x = 0.$$

Applying Lemma 3.1 (with $p = q = r = 0$), we see that both (3.6) and (3.7) are equivalent to the following formulation of the Runge-Kutta method,

$$(3.8) \quad u_k = u_{k-1} + \mathbf{b}^T (F_1 + I_2)z, \quad Hz = 0.$$

If any numerical procedure is applied to solve the equation $H\tilde{z} = 0$, we obtain, in general, only an approximation, say \tilde{z} , to the true z . Denoting the corresponding numerical approximation to u_k by \tilde{u}_k we thus have

$$(3.9a) \quad \tilde{u}_k = u_{k-1} + \mathbf{b}^T (F_1 + I_2)\tilde{z},$$

$$(3.9b) \quad H\tilde{z} = r$$

with a residual vector $r \in \mathbb{K}^{nm}$, $r \approx 0$. We note that the relations (3.9) with $(\mathcal{M}_1 = \{1, 2, \dots, m\})$ and a different interpretation of the vector r also occur in the interesting investigations of B -consistency by Frank, Schneid and Ueberhuber (cf. [13], [14]). We call the components $r_i \in \mathbb{K}^n$ of $r = [r_i] \in \mathbb{K}^{nm}$ *internal perturbations* in the Runge-Kutta step (3.8).

A question of great practical and theoretical importance is whether $\|\tilde{z} - z\|$ and $|\tilde{u}_k - u_k|$ are small (uniformly for all f satisfying (2.1)) whenever $\|r\|$ is small (cf. (3.8), (3.9)). The results of § 3.3 are relevant to this question for $\|\tilde{z} - z\|$, and those of § 3.4 for $|\tilde{u}_k - u_k|$.

In practice one usually computes u_k from (3.6) or from (3.7). These cases are covered by our considerations since (3.8), (3.9) reduce to (3.6), (3.16) when $\mathcal{M}_1 = \{1, 2, \dots, m\}$, while (3.8), (3.9) reduce to (3.7), (3.17) when $\mathcal{M}_2 = \{1, 2, \dots, m\}$.

3.3. Internal stability. We shall investigate, for arbitrary z , $\tilde{z} \in \mathbb{K}^{nm}$, the sensitivity of $\tilde{z} - z$ with respect to $H\tilde{z} - Hz$, where the latter difference can be interpreted as the difference between two (different) internal perturbations (cf. (3.9b)). The results we obtain are basic for the proof in § 4 of Theorem 2.1.

Let z, \tilde{z} be arbitrary vectors in \mathbb{K}^{nm} . In view of Lemma 3.1(c) we define

$$(3.10) \quad \begin{aligned} x &= (F_1 + I_2)z, & y &= I_1z + A_2x, \\ \tilde{x} &= (F_1 + I_2)\tilde{z}, & \tilde{y} &= I_1\tilde{z} + A_2\tilde{x}. \end{aligned}$$

LEMMA 3.2. Assume (2.1), (2.2), (2.3). Then there is a constant γ_0 (only depending on $D, S, T, h^{-1}\alpha, h\beta$) such that

$$\|I_1(\tilde{x} - x)\| + \|I_2(\tilde{y} - y)\| \leq \gamma_0 \|H\tilde{z} - Hz\|$$

whenever $z, \tilde{z} \in \mathbb{K}^{nm}$ and $x, \tilde{x}, y, \tilde{y}$ are defined by (3.10).

