stichting mathematisch centrum

≥ MC

AFDELING NUMERIEKE WISKUNDE (DEPARTMENT OF NUMERICAL MATHEMATICS)

NW 138/82

SEPTEMBER

K. DEKKER

ON THE ITERATION ERROR IN ALGEBRAICALLY STABLE RUNGE-KUTTA METHODS

Preprint

kruislaan 413 1098 SJ amsterdam

MINIOTHEEK MATHEMATISCH CLIVING

Printed at the Mathematical Centre, 413 Kruislaan, Amsterdam.

The Mathematical Centre, founded the 11-th of February 1946, is a non-profit institution aiming at the promotion of pure mathematics and its applications. It is sponsored by the Netherlands Government through the Netherlands Organization for the Advancement of Pure Research (Z.W.O.).

On the iteration error in algebraically stable Runge-Kutta methods*)

bу

K. Dekker

ABSTRACT

In the implementation of implicit Runge-Kutta methods inaccuracies are introduced due to the solution of the implicit equations. It is shown that the effect of these errors remains bounded, provided that a dissipative equation is solved with an algebraically stable method which satisfies an additional condition. Moreover, the implicit equations have a unique solution when this condition is satisfied.

KEY WORDS & PHRASES: Numerical analysis, ordinary differential equations,
Runge-Kutta methods, algebraic stability

^{*)} This report will be submitted for publication elsewhere.



1. INTRODUCTION

We consider the class of ordinary differential equations

(1.1)
$$y'(x) = f(x,y(x)), f : \mathbb{R}^{N+1} \to \mathbb{R}^{N},$$

satisfying the contractivity condition

(1.2)
$$\langle f(x,y)-f(x,z), y-z \rangle \leq 0$$
 for all $y,z \in \mathbb{R}^N$ and $x \in \mathbb{R}$,

<., .> being an innerproduct on \mathbb{R}^N with $\|\cdot\|$ the corresponding norm. This class of equations is of particular interest in the study of stiff nonlinear systems, and it has been the subject of much recent analysis, e.g. BURRAGE and BUTCHER [1], DAHLQUIST [4]. A common property of equations of this type is that the difference between two solutions, y(x) and z(x), does not increase as x increases and it seems natural to require that a stable numerical method shares this property. BURRAGE and BUTCHER [1] associate the concept of BN-stability with this property for implicit Runge-Kutta methods and they prove that BN-stability is equivalent to algebraic stability.

In their analysis they assume that the implicit equations arising from the implicit Runge-Kutta scheme are solved exactly. However, in practical situations we are left with errors made in the iteration process used to solve the implicit equations and one may wonder whether or not these errors contaminate the final results. VERWER [11] questions the practical value of implemented BN-stable methods. He suggests that any implementation might yield unbounded errors, when applied to a judiciously chosen problem satisfying (1.2).

Recently, HUNSDORFER and SPIJKER [8] have constructed an example, in which an algebraically stable method applied to an equation satisfying (1.2) generated a system of nonlinear algebraic equations without a solution. They proved that uniqueness and existence of a solution is guaranteed if (1.2) is replaced by a slightly stronger condition. We show that a similar result holds for equations satisfying (1.2) if we impose on the Runge-Kutta method a condition somewhat stronger than algebraic stability. Moreover, we derive bounds on the errors due to the iteration process and show that these bounds

can be made as small as necessary. Finally we present some examples of algebraically stable methods and check whether the additional condition is satisfied.

2. IMPLICIT RUNGE-KUTTA METHODS

Let ..., y_{n-1},y_n,\ldots denote a sequence of approximations computed by the implicit Runge-Kutta method

with stepsize h. The approximations are defined by the solution of the equations

(2.2)
$$y_{n} = y_{n-1} + h \sum_{j=1}^{s} a_{ij} f(x_{n-1} + hc_{j}, Y_{j}), \quad i = 1, ..., s,$$

$$y_{n} = y_{n-1} + h \sum_{j=1}^{s} b_{j} f(x_{n-1} + hc_{j}, Y_{j}),$$

for $n = 1, 2, \ldots$. We quote the following definitions and theorems from BURRAGE and BUTCHER [1].

<u>DEFINITION</u>. Method (2.1) is said to be BN-stable if for two solution sequences ..., y_{n-1}, y_n, \ldots and ..., z_{n-1}, z_n, \ldots applied to any problem (1.1) such that (1.2) holds, $\|y_n - z_n\| \le \|y_{n-1} - z_{n-1}\|$.

The algebraic stability criterion is concerned with the quadratic form $(\xi_1,\xi_2,\ldots,\xi_s)^T$ M $(\xi_1,\xi_2,\ldots,\xi_s)$, where

(2.3)
$$M = diag(b_1, ..., b_s) A + A^T diag(b_1, ..., b_s) - bb^T$$
.

In the sequel we will denote $diag(b_1,...,b_s)$ by the diagonal matrix B.

<u>DEFINITION</u>. Method (2.1) is said to be *algebraically stable* if B is non-negative and M is non-negative.

THEOREM 2.1. BN-stability is equivalent to algebraic stability.

<u>PROOF.</u> See BURRAGE and BUTCHER [1], theorem 2.2 and 3.3, and for the confluent case (not all c_i distinct) HUNSDORFER and SPIJKER [7].

If one of the weights b_i , $1 \le i \le s$, is zero, then algebraic stability implies that the corresponding column of A with elements $a_{j,i}$, $j=1,2,\ldots,s$, is zero too, so that the method is reducible (DAHLQUIST and JELTSCH [5]). As we will consider irreducible methods only, we assume in the sequel that B is positive.

3. SOLUTION OF THE IMPