

RUNGE–KUTTA METHODS REVISITED

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Abstract.

The exact relation between a Cooper-like reducibility concept and the reducibilities introduced by Hundsdorfer, Spijker and by Dahlquist and Jeltsch is given. A shifted Runge–Kutta scheme and a transplanted differential equation is introduced in such a fashion that the input/output relation remains unchanged under these transformations. This gives a technique to prove stability and contractivity results. This is demonstrated on the example of contractivity disks.

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1 Introduction.

In [6] we have studied contractivity of explicit Runge–Kutta methods. A close look at the proofs shows that these are similar to the ones in [1], [5] concerning *BN*-stability. A similar relation between proofs in [2] and [3] can be observed. Here we shall link some of these results by introducing shifted Runge–Kutta schemes and the corresponding transplanted differential equation. These transformations are done in such a fashion that the input/output relation in the transformed situation is the same one as in the original scheme. This gives us a tool to prove new results by transforming these back to known theorems. We shall present this proving technique in Section 3. To show how it works we apply it to prove *r*-circle contractivity in Section 4. To present these results in their sharpest version we need the concept of irreducibility. We shall introduce in Section 2 a reducibility concept which has been implicitly suggested by G. J. Cooper [4] and then give the exact relation to the reducibility concepts

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of Hundsdorfer and Spijker [11] and of Dahlquist and Jeltsch [6]. The results in this report have been announced in [7].

2 Irreducible methods.

To solve the initial value problem

$$(2.1) \quad y'(t) = f(t, y(t)), \quad y(0) \text{ given, } y, f \in \mathbb{R}^s \text{ or } \mathbb{C}^s$$

we consider m -stage Runge–Kutta methods. Let y_n and y_{n+1} be the numerical approximations to the exact solution at t_n and $t_{n+1} = t_n + h$, respectively, where the stepsize h is always assumed to be positive. Then y_{n+1} is computed by

$$(2.2) \quad y_{n+1} = y_n + h \sum_{j=1}^m b_j f(t_n + c_j h, Y_j),$$

where

$$(2.3) \quad Y_i = y_n + h \sum_{j=1}^m a_{ij} f(t_n + c_j h, Y_j), \quad i = 1, 2, \dots, m.$$

We shall always request the **consistency condition**

$$(2.4a) \quad \sum_{i=1}^m b_i = 1$$

and

$$(2.4b) \quad c_i = \sum_{j=1}^m a_{ij}.$$

While (2.4a) is a necessary condition for convergence, (2.4b) is not [13]. However (2.4b) ensures that the Runge–Kutta scheme gives the same result, whether it is applied to a nonautonomous problem or the corresponding autonomous problem obtained by augmenting the system of equations by the equation $dt/dt = 1$. Even so (2.4b) is not necessary for the results presented here it is convenient to assume it and practically all known methods satisfy it. The scheme is called **explicit** if

$$(2.5) \quad A := (a_{ij})_{i,j=1}^m$$

is a strictly lower triangular matrix. A Runge–Kutta method is called **confluent** if $c_i = c_j$ for some $i \neq j$ and **nonconfluent** otherwise. For compactness of notations we introduce the vectors

$$Y, F(t_n e_m + ch, Y) \in \mathbb{R}^{ms} \text{ or } \mathbb{C}^{ms}, \quad \text{and } c, e_m \in \mathbb{R}^m$$

are defined by

$$(2.6) \quad Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_m \end{pmatrix}, \quad F(t_n e_m + ch, Y) = \begin{pmatrix} f(t_n + c_1 h, Y_1) \\ f(t_n + c_2 h, Y_2) \\ \vdots \\ f(t_n + c_m h, Y_m) \end{pmatrix}$$

$$e_m = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \quad c = A e_m = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix}.$$

Using the Kronecker-product symbol \otimes , see for example [9, p. 116], or [12] we can simplify the notation. In order to cut down on the number of parentheses we assume that \otimes has higher priority than ordinary matrix multiplication. Let I_s be the $s \times s$ identity matrix, and let $b^T = (b_1, b_2, \dots, b_m)$. Then (2.2) and (2.3) take the form

$$(2.7) \quad y_{n+1} = y_n + hb^T \otimes I_s F(t_n e_m + ch, Y)$$

and

$$(2.8) \quad Y = e_m \otimes y_n + hA \otimes I_s F(t_n e_m + ch, Y).$$

The aim in research on Runge–Kutta scheme is very often to express a property of the scheme in terms of properties of the coefficients a_{ij} and b_j . However one can often, for example by adding redundant stages, destroy the latter while keeping the former. Thus one would like to get rid of all possible redundancies in a scheme to get sharpest results. This lead to the introduction of several notions of reducibility [4, 6, 8, 11, 15]. Before discussing reducibility we observe that a permutation of the numbering of the stages does not change the numerical result of the Runge–Kutta scheme. In terms of the coefficients matrix A and b this is expressed by the obvious

LEMMA 2.1. *Let Π be a permutation matrix. Then the Runge–Kutta schemes defined by A, b, c and $\pi A \pi^T, \pi b, \pi c$ give identical results.*

In a strict sense one should call a Runge–Kutta scheme reducible, if there is a Runge–Kutta scheme with fewer stages which gives in all situation identical results as the original scheme. This reducibility has the drawback of being too stringent and not being expressed in terms of the coefficients. Four our results we shall use the following reducibility definition, which has been implicitly suggested by G. J. Cooper [4].

DEFINITION 2.1. *An m -stage Runge–Kutta scheme A, b is called **reducible**, if there exists an $m_r < m$ and an m_r -stage Runge–Kutta scheme A_r, b_r which*

satisfies the following property. There exists an $m \times m$ matrix M with exactly one element 1 in each row and 0 otherwise such that

$$(2.9) \quad AM = M \begin{pmatrix} A_r & 0 \\ & D \end{pmatrix}, \quad M^T b = \begin{pmatrix} b_r \\ 0 \end{pmatrix}.$$

Here D is an $(m - m_r) \times m$ matrix. The method is called **irreducible** if it is not reducible.