Proof. We define $u = [u_i], v = [v_i], w = [w_i], p = [p_i], q = [q_i] \in \mathbb{K}^{nm}$ by

$$\begin{aligned} u &= \tilde{x} - x, & v &= \tilde{y} - y, & w &= F\tilde{y} - Fy, \\ p &= I_1(H\tilde{z} - Hz), & q &= I_2(H\tilde{z} - Hz). \end{aligned}$$

By the last part of Lemma 3.1 we thus have

$$(3.11) \quad v - Au = p, \quad u - w = q.$$

From (2.1) it follows that

$$\operatorname{Re} \langle v_i, w_i \rangle \leq \bar{\alpha} |w_i|^2 + \bar{\beta} |v_i|^2$$

where $\bar{\alpha} = h^{-1}\alpha, \bar{\beta} = h\beta$. Substituting $v_i = \mathbf{a}_i^T u + p_i, w_i = u_i - q_i$ (cf. (3.11)) in this inequality and using $\langle p_i, q_i \rangle = 0$, we obtain

$$\operatorname{Re} \langle \mathbf{a}_i^T u, u_i \rangle - \bar{\alpha} |u_i|^2 - \bar{\beta} |\mathbf{a}_i^T u|^2 \leq \operatorname{Re} \langle u_i, -p_i - 2\bar{\alpha}q_i \rangle + \operatorname{Re} \langle \mathbf{a}_i^T u, q_i + 2\bar{\beta}p_i \rangle + \bar{\beta} |p_i|^2 + \bar{\alpha} |q_i|^2.$$

From (2.2) and Lemma 2.2 in [7] it can be seen that

$$\sum_{i=1}^m 2\delta_i \operatorname{Re} \langle \mathbf{a}_i^T u, u_i \rangle \geq \sum_{i=1}^m \sigma_i |u_i|^2 + \sum_{i=1}^m \tau_i |\mathbf{a}_i^T u|^2.$$

A combination of the last two inequalities yields

$$(3.12) \quad \begin{aligned} &\sum_{i=1}^m \left(\frac{1}{2} \sigma_i - \bar{\alpha} \delta_i \right) |u_i|^2 + \sum_{i=1}^m \left(\frac{1}{2} \tau_i - \bar{\beta} \delta_i \right) |\mathbf{a}_i^T u|^2 \\ &\leq \sum_{i=1}^m \delta_i \{ |u_i| \cdot |p_i + 2\bar{\alpha}q_i| + |\mathbf{a}_i^T u| \cdot |q_i + 2\bar{\beta}p_i| + \bar{\beta} |p_i|^2 + \bar{\alpha} |q_i|^2 \}. \end{aligned}$$

Let $\xi, \eta, \lambda, \mu \in \mathbb{R}^m$ be column-vectors with components $\xi_i = (\frac{1}{2}\sigma_i - \bar{\alpha}\delta_i)^{1/2} |u_i|, \eta_i = (\frac{1}{2}\tau_i - \bar{\beta}\delta_i)^{1/2} |\mathbf{a}_i^T u|, \lambda_i = (\frac{1}{2}\sigma_i - \bar{\alpha}\delta_i)^{-1/2} \delta_i |p_i + 2\bar{\alpha}q_i|, \mu_i = (\frac{1}{2}\tau_i - \bar{\beta}\delta_i)^{-1/2} \delta_i |q_i + 2\bar{\beta}p_i|$ ($1 \leq i \leq m$) (we use the convention $0^{-1/2} = 0$). Putting

$$\varepsilon = \sum_{i=1}^m \delta_i \{ \bar{\beta} |p_i|^2 + \bar{\alpha} |q_i|^2 \},$$

we see from (2.3) that (3.12) is equivalent to

$$\xi^T \xi + \eta^T \eta \leq \xi^T \lambda + \eta^T \mu + \varepsilon.$$

After an application of Schwarz's inequality a little calculation shows that

$$(\xi^T \xi + \eta^T \eta)^{1/2} \leq \frac{1}{2} (\lambda^T \lambda + \mu^T \mu)^{1/2} + \frac{1}{2} (\lambda^T \lambda + \mu^T \mu + 4\varepsilon)^{1/2}.$$

Hence

$$(3.13) \quad \sum_{i=1}^m (\sigma_i - 2\bar{\alpha}\delta_i) |u_i|^2 + \sum_{i=1}^m (\tau_i - 2\bar{\beta}\delta_i) |\mathbf{a}_i^T u|^2 \leq \gamma_1 \sum_{i=1}^m |h_i(\tilde{z}) - h_i(z)|^2$$

with a constant γ_1 only depending on the parameters $\delta_i, \sigma_i, \tau_i, \bar{\alpha}, \bar{\beta}$.

The proof is completed by applying (2.3) and substituting $\mathbf{a}_i^T u = v_i$ (for $i \in \mathcal{M}_2$; see (3.11)) into (3.13). \square

Using the above lemma we shall prove the following theorem, which is the main result of this section.

THEOREM 3.3. *Assume (2.1), (2.2), (2.3). Then there exists a function $\phi : \mathbb{K}^{nm} \times [0, \infty) \rightarrow [0, \infty)$ with the properties*

- (i) $\phi(z; \cdot)$ is isotone on $[0, \infty)$ (for each $z \in \mathbb{K}^{nm}$),
- (ii) $\phi(z; \rho) \rightarrow \phi(z; 0) = 0$ (as $\rho \rightarrow 0+$; for each $z \in \mathbb{K}^{nm}$),
- (iii) $\|\tilde{z} - z\| \leq \phi(z; \|H\tilde{z} - Hz\|)$ (for all $z, \tilde{z} \in \mathbb{K}^{nm}$).

Moreover, if $\mathcal{M}_2 = \emptyset$, then (i), (ii) and (iii) hold with $\phi(z, \rho) \equiv \gamma\rho$ where γ is a constant only depending on $A, h^{-1}\alpha, h\beta$ (and not on z, f or the dimension n).

Proof. Let $z, \tilde{z} \in \mathbb{K}^{nm}$ be given. Defining u, v, w, p, q as in the proof of Lemma 3.2, we have the representation

$$\tilde{z} - z = I_1 v + I_2 u.$$

From (3.11) and Lemma 3.2 we obtain

$$\|I_2 u\| \leq \|q\| + \|F_2 \tilde{y} - F_2 y\| \leq \|q\| + \psi(z; \gamma_0 \|H\tilde{z} - Hz\|)$$

where

$$(3.14) \quad \psi(z; \rho) = \sup \{ \|F_2(y + e) - F_2 y\| : e \in \mathbb{K}^{nm} \text{ with } \|I_2 e\| \leq \rho \},$$

$$y = I_1 z + A_2(F_1 + I_2)z.$$

Using (3.11) and Lemma 3.2 once more, we thus obtain

$$\begin{aligned} \|I_1 v\| &\leq \|p\| + \|A_1 I_1\| \cdot \|I_1 u\| + \|A_1 I_2\| \cdot \|I_2 u\| \\ &\leq \|p\| + \|A_1 I_1\| \cdot \gamma_0 \cdot \|H\tilde{z} - Hz\| + \|A_1 I_2\| \{ \|q\| + \psi(z; \gamma_0 \|H\tilde{z} - Hz\|) \}. \end{aligned}$$

It follows that property (iii) holds with

$$(3.15) \quad \phi(z; \rho) = (2 + \|A_1 I_2\| + \gamma_0 \|A_1 I_1\|)\rho + (1 + \|A_1 I_2\|)\psi(z; \gamma_0 \rho).$$

The remaining properties stated in the theorem follow from the continuity of f (see (2.1)) and from the fact that for any $m \times m$ matrix M the norm $\|M \otimes I^{(n)}\|$ is independent of n (which can be proved e.g. by using Lemma 2.2 in [7]). \square

If $\mathcal{M}_2 \neq \emptyset$ the function ϕ defined by (3.15) depends through ψ on the (local) Lipschitz constant of f . If $\alpha \geq 0$ this Lipschitz constant can be arbitrarily large. In this case the upper bound on $\|\tilde{z} - z\|$ provided by the theorem thus only holds for the particular function f under consideration, and not uniformly for all f satisfying (2.1).