In [4] M is called reducing matrix. The reduced m_r -stage Runge–Kutta method is given by

$$(2.10) \quad Z = e_{m_r} \otimes y_n + h A_r \otimes I_s F(t_n e_{m_r} + h A_r e_{m_r}, Z)$$

and

$$(2.11) \quad z_{n+1} = y_n + h b_r^T \otimes I_s F(t_n e_{m_r} + h A_r e_{m_r}, Z).$$

Before relating z_{n+1} , Z of (2.11), (2.10) with y_{n+1} , Y of (2.7), (2.8) we observe the following simplification.

LEMMA 2.2. *If the Runge–Kutta scheme A, b is reducible then there exists a permutation matrix π such that the reducing matrix M of the Runge–Kutta method $\pi A \pi^T$, πb has the product representation*

$$(2.12) \quad M = M_S P,$$

where P is a permutation matrix and

$$(2.13) \quad M_S = \begin{pmatrix} & I_\mu & 0 \\ \underbrace{0}_\sigma & & L & 0 \end{pmatrix},$$

where L is an $(m - \mu) \times (\mu - \sigma)$ matrix with exactly one 1 in each row, at least one 1 in each column and zeros otherwise.

PROOF. First we observe that pre-multiplication (post-multiplication) with a permutation matrix corresponds to a permutation of the rows (columns) of a matrix. Let M' be the reducing matrix of the scheme. By definition M' has columns with no 1, exactly one 1 and more than one 1. Hence there exists a permutation matrix P^T such that $M'P^T$ has in the first σ columns exactly one 1, in the next $\mu - \sigma$ columns more than one 1 and no ones in the last $m - \mu$ columns. Since there is exactly one 1 in each row of M' and thus of $M'P^T$ there exists a permutation matrix π such that $M_S := \pi M'P^T$ has the form (2.13). Clearly $M := \pi M'$ has the required form (2.12) and we find using (2.9) that

$$\pi A \pi^T M = \pi A M' = \pi M' \begin{pmatrix} A_r & 0 \\ & D \end{pmatrix} = M \begin{pmatrix} A_r & 0 \\ & D \end{pmatrix}$$

and

$$M^T \pi b = M'^T b = \begin{pmatrix} b_r \\ 0 \end{pmatrix}.$$

□

Due to Lemma 2.1 and Lemma 2.2 we can always assume, without loss of generality, that a reducible Runge–Kutta scheme is in the form such that M has the product representation (2.12). The two factors are associated with two well-known reducibility concepts, namely reducibility in the sense of Dahlquist and Jeltsch [6] and reducibility in the sense of Hundsdorfer and Spijker [11]. To simplify the referencing within this section we give these two special reducibility concepts the following working names:

DEFINITION 2.2 (Dahlquist/Jeltsch [6]). *An m -stage Runge–Kutta A, b method is called **DJ-reducible** if there exist two sets T and U such that $T \neq \phi$, $U \neq \phi$, $T \cap U = \phi$, $T \cup U = S := \{1, 2, \dots, m\}$ and*

$$(2.14) \quad b_j = 0 \quad \text{if } j \in T$$

$$(2.15) \quad a_{ij} = 0 \quad \text{if } i \in U \text{ and } j \in T.$$

Clearly, a Runge–Kutta method is DJ-reducible if and only if it is reducible with an M which is a permutation matrix. The reduced scheme is obtained by deleting all stages Y_j with $j \in T$. Hence, one can reduce the scheme by $|T|$ -stages to an $|U|$ -stage Runge–Kutta method. DJ-reducible schemes can be thought of schemes where one has artificially added stages together with zeros at appropriate locations to ensure that the additional stages have no influence on the old ones. The only influence is on the solvability of the whole system. One can add the new stags such that the enlarged method has $0, 1, 2, \dots$ up to infinitely many solution. However, due to the appropriate zeros one has that if the enlarged scheme has solutions then the y_{n+1} value is the same as in the original method.

A different reducibility concept was introduced in [11] (see also [15] for a special case). Here the idea was that existing stages are duplicated in order to give additional stages, all providing the same Y_j and therefore the same $f(t_n + c_j h, Y_j)$. Hence, wherever an $f(t_n + c_j h, Y_j)$ occurs in the scheme it can be replaced by a sum over these identical values. The formal definition is:

DEFINITION 2.3 (Hundsdorfer/Spijker [11]). *Let $\rho \geq 1$, S_1, S_2, \dots, S_ρ are pairwise disjoint subsets of $S := \{1, 2, \dots, m\}$ each containing at least two elements. Let*

$$S_0 = S - \bigcup_{j=1}^{\rho} S_j.$$

The method is $\{S_1, S_2, \dots, S_\rho\}$ -reducible, if for $k = 1, 2, \dots, \rho$ one has for $i, j \in S_k$ that

$$(2.16) \quad \sum_{\nu \in S_\ell} a_{i\nu} = \sum_{\nu \in S_\ell} a_{j\nu}, \quad \ell = 1, 2, \dots, \rho$$

and

$$(2.17) \quad a_{i\ell} = a_{j\ell}, \quad \ell \in S_0.$$

Clearly, if a Runge–Kutta A, b is $\{S'_1, S'_2, \dots, S'_\rho\}$ -reducible then there exists a permutation matrix π such that the scheme $\pi A \pi^T, \pi b$ is $\{S_1, S_2, \dots, S_\rho\}$ -reducible where S_i satisfies the following condition

$$(2.18) \quad S_0 = \{1, 2, \dots, s_0\} \quad s_0 + i \in S_i \quad \text{for } i = 1, 2, \dots, \rho.$$

The idea behind this reducibility is that for each fixed $i \geq 1$, all stages Y_j with $j \in S_i$ give identical Y_j values. The scheme can then be reduced, assuming that (2.18) holds, to the scheme A', b'

$$(2.19) \quad \begin{aligned} a'_{ij} &= a_{ij} & i = 1, 2, \dots, s_0 + \rho; \quad j = 1, 2, \dots, s_0 \\ a'_{i, s_0+k} &= \sum_{\ell \in S_k} a_{i\ell} & i = 1, 2, \dots, s_0 + \rho; \quad k = 1, 2, \dots, \rho \end{aligned}$$

$$(2.20) \quad \begin{aligned} b'_i &= b_i & i = 1, 2, \dots, s_0 \\ b'_{s_0+k} &= \sum_{\ell \in S_k} b_\ell & k = 1, 2, \dots, \rho. \end{aligned}$$

This scheme has $|S_0| + \rho$ stages. From the idea of this reducibility concept it is clear that if the reduced scheme has a solution then the unreduced one has a solution too. However, the large system may have additional solutions where the stages with the indices in the same S_j are not identical. We give now the final relation between the three reducibility concepts.