We note that when $\mathcal{M}_2 = \emptyset$ and $\alpha = 0$, the content of Theorem 3.3 is similar to the (so-called BSI-stability) results formulated in [13, Thm. 4.1, Cor. 4.1], [12, Thm. 5.3.7].

3.4. External stability. We deal with the effect of the internal perturbation r on the difference $\tilde{u}_k - u_k$ where u_k, \tilde{u}_k satisfy (3.8), (3.9). The following theorem provides a condition under which a bound for $|\tilde{u}_k - u_k|$ in terms of $\|r\|$ holds uniformly for all f satisfying (2.1). This condition can be fulfilled in cases where no analogous uniform bound holds for $\|\tilde{z} - z\|$.

THEOREM 3.4. *Assume (2.1), (2.2), (2.3). Suppose there exist real d_j (for $j \in \mathcal{M}_2$) such that*

$$b_i = \sum_{j \in \mathcal{M}_2} d_j a_{ji} \quad (\text{for all } i \in \mathcal{M}_2).$$

Then there is a constant γ only depending on $A, b, h^{-1}\alpha, h\beta$ (and not on u_{k-1}, z, f or the dimension n) such that

$$|\tilde{u}_k - u_k| \leq \gamma \|r\|$$

whenever u_k, \tilde{u}_k, r satisfy (3.8), (3.9).

Proof. We define

$$d_i = b_i - \sum_{j \in \mathcal{M}_2} d_j a_{ji} \quad (\text{for all } i \in \mathcal{M}_1),$$

and

$$d = (d_1, d_2, \dots, d_m)^T, \quad \mathbf{d} = d \otimes I^{(n)}.$$

One easily verifies that, with these definitions,

$$\mathbf{b}^T = \mathbf{d}^T I_1 + \mathbf{d}^T A_2.$$

From (3.8), (3.9) it follows that

$$\tilde{u}_k - u_k = [\mathbf{d}^T I_1 + \mathbf{d}^T A_2][(F_1 \tilde{z} - F_1 z) + I_2(\tilde{z} - z)].$$

Defining $x, \tilde{x}, y, \tilde{y}$ by (3.10) we have

$$F_1 \tilde{z} - F_1 z = I_1(\tilde{x} - x), \quad A_2[(F_1 \tilde{z} - F_1 z) + I_2(\tilde{z} - z)] = A_2(\tilde{x} - x) = I_2(\tilde{y} - y).$$

Consequently

$$\tilde{u}_k - u_k = \mathbf{d}^T [I_1(\tilde{x} - x) + I_2(\tilde{y} - y)].$$

An application of Lemma 3.2 completes the proof. \square

In order to formulate some interesting corollaries to the above theorem, we define for any index set $\mathcal{N} \subset \{1, 2, \dots, m\}$ the $m \times m$ matrix $A(\mathcal{N})$ by

$$A(\mathcal{N}) = (c_{ij}), \quad c_{ij} = a_{ij} \quad (\text{if } i \in \mathcal{N}, j \in \mathcal{N}), \quad c_{ij} = \delta_{ij} \quad (\text{otherwise}),$$

where δ_{ij} denotes the Kronecker delta.

COROLLARY 3.5. *Suppose (2.2) holds with*

$$\delta_i \geq 0, \quad \sigma_i \geq 0, \quad \tau_i \geq 0, \quad \sigma_i + \tau_i > 0 \quad (\text{for } 1 \leq i \leq m).$$

Let $\mathcal{M}_1, \mathcal{M}_2$ be disjoint, $\mathcal{M}_1 \cup \mathcal{M}_2 = \{1, 2, \dots, m\}$, with

$$\{i \mid \sigma_i = 0\} \subset \mathcal{M}_2 \subset \{i \mid \tau_i > 0\},$$

and $\text{Rank}[A(\mathcal{M}_2)^T, b] = \text{Rank}[A(\mathcal{M}_2)^T]$. Then there is a constant γ (only depending on A, b) such that

$$|\tilde{u}_k - u_k| \leq \gamma \|r\|,$$

whenever u_k, \tilde{u}_k, r satisfy (3.8), (3.9) and the continuous $f: \mathbb{R} \times \mathbb{K}^n \rightarrow \mathbb{K}^n$ fulfills (1.2).