PROPOSITION 2.3. *An m -stage Runge–Kutta method A, b is reducible to an m_r -stage Runge–Kutta A_r, b_r if and only if it is either DJ-reducible or $\{S_1, \dots, S_\rho\}$ -reducible or both. More precisely:*

- i) *A Runge–Kutta scheme is DJ-reducible if and only if there exists a reducing matrix M of $\text{rank}(M) = m$.*
- ii) *A Runge–Kutta scheme is $\{S_0, S_1, \dots, S_\rho\}$ -reducible if and only if $\mu := \text{rank}(M) < m$. It can be reduced to an μ -stage scheme and one has*

$$(2.21) \quad \mu = \rho + \sigma.$$

In addition, after suitable numbering of the stages one has

$$(2.22) \quad S_0 = \{1, 2, \dots, \sigma\}$$

and

$$(2.23) \quad S_k = \{i | m_{i, \sigma+k} = 1\}, \quad k = 1, 2, \dots, \rho,$$

where

$$M_S = (m_{ij})_{i,j=1}^m.$$

iii) *If we assume that M is chosen such as to minimize m_r then after reducing the scheme to a rank (M) -stage method using $\{S_1, S_2, \dots, S_\sigma\}$ -reducibility the remaining scheme can be reduced by rank $(M) - m_r$ -stages using DJ-reducibility.*

REMARKS.

1. The reducibility of Definition 2.1 is nothing more than a combination of the two-well established reducibility concepts.
2. Since in [11], [8, p. 111], an algorithm to determine $\{S_1, \dots, S_\rho\}$ -reducibility is given and it is obvious how to determine DJ-reducibility one just joins the two algorithms together to get an algorithm for determining reducibility.

PROOF OF PROPOSITION 2.3. As already observed in [4], part i), is trivial. To show ii) we first assume that the scheme is $\{S_1, \dots, S_\rho\}$ -reducible. Without loss of generality we can assume that the stage numbers have been permuted such that the S_i are as follows:

$$(2.24) \quad S_0 = \{1, 2, \dots, \sigma\} \quad \sigma + i \in S_i \quad \text{for } i = 1, 2, \dots, \rho.$$

Let $M = (m_{ij})_{i,j=1}^m$ be defined by

$$(2.25) \quad m_{ij} = \begin{cases} 1 & \text{for } i \in S_0, j = i \\ 1 & \text{for } i \in S_k, j = \sigma + k, \text{ for } k = 1, 2, \dots, \rho \\ 0 & \text{elsewhere.} \end{cases}$$

Clearly, $\text{rank}(M) = \sigma + \rho < m$ and M satisfies (2.23) and with $\mu := \text{rank}(M)$ (2.21) too. It remains to show that M is a reducing matrix. Let $A' = AM = (a'_{ij})_{i,j=1}^m$. Hence

$$a'_{ij} = \begin{cases} a_{ij} & j \in S_0 \\ \sum_{\ell \in S_k} a_{i\ell} & j = \sigma + k, k = 1, 2, \dots, \rho \\ 0 & j > \sigma + \rho. \end{cases}$$

One easily verifies that

$$MA' = A' = \begin{pmatrix} A'_{11} & 0 \\ A'_{22} & 0 \end{pmatrix}$$

and

$$b' := M^T b = \begin{pmatrix} b'_1 \\ 0 \end{pmatrix},$$

where A'_{11} is a $\mu \times \mu$ matrix and $b'_1 \in \mathbb{R}^\mu$. Hence, the Runge–Kutta scheme A, b is reducible. In fact M has the standard form of M_S in (2.13). We now show

the converse, namely that a reducible scheme with the reducing matrix M of rank $(M) = \mu < m$ is $\{S_1, \dots, S_\rho\}$ -reducible with (2.21)–(2.23) after suitable renumbering of the stage numbers. We choose the numbering of the stage numbers such that M has the form (2.12), (2.13). This defines σ . We choose ρ and S_i according to (2.21)–(2.23). Since there is exactly one 1 in each row of M_S we have

$$\bigcup_{j=0}^{\rho} S_j = \{1, 2, \dots, m\}$$

and the sets S_j are pairwise disjoint. Moreover each S_j with $j > 0$ has at least two elements. For brevity we rewrite M_S as

$$M_S = \begin{pmatrix} I_\mu & 0 \\ L' & 0 \end{pmatrix}, \quad A' = P \begin{pmatrix} A_r & 0 \\ & D \end{pmatrix} P^T,$$

where I_μ is the $\mu \times \mu$ identity matrix and L' is the $(m - \mu) \times \mu$ matrix

$$L' = (0 \quad L).$$

With the corresponding partitioning of A and A' we find from (2.9)

$$(2.26) \quad AM_S = \begin{pmatrix} A_{11} + A_{12}L' & 0 \\ A_{21} + A_{22}L' & 0 \end{pmatrix} = \begin{pmatrix} A'_{11} & A'_{12} \\ L'A'_{11} & L'A'_{12} \end{pmatrix} = M_S A'.$$