This corollary completes some results on external stability for $\mathcal{M}_1 = \{1, 2, \dots, m\}$ derived under assumptions (1.4), (1.2) in [10, Cor. 4.3].

COROLLARY 3.6. *Let $h > 0$ and $\alpha, \beta, \kappa, \lambda \in \mathbb{R}$ be given numbers, $D = \text{diag}(\delta_1, \delta_2, \dots, \delta_m)$, and let $\mathcal{M}_1, \mathcal{M}_2$ be disjoint index sets with $\mathcal{M}_1 \cup \mathcal{M}_2 = \{1, 2, \dots, m\}$. Assume the following four conditions hold.*

- (i) $DA + A^T D - \kappa D - \lambda A^T D A$ is positive semidefinite;
- (ii) $\delta_i > 0$ ($1 \leq i \leq m$), $2\alpha h^{-1} \leq \kappa$, $2\beta h \leq \lambda$, $2\alpha h^{-1} + 2\beta h < \kappa + \lambda$;
- (iii) $\text{Rank}[A(\mathcal{M}_2)^T, b] = \text{Rank}[A(\mathcal{M}_2)^T]$;
- (iv) if $\alpha = \kappa = 0$ then either $\mathcal{M}_1 = \emptyset$ or A is regular.

Then there is a constant γ (only depending on $A, b, \alpha h^{-1}$ and βh) such that

$$|\tilde{u}_k - u_k| \leq \gamma \|r\|$$

whenever \tilde{u}_k, u_k, r satisfy (3.8), (3.9) and f fulfills (2.1).

Proof. By applying Lemma 2.2 to the function hf , the proof follows from Theorem 3.4 for the case $[2\alpha h^{-1} \leq \kappa, 2\beta h < \lambda, \alpha \neq 0]$.

If $[\alpha = \kappa = 0, 2\beta h < \lambda, \mathcal{M}_1 = \emptyset]$, Theorem 3.4 may be applied directly.

In case $[\alpha = \kappa = 0, 2\beta h < \lambda, A \text{ regular}]$ we take $S = \kappa_1 D, T = \lambda_1 D$ in (2.2) with $\lambda_1 \in (2\beta h, \lambda), \kappa_1 > \kappa$ and $\kappa_1 - \kappa$ sufficiently small. The assumptions of Theorem 3.4 are then fulfilled.

Similarly, if $[2\alpha h^{-1} < \kappa, 2\beta h \leq \lambda]$ we choose $S = \kappa_1 D, T = \lambda_1 D$ with $\kappa_1 \in (2\alpha h^{-1}, \kappa), \lambda_1 > \lambda$ and $\lambda_1 - \lambda$ sufficiently small. \square

Let the Runge-Kutta method (1.3) be *algebraically stable*. Consider along with (3.6), (3.7), the perturbed relations

$$(3.16) \quad \tilde{u}_k = u_{k-1} + \mathbf{b}^T F \tilde{y}, \quad \tilde{y} - \mathbf{A} F \tilde{y} = p,$$

$$(3.17) \quad \tilde{u}_k = u_{k-1} + \mathbf{b}^T \tilde{x}, \quad \tilde{x} - \mathbf{F} \mathbf{A} \tilde{x} = q,$$

respectively. For given $h > 0, \alpha \leq 0, \beta \leq 0, \alpha + \beta < 0$, Corollary 3.6 (with $\kappa = \lambda = 0$) proves the existence of a constant γ such that