Hence $A'_{12} = 0$ and A'_{11} is uniquely determined. Let $i \in S_j$, $j > 0$ and $k \in S_0$. Hence one finds by (2.26) that the (i, k) th element of AM is a_{ik} while the (i, k) th element of MA' is $a'_{\sigma+j,k}$. Hence by (2.26) one has

$$(2.27) \quad a_{ik} = a'_{\sigma+j,k}.$$

Since this is true for all $i \in S_j$ we have shown (2.17). Let $i \in S_j$, $j > 0$ and $k > 0$. As before one finds by equating the $(i, \sigma + k)$ th element in (2.26) that

$$(2.28) \quad \sum_{\nu \in S_k} a_{i\nu} = a'_{\sigma+j,\sigma+k}.$$

Since the right-hand side is the same for all $i \in S_j$ we have shown (2.16). To show iii) assume that M is chosen such that it minimizes m_r . In addition we can assume by Lemma 2.2 that M is in the standard form $M = M_S P$ where M_S is given by (2.13). We have already shown that M_S determines the $\{S_1, \dots, S_\rho\}$ -reducibility, and

$$AM_S = M_S A'$$

and

$$(2.29) \quad A' = \begin{pmatrix} A'_{11} & 0 \\ A'_{21} & A'_{22} \end{pmatrix} = P \begin{pmatrix} A_r & 0 \\ & D \end{pmatrix} P^T.$$

Here A'_{11} is a $\mu \times \mu$ matrix. Let

$$(2.30) \quad b' = M_S^T b = P^T \begin{pmatrix} b_r \\ 0 \end{pmatrix}.$$

From the form of M_S we see that the Runge–Kutta method A', b' is DJ-reducible to an μ -stage scheme. In addition one sees from (2.29), (2.30) that the scheme A', b' is also DJ-reducible to an m_r -stage scheme. Since m_r is minimal the scheme A'_{11}, b'_1 , where b'_1 is the vector in \mathbb{R}^μ consisting of the first μ components of b' is DJ-reducible by $\mu - m_r$ -stages to the scheme A_r, b_r . One verifies easily that the scheme A'_{11}, b'_1 is the one obtained by the $\{S_1, \dots, S_\sigma\}$ -reduction. \square

Part iii) of Proposition 2.3 gives the best insight in the relation between the solvability of (2.10) of the completely reduced scheme A_r, b_r and (2.8) of the original scheme A, b and the relation between y_{n+1} in (2.7) and z_{n+1} in (2.11). First let ν_r, ν be the number of solutions of (2.10) and (2.8) respectively. It is illuminating to consider also the scheme A'_{11}, b'_1 which is obtained from A, b by using $\{S_1, \dots, S_\sigma\}$ -reducibility. This intermediate method has the form

$$(2.31) \quad W = e_\mu \otimes y_n + h A'_{11} \otimes I_s F(t_n e_\mu + h A'_{11} e_\mu, W)$$

and

$$(2.32) \quad w_{n+1} = y_n + h b'^T \otimes I_s F(t_n e_\mu + h A'_{11} e_\mu, W).$$

Let ν' be the number of solutions of (2.31). Clearly, there is no relation whatsoever between ν_r and ν' since the system (2.31) can be thought of being created from the smaller system (2.10) by adding a system of redundant stages which may have no or any number of solutions, i.e. all three possibilities $\nu_r < \nu'$, $\nu_r = \nu'$ and $\nu_r > \nu'$ can occur. However one always has $\nu' \leq \nu$ since from each solution of (2.31) one can construct a solution of (2.8) by duplication of the appropriate stages. If $\nu_r \cdot \nu' > 0$ then one always has $w_{n+1} = z_{n+1}$. However since (2.8) admits sometimes solutions which did not arise from duplication of stages in (2.31) one may have that $y_{n+1} \neq w_{n+1}$. Therefore it is possible that the system (2.8) of the original scheme has a unique solution and the system of the completely reduced scheme (2.10) has a unique solution but $y_{n+1} \neq z_{n+1}$. To demonstrate this we give the following example.

EXAMPLE. The scalar initial value problem is the following

$$y' = f(t, y) = \begin{cases} y^2 & \text{if } y \geq 0 \\ 0 & \text{if } y < 0 \end{cases}$$

$$y(0) = 1.$$

The reducible scheme is given by

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -\frac{1}{2} \\ 0 & \frac{1}{2} & 0 \end{pmatrix}$$

$$b^T = (1 \quad b_2 \quad -b_2)$$

and the completely reduced scheme is Euler's method

$$A_r = (0) \quad b_r^T = (1).$$

One easily verifies that for $y_0 = 1$, $h = 2$ the implicit equation (2.8) with A has the unique solution

$$Y = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

and hence

$$y_1 = 3 - 2b_2.$$

Since the reduced scheme is Euler's scheme it has a unique solution and $z_1 = 3$.

3 Shifted Runge–Kutta methods and the transplanted differential equation.

In this section we transform the Runge–Kutta method and the differential equation such that the input/output relation in the transformed situation is the same one as in the original scheme if one uses the same stepsize h in both cases. The transformed scheme is called **shifted** Runge–Kutta method.

DEFINITION 3.1. *Let A, b, c represent an m -stage Runge–Kutta scheme with $c = A e_m$. Then the Runge–Kutta scheme A^*, b^*, c^* shifted by σ is defined as follows*

$$(3.1) \quad \begin{aligned} A^* &= A + \sigma I_m \\ b^* &= b \end{aligned}$$

$$(3.2) \quad c^* = c + \sigma e_m.$$

Clearly, the shifted Runge–Kutta scheme satisfies (2.4b). We shall now “transplant” the differential equation. To do this we introduce the non-linear map $T_\sigma : \mathbb{R}^{s+1} \rightarrow \mathbb{R}^{s+1}$ given by

$$(3.3) \quad \begin{pmatrix} t^* \\ y^* \end{pmatrix} = T_\sigma \begin{pmatrix} t \\ y \end{pmatrix} = \begin{pmatrix} t + \sigma h \\ y + \sigma h f(t, y) \end{pmatrix}.$$

In order not to overload the notations we do not indicate the dependance of T_σ on h and f explicitly.

DEFINITION 3.2. *The function $f^*(t^*, y^*)$ defined by*

$$(3.4) \quad f^*(t^*, y^*) := f(t, y)$$

where t, y are given by

$$\begin{pmatrix} t \\ y \end{pmatrix} = T_\sigma^{[-1]} \begin{pmatrix} t^* \\ y^* \end{pmatrix}$$

is called the **transplant of f under the map T_σ** .

Thus the value of f^* at t^*, y^* is equal to the value of f at the pre-image of t^*, y^* under the map T_σ .

PROPOSITION 3.1. *Let A, b be an m -stage Runge–Kutta scheme with $c = Ae_m$ and A^*, b^* the scheme shifted by σ . Let f^* be the transplant of f under the map T_σ . Then one integration step to solve the initial value problem*

$$y'(t) = f(t, y(t)), \quad y(t_n) = y_n$$

using the Runge–Kutta scheme A, b yields the same result as one step to solve the “transplanted” initial value problem

$$z'(t) = f^*(t, z(t)), \quad z(t_n) = y_n$$

using the shifted Runge–Kutta method A^*, b^*, c^* .

PROOF. From (3.4) follows that

$$(3.5) \quad F^*(t_n e_m + c^* h, Y^*) = F(t_n e_m + c^* h - \sigma h e_m, Y)$$

if

$$(3.6) \quad Y^* = Y + \sigma h F(t_n e_m + c^* h - \sigma h e_m, Y).$$

Substitution of (3.5) and (3.6) in

$$Y^* = e_m \otimes y_n + h A^* \otimes I_s F^*(t_n e_m + c^* h, Y^*)$$

gives using (3.1), (3.2)

$$Y + \sigma h F(t_n e_m + c h, Y) = e_m \otimes y_n + h(A + \sigma I_m) \otimes I_s F(t_n e_m + c h, Y).$$

Thus Y satisfies (2.8). Hence

$$\begin{aligned} z_{n+1} &= y_n + h b^{*T} \otimes I_s F^*(t_n e_m + c^* h, Y^*) \\ &= y_n + h b^T \otimes I_s F(t_n e_m + c h, y) = y_{n+1}. \end{aligned}$$

□

Since the input/output relation of the original and the transformed situation are identical a boundedness result

$$(3.7) \quad \|y_{n+1}\| \leq k \|y_n\|$$

or a result of the form

$$(3.8) \quad \|y_{n+1} - \tilde{y}_{n+1}\| \leq k \|y_n - \tilde{y}_n\|$$

for the transformed situation must imply the corresponding result in the original situation and vice versa. Before exploiting this fact by giving examples in the next section, we collect here some basic properties on the transformation.

Clearly, the order of a Runge–Kutta scheme can vary under a shift by σ as one easily sees from the example of the one stage Gauss–Legendre method $A = (\frac{1}{2})$, $b = (1)$. This method has order 2 while the scheme shifted by $-\frac{1}{2}$ is Euler’s method which has order one. However, from Definition 3.1 the following lemma is obvious.

LEMMA 3.2. *A shifted Runge–Kutta scheme is consistent if and only if the original scheme is consistent.*

LEMMA 3.3. *A shifted Runge–Kutta scheme is reducible if and only if the original scheme is reducible.*

PROOF. Assume the scheme A, b is reducible; i.e. (2.9) holds with the reducing matrix M . Let A^*, b^* be the Runge–Kutta scheme shifted by σ . Hence

$$(3.9) \quad \begin{aligned} A^*M &= AM + \sigma M = MA' + \sigma M \\ &= M(A' + \sigma I_m). \end{aligned}$$

Since $A' + \sigma I_m$ has the same structure A' and $b^* = b$ we find by (3.9) that the shifted method is reducible too. Since the sign of σ is arbitrary we have that the shifted scheme is reducible if and only if the original method is reducible. \square

In the next sections we shall impose some conditions on the differential equations. Let $\langle \cdot, \cdot \rangle$ be a semi-innerproduct and $\|u\| := \langle u, u \rangle^{\frac{1}{2}}$ be a semi-norm on \mathbb{R}^s or \mathbb{C}^s . One imposes on the differential equation either the condition

$$(3.10) \quad \operatorname{Re} \langle \alpha u + \beta f(u), \gamma u + \delta f(u) \rangle \leq 0 \quad \text{for all } u \in \mathbb{R}^s \text{ or } \mathbb{C}^s$$

or

$$(3.11) \quad \operatorname{Re} \langle \alpha(u - v) + \beta(f(t, u) - f(t, v)), \gamma(u - v) + \delta(f(t, u) - f(t, v)) \rangle \leq 0$$

for all $u, v \in \mathbb{R}^s$ or \mathbb{C}^s .

Here, $\alpha, \beta, \gamma, \delta$ are real numbers.

Since we always want that these conditions involve f we can without loss of generality assume $\delta = 1$. Condition (3.10) is very often used with

$$\alpha = \delta = 1, \quad \beta = \gamma = 0$$

to prove monotonicity, i.e.

$$(3.12) \quad \|y_{n+1}\| \leq \|y_n\|,$$

see for example [2, 14]. For proving contractivity, i.e.

$$(3.13) \quad \|y_{n+1} - \tilde{y}_{n+1}\| \leq \|y_n - \tilde{y}_n\|$$

one usually request (3.11) with either $\alpha = \delta = 1, \beta = 0$, see e.g. [1], or $\alpha = \delta = 1, \gamma = 0$, see e.g. [6].

LEMMA 3.4. *Assume that f satisfies either (3.10) or (3.11) respectively with $\delta = 1$. If $1 - \gamma\sigma h > 0$ then the transplant f^* of f under T_σ satisfies (3.10) or (3.11) respectively with $\alpha, \beta, \gamma, \delta$ replaced by*

$$(3.14) \quad \alpha^* := \frac{\alpha}{1 - \gamma\sigma h}, \quad \beta^* := \frac{\beta - \alpha\sigma h}{1 - \gamma\sigma h}, \quad \gamma^* := \frac{\gamma}{1 - \gamma\sigma h}, \quad \delta^* := 1.$$

PROOF. The map T_σ is given by

$$u^* = T_\sigma(u) = u + \sigma h f(u)$$

and the transplant f^* of f under T_σ is given by

$$f^*(u^*) := f(u).$$

If (3.10) holds one easily finds

$$\begin{aligned} 0 &\geq \operatorname{Re} \langle \alpha u + \beta f(u), \gamma u + f(u) \rangle \\ &= \operatorname{Re} \langle (u + \sigma h f(u) + (\beta - \alpha\sigma h) f(u), \gamma(u + \sigma h f(u)) + (1 - \gamma\sigma h) f(u) \rangle \\ &= \operatorname{Re} \left\langle \frac{\alpha}{1 - \gamma\sigma h} u^* + \frac{\beta - \alpha\sigma h}{1 - \gamma\sigma h} f^*(u^*), \frac{\gamma}{1 - \gamma\sigma h} u^* + f^*(u^*) \right\rangle. \end{aligned}$$