$$(3.7), (3.17) \Rightarrow |\tilde{u}_k - u_k| \leq \gamma \|q\|$$

uniformly for all f satisfying (2.1) (note that $\text{Rank}[A^T, b] = \text{Rank}[A^T]$ since $x^T(A^T Bx) \geq \frac{1}{2}(x^T b)^2$ (for all $x \in \mathbb{R}^m$)). Under the same assumptions the corollary also proves the existence of a γ such that

$$(3.6), (3.16) \Rightarrow |\tilde{u}_k - u_k| \leq \gamma \|p\|$$

uniformly for all f satisfying (2.1), provided we assume additionally that

$$\alpha < 0, \text{ or } A \text{ is regular.}$$

We note that when $\alpha = 0$ this stability result for (3.16) also follows from [12, Thm. 5.3.7]. On the other hand, Corollary 3.6 implies the general bound for $|\tilde{u}_k - u_k|$ in terms of $\|p\|$ (cf. (3.6), (3.16)) that also follows from [12, Thm. 5.3.7].

3.5. Examples.

Example 3.7. Consider the 3-stage Labotto IIIC method (cf. Example 2.5) and let f satisfy (1.2). Choosing $\mathcal{M}_1 = \{2\}, \mathcal{M}_2 = \{1, 3\}$, it follows from Corollary 3.5 that

$$|\tilde{u}_k - u_k| \leq \gamma \cdot \|r\|$$

whenever (3.8), (3.9) hold. Here γ is independent of $h > 0$ and f . The formulation (3.8) of the Runge-Kutta step for which this stability result is valid, reads in full

$$(3.18a) \quad u_k = u_{k-1} + \frac{1}{6}(z_1 + 4f_2(z_2) + z_3),$$

$$z_1 = f_1(\frac{1}{6}(z_1 - 2f_2(z_2) + z_3)),$$

$$(3.18b) \quad z_2 = \frac{1}{12}(2z_1 + 5f_2(z_2) - z_3),$$

$$z_3 = f_3(\frac{1}{6}(z_1 + 4f_2(z_2) + z_3))$$

with $f_i(\xi) = hf(t_{k-1} + c_i h, u_{k-1} + \xi), c_0 = 0, c_1 = \frac{1}{2}, c_2 = 1$.

For $\|\tilde{z} - z\|$ there is no analogous upper bound valid in terms of $\|r\|$.

If we define \tilde{u}_k, \tilde{y} by (3.16), it can be proved that not only

$$\sup \{ \|\tilde{y} - y\| : p \in \mathbb{K}^{3n}, \|p\| \leq 1, f \text{ satisfies (1.2)} \} = \infty$$

(cf. [10, ex. 4.4], [12, ex. 5.9.2]), but also

$$\sup \{ |\tilde{u}_k - u_k| : p \in \mathbb{K}^{3n}, \|p\| \leq 1, f \text{ satisfies (1.2)} \} = \infty.$$

In practical applications the use of (3.18) thus seems to have an advantage over the use of (1.3). A small residual vector in the process (3.18) has generally a substantially smaller effect on the approximation to $U(t_k)$ than in the process (1.3).

Example 3.8. Consider an arbitrary method satisfying condition (1.4) (e.g. Gauss, Radau IA or IIA—see [13]).

Applying Corollary 3.6 it can be seen that, for any disjoint $\mathcal{M}_1, \mathcal{M}_2$ with $\mathcal{M}_1 \cup \mathcal{M}_2 = \{1, 2, \dots, m\}$, there exist $\kappa_0 > 0, \lambda_0 > 0, \gamma > 0$ such that

$$(3.8), (3.9) \Rightarrow |\tilde{u}_k - u_k| \leq \gamma \|r\|$$

uniformly for all $h > 0$ and f satisfying (2.1) with

$$\alpha h^{-1} \leq \kappa_0, \quad \beta h \leq \lambda_0.$$

In particular we thus have

$$(3.6), (3.16) \Rightarrow |\tilde{u}_k - u_k| \leq \gamma \|p\| \quad \text{and} \quad (3.7), (3.17) \Rightarrow |\tilde{u}_k - u_k| \leq \gamma \|q\|$$

uniformly for $h > 0$ and f as above. This completes a so-called BS-stability result on (3.6), (3.16) with $\alpha = 0$ given in [13, Thm. 4.1, Cor. 4.1], [12, Thm. 7.4.1].