Here we have used in the last step that $1 - \gamma\sigma h > 0$. The result for (3.11) is proved in the same way. □

In order to get a feeling for the conditions (3.10) and (3.11) we observe that for the linear equation $y' = \lambda y$ the conditions become, provided that $\|y\| \neq 0$,

$$(3.15) \quad \operatorname{Re} \frac{\alpha + \beta\lambda}{\gamma + \lambda} \leq 0.$$

Since $w(\lambda) = (\alpha + \beta\lambda)/(\gamma + \lambda)$ is a Möbius transformation the set $\{\lambda \mid \operatorname{Re} w(\lambda) \leq 0\}$ is either a circle or a halfplane.

4 r -circle contractivity.

In this section we show on the example of contractivity how Proposition 3.1 can be used to prove new results. We talk of **numerical contractivity** if any two numerical solutions

$$\{y_n\}_{n=0,1,\dots}, \quad \{\tilde{y}\}_{n=0,1,\dots},$$

which are computed with the same h satisfy

$$(4.1) \quad \|y_{n+1} - \tilde{y}_{n+1}\| \leq \|y_n - \tilde{y}_n\|, \quad n = 0, 1, \dots, .$$

Here we assume that $\|u\|$ is an innerproduct norm as introduced in the Section 3. In order that one has numerical contractivity one has to impose conditions on the differential equations and on the methods. For the differential equation we request that (3.10) holds with $\alpha = \delta = 1, y = 0$, i.e.

$$(4.2) \quad \operatorname{Re} \langle u - v, f(t, u) - f(t, v) \rangle \leq -\beta \|f(t, u) - f(t, v)\|^2 \quad \text{for all } u, v \in \mathbb{R}^s \text{ or } \mathbb{C}^s .$$

For brevity let us introduce the generalized disks

$$(4.3) \quad D(r) := \begin{cases} \{ \lambda \in \mathbb{C} \mid |\lambda + r| \leq r \} & \text{if } r > 0 \\ \{ \lambda \in \overline{\mathbb{C}} \mid \operatorname{Re} \lambda \leq 0 \} & \text{if } r = \infty \\ \{ \lambda \in \overline{\mathbb{C}} \mid |\lambda + r| \geq -r \} & \text{if } r < 0 . \end{cases}$$

Hence (4.2) corresponds for $y' = \lambda y$ to the condition $\lambda \in D(1/(2\beta))$.

To motivate the condition on the Runge–Kutta scheme we consider the scalar test equation

$$(4.4) \quad y' = \lambda(t) y(t), \quad \lambda(t) \in \mathbb{C} .$$

If one applies (2.7), (2.8) to (4.3) the numbers

$$(4.5) \quad \zeta_i = h\lambda(t_n + c_i h), \quad i = 1, 2, \dots, m$$

and $\zeta = (\zeta_1, \zeta_2, \dots, \zeta_m)^T$ are needed. Assume that (4.4) satisfies (4.2) then $\zeta_i \in D(r)$ with $r = h/(2\beta)$. If the c_i are distinct then one can choose any m complex numbers $\zeta_i \in D(r)$ and find a smooth $\lambda(t)$ such that (4.5) holds. Applying (2.7), (2.8) to (4.4) leads to

$$(4.6) \quad y_{n+1} = K(\zeta) y_n ,$$

where

$$(4.7) \quad K(\zeta) = 1 + b^T Z (I_m - AZ)^{-1} e_m$$

with

$$(4.8) \quad Z = \operatorname{diag}(\zeta_1, \zeta_2, \dots, \zeta_m) ,$$

see [1]. Clearly we have numerical contractivity if $|K(\zeta)| \leq 1$. This leads to the

DEFINITION 4.1. A Runge–Kutta method is called ***r*-circle contractive** if $D(r)$ is the largest generalized disk with $r \neq 0$ and

$$(4.9) \quad |K(\zeta)| \leq 1 \quad \text{for all } \zeta \in D(r)^m .$$

A method is called ***circle contractive*** if (4.9) holds for some $r \neq 0$.

With largest generalized disk we mean largest in the sense of the natural ordering by set inclusion. Note that this is equivalent to the ordering of $-\frac{1}{r}$ in the reals. Note that for a confluent method applied to (4.4) one never has $\zeta_i \neq \zeta_j$ if $c_i = c_j$. Nevertheless we request (4.9). One reason for this is, that with the present definition $\frac{1}{r}$ is a continuous function of the coefficients a_{ij} and b_j if the method is irreducible as one easily sees from the next theorem below. Another is that Theorem 4.1 will hold. Clearly $D(r) \subset S$, where S is the stability region of the method, given by

$$S = \{ \mu \in \overline{\mathbb{C}} \mid |K(\mu I_m)| \leq 1 \} .$$

Following Burrage and Butcher [1] we introduce the matrix,

$$(4.10) \quad Q = BA + A^T B - bb^T ,$$

where

$$(4.11) \quad B = \text{diag}(b_1, b_2, \dots, b_m) .$$

THEOREM 4.1. Assume that the Runge–Kutta scheme is irreducible. Then the following conditions are equivalent:

- i) The method is *r*-circle contractive.
- ii) $b_i > 0$ for $i = 1, 2, \dots, m$ and

$$(4.12) \quad -\frac{1}{r} = \inf_{\substack{w \in \mathbb{R}^m \\ w \neq 0}} \frac{w^T Q w}{w^T B w} = \min_{i=1,2,\dots,m} \nu_i ,$$

where ν_i are the eigenvalues $B^{-\frac{1}{2}} Q B^{-\frac{1}{2}}$.

- iii) $\frac{1}{r}$ is the smallest number such that the following holds. If two numerical solutions $\{y_n\}, \{\tilde{y}_n\}$ of a differential equation with (4.2) are computed with the same stepsize h satisfying

$$(4.13) \quad \frac{h}{2r} \leq \beta ,$$

then one has

$$(4.14) \quad \|y_{n+1} - \tilde{y}_{n+1}\| \leq \|y_n - \tilde{y}_n\| .$$

From this theorem one easily notes that *r*-circle contractivity is equivalent to $(1, 0, \frac{1}{2})$ algebraic stability of G. J. Cooper [3]. Instead of proving the theorem

directly we show how one can use the transformation described in Section 3 to make use of existing theorems concerning the “half plane” situation. Hence, let us first recall these results.

DEFINITION 4.2. A Runge–Kutta scheme is called **algebraically stable** if $b_i \geq 0$ for $i = 1, \dots, m$ and Q is nonnegative definite.

It is easy to show that, if the method is irreducible then one has in fact $b_i > 0$ [6], [8, p. 114].

DEFINITION 4.3. A Runge–Kutta method is called **BN-stable** if for all f satisfying (4.2) with $\beta = 0$, all y_n, \tilde{y}_n and all $h > 0$ inequality (4.14) holds.

THEOREM 4.2 ([10]). A Runge–Kutta scheme is algebraically stable if and only if

$$(4.15) \quad |K(\zeta)| \leq 1 \quad \text{for all } \zeta \in (\overline{\mathbb{C}^-})^m.$$

THEOREM 4.3 ([1, 5, 11]). An irreducible Runge–Kutta scheme is BN-stable if and only if it is algebraically stable.

We shall need the following two lemmata. The first one corresponds to Proposition 3.1 and relates $K(\zeta)$ to $K^*(\zeta^*)$.

LEMMA 4.4. Let $K(\zeta)$ belong to the Runge–Kutta method A, b and $K^*(\cdot)$ belong to the Runge–Kutta scheme shifted by $\frac{1}{2r}$. Moreover let

$$\zeta^* = (\zeta_1^*, \zeta_2^*, \dots, \zeta_m^*)^T,$$

where

$$(4.16) \quad \zeta_i^* = \frac{\zeta_i}{1 + \frac{1}{2r} \zeta_i}.$$

Then

$$(4.17) \quad K^*(\zeta^*) = K(\zeta).$$

Moreover

$$(4.18) \quad |K(\zeta)| \leq 1 \quad \text{for all } \zeta \in D(r)^m$$

if and only if

$$(4.19) \quad |K^*(\zeta^*)| \leq 1 \quad \text{for all } \zeta \in (\overline{\mathbb{C}^-})^m.$$

PROOF. Clearly

$$Z^* = \text{diag}(\zeta_1^*, \dots, \zeta_m^*) = Z \left(I_m + \frac{1}{2r} Z \right)^{-1}.$$

Hence

$$\begin{aligned} K^*(\zeta^*) &= 1 + b^T Z \left(I_m + \frac{1}{2r} Z \right)^{-1} \left(I_m - \left(A + \frac{1}{2r} I_m \right) Z \left(I_m + \frac{1}{2r} Z \right)^{-1} \right)^{-1} e_m \\ &= 1 + b^T Z \left(I_m + \frac{1}{2r} Z - \left(A + \frac{1}{2r} I_m \right) Z \right)^{-1} e_m = K(\zeta) \end{aligned}$$

and thus (4.17) holds. The equivalence of (4.18) and (4.19) is trivial since the map $\zeta \rightarrow \zeta / (1 - \frac{1}{2r} \zeta)$ is a Möbius transformation which maps $D(r)$ one-to-one onto $\overline{\mathbb{C}^-}$. □

LEMMA 4.5. *Let Q belong to the Runge–Kutta method A, b . Then*

$$(4.20) \quad \inf_{\substack{w \in \mathbb{R}^m \\ w \neq 0}} \frac{w^T Q w}{w^T B w} \geq -\frac{1}{r},$$

if and only if the Runge–Kutta method A^, b^* shifted by $\frac{1}{2r}$ is algebraically stable.*

PROOF. The proof follows immediately from $b^* = b$ and the relation

$$\begin{aligned} Q^* &= B A^* + A^{*T} B - b b^T \\ &= B \left(A + \frac{1}{2r} I_m \right) + \left(A + \frac{1}{2r} I_m \right)^T B - b b^T \\ &= Q + \frac{1}{r} B. \end{aligned} \quad \square$$

PROOF OF THEOREM 4.1. To prove the equivalence of i) and ii) it is enough to show that one has

$$|K(\zeta)| \leq 1 \quad \text{for all } \zeta \in D(r)^m,$$

if and only if

$$(4.21) \quad \inf_{\substack{w \in \mathbb{R}^m \\ w \neq 0}} \frac{w^T Q w}{w^T B w} \geq -\frac{1}{r}.$$

This follows however immediately from the Lemma 4.4, 4.5 and Theorem 4.2. To show the equivalence of ii) and iii) it is enough to show that (4.21) is equivalent to the following statement: If two numerical solutions $\{y_n\}, \{\tilde{y}_n\}$ of a differential equation with (4.2) are computed with the same stepsize satisfying

$$(4.22) \quad \frac{h}{2r} \leq \beta,$$

then one has

$$(4.23) \quad \|y_{n+1} - \tilde{y}_{n+1}\| \leq \|y_n - \tilde{y}_n\|.$$

However this last statement is equivalent to the statement that the Runge–Kutta method shifted by $\frac{1}{2r}$ is BN -stable since by Proposition 3.1 the input/output

relation is invariant under the transformation and by Lemma 3.4 and (4.22) the β^* of the transformed differential equation is nonnegative. By Theorem 4.3 the transformed method is algebraically stable and hence by Lemma 4.5 we have (4.21). \square

In similar ways one can use the presented technique to generalize other known results. We mention, just as an example results by M. N. Spijker [14] on monotonicity which could be extended most easily.

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Appendix 1.

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One of the referees made the following correct remark:

In Section 3 the authors fail to require (in Definition 3.2, in Proposition 3.1, in Lemma 3.4) that the map T_σ is a bijection, so as to ensure that $f^* = f \circ (T_\sigma)^{-1}$ actually exists. Partly due to this omission, their proof of Theorem 4.1 on p. 583 seems to be incomplete. To be more specific, let F_β denote the class of *all* f satisfying (4.2) for some inner product and some $s \geq 1$. On p. 583 the authors claim the following statement (a) and (b) to be equivalent.