It thus follows that a small residual, e.g. in the numerical solution of either (1.3b) or (1.5b), only slightly disturbs the corresponding u_k computed via (1.3a) or (1.5a), respectively (uniformly for $\alpha h^{-1} \leq \kappa_0, \beta h \leq \lambda_0$).

Example 3.9. We finally give a counterexample showing that assumption (iv) in Corollary 3.6 cannot be omitted.

Consider Euler's method ($m = 1, A = 0, b = 1$). The conditions (i), (ii), (iii) of the corollary are fulfilled with

$$\delta_1 = 1, \quad \kappa = 0, \quad \lambda = 1, \quad \alpha = 0, \quad \beta = 0, \quad h = 1, \quad \mathcal{M}_2 = \emptyset.$$

Applying (3.6), (3.16) with $u_{k-1} = 0, f(t, \xi) \equiv \mu \xi, \mu < 0$, we have

$$\tilde{u}_k - u_k = \mu p.$$

Letting $\mu \rightarrow -\infty$ we see that the conclusion of Corollary 3.6 is not valid.

4. The proof of Theorem 2.1. Theorem 2.1 is easily proved by using Lemma 4.1 and by a combination of Theorem 3.3 with the subsequent Lemma 4.2.

LEMMA 4.1. *Each of the following systems (4.1)–(4.4) has a unique solution iff any of the other systems has a unique solution.*

$$(4.1) \quad y - \mathbf{A}Fy = 0,$$

$$(4.2) \quad x - F\mathbf{A}x = 0,$$

$$(4.3) \quad Hz = 0,$$

$$(4.4) \quad y - \mathbf{A}x = 0, \quad x - Fy = 0.$$

Proof. Apply Lemma 3.1. \square

LEMMA 4.2. *Let E be a finite dimensional vector space over \mathbb{K} with norm $\|\cdot\|$, and let $G: E \rightarrow E$ be a given continuous function. Assume $\phi: E \times [0, \infty) \rightarrow [0, \infty)$ has the properties*

(a) $\phi(z; \cdot)$ is isotone on $[0, \infty)$ (for all $z \in E$),

(b) $\phi(z; 0) = 0$ (for all $z \in E$),

(c) $\|\tilde{z} - z\| \leq \phi(z; \|G\tilde{z} - Gz\|)$ (for all $z, \tilde{z} \in E$).

Then there is a unique $z^ \in E$ with $Gz^* = 0$.*

Proof. G is a continuous one-to-one mapping defined on E . The domain-invariance theorem (cf. [18]) thus implies that $G(E)$ is open.

Property (c) implies that $\|Gz\| \rightarrow \infty$ (when $\|z\| \rightarrow \infty$). Therefore a *bounded* sequence $z_1, z_2, z_3 \dots$ exists with

$$\lim_{k \rightarrow \infty} \|Gz_k\| = r, \quad r = \inf \{ \|Gz\| : z \in E \}.$$

Consequently there is a subsequence $\{y_k\}$ of $\{z_k\}$ with

$$\lim_{k \rightarrow \infty} y_k = z^*, \quad \lim_{k \rightarrow \infty} Gy_k = Gz^*, \quad \|Gz^*\| = r$$

for some $z^* \in E$.

Since $G(E)$ is open, we have $r = 0$. \square

We note that theorems with much resemblance to the above lemma can be found in the literature (see e.g. [16, Thm. 13.5], [19, Thm. 5.3.8]).

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