- (a)... There is contractivity for A , whenever $f \in F_\beta, \frac{h}{2r} \leq \beta$,
- (b)... There is contractivity for $A^* = (A + \frac{1}{2r})$, whenever $f \in F_0, h < \infty$.
However, their proof of this equivalence seems to require that the dubious statement (c), (d) are true.
- (c)... f^* , with $\sigma = \frac{1}{2r}$, actually exists, whenever $f \in F_\beta, \frac{h}{2r} \leq \beta$,
- (d)... There is an $f \in F_\beta$ with $\beta \geq \frac{h}{2r}, f^* = g, \sigma = \frac{1}{2r}$, whenever $g \in F_0$ is given.

This remark by the referee is correct. We show this with the following example:

Let $\sigma h = 1$ and $f(t, y) = -y$ then by (3.3) in Definition 3.1 we have

$$T_\sigma \begin{pmatrix} t \\ y \end{pmatrix} = \begin{pmatrix} t + 1 \\ 0 \end{pmatrix}.$$

Clearly $T_\sigma^{[-1]}$ does not exist.

This problem can be removed by making the changes suggested by the referee. Hence we replace Definition 3.2 by

DEFINITION 4.4 (new version of Definition 3.2). *Assume the map $T_\sigma: \mathbb{R}^{s+1} \rightarrow \mathbb{R}^{s+1}$ given by (3.3) is a bijection. Then the function $f^*(t^*, y^*)$ defined by*

$$(4.24) \quad f^*(t^*, y^*) := f(t, y),$$

where t, y are given by

$$\begin{pmatrix} t \\ y \end{pmatrix} = T_\sigma^{[-1]} \begin{pmatrix} t^* \\ y^* \end{pmatrix}$$

is called the **transplant of f under the map T_σ** .

Replace Proposition 3.1 by

PROPOSITION 4.6 (new version of Proposition 3.1). *Let A, b be an m -stage Runge–Kutta scheme with $c = Ae_m$ and A^*, b^* the scheme shifted by σ . Assume*

hat the map T_σ defined by σ and $f(t, y)$ is a bijection. Let f^* be the transplant of f under the map T_σ . Then one integration step to solve the initial value problem

$$y'(t) = f(t, y(t)), \quad y(t_n) = y_n$$

using the Runge–Kutta scheme A, b yields the same result as one step to solve the “transplanted” initial value problem

$$z'(t) = f^*(t, y(t)), \quad z(t_n) = z_n$$

using the shifted Runge–Kutta method A^*, b^*, c^* .

Further we replace Lemma 3.4 by

LEMMA 4.7 (new version of Lemma 3.4). *Assume that f satisfies either (3.10) or (3.11) respectively with $\delta = 1$. Assume that the map T_σ defined by σ and $f(t, y)$ is a bijection. If $1 - \gamma\sigma h > 0$ then the transplant f^* of f under T_σ satisfies (3.10) or (3.11) respectively with $\alpha, \beta, \gamma, \delta$ replaced by*

$$(4.25) \quad \alpha^* := \frac{\alpha}{1 - \gamma\sigma h}, \quad \beta^* := \frac{\beta - \alpha\sigma h}{1 - \gamma\sigma h}, \quad \gamma^* := \frac{\gamma}{1 - \gamma\sigma h}, \quad \delta^* := 1.$$

At this point we should note that for the differential equation

$$(4.26) \quad y' = \lambda(t)y \quad \lambda \in \mathbb{C}$$

satisfying (4.2) one has $\lambda \in D(\frac{1}{2\beta})$. If we transplant (4.26) with $\sigma = \frac{1}{2\beta}$ one has for $h\sigma \leq \beta$ that $1 + \sigma h\lambda \neq 0$ except in the case $\lambda = -\frac{1}{\beta}$ and $h\sigma = \beta$. Hence except for the particular case of $\lambda = -\frac{1}{\beta}$ the transformation T_σ is a bijection. Applying a Runge–Kutta method to (4.26) yields

$$(4.27) \quad y_{n+1} = K(\zeta)y_n.$$

Note that if $\zeta_i = -2r$ this corresponds by (4.16) to $\zeta_i^* = \infty$. However $-2r$ is a boundary point of $D(r)$ and ∞ is a boundary point of $\overline{\mathbb{C}^-}$. As $K(\zeta)$ is a rational function (4.9) and (4.15) are true independently whether this boundary points are included or not. Hence Lemma 4.4 remains valid. The same is true for Lemma 4.5, We modify Theorem 4.1 as follows:

THEOREM 4.8 (new version of Theorem 4.1). *Assume the Runge–Kutta scheme is irreducible. Then the following conditions are equivalent*

- i) (as in Theorem 4.1)
- ii) (as in Theorem 4.1)
- iii) (new) $\frac{1}{r}$ is the smallest number such that the following holds.

Let two numerical solutions $\{y_n\}, \{\tilde{y}_n\}$ of a differential equation satisfying (4.2) be computed with the same stepsize h satisfying

$$(4.28) \quad \frac{h}{2r} \leq \beta$$

and assume that the transformation T_σ with $\sigma = \frac{1}{2r}$ is bijective then one has

$$\|y_{n+1} - \tilde{y}_{n+1}\| \leq \|y_n - \tilde{y}_n\|.$$

The proof of Theorem 4.8 can now be done exactly the same way as in the original report. However we have now requested in statement iii) that the transformation T_σ with $\sigma = \frac{1}{2r}$ is bijective.

Remarks added by the editors.

This article appeared first as a report by the Institute for Geometry and Practical Mathematics, RWTH Aachen, May 1987. G. Dahlquist worked on a report while visiting the R. Jeltsch in Aachen in June of 1983. On his way home G. Dahlquist bought a postcard in transit in Brussels which he posted while being in Copenhagen on June 13. The text of this postcard is given here, because the main idea of the second half of the article, Sections 3 and 4, namely the transformation T_σ is described on the back of the postcard. The report was submitted to BIT in Summer of 1987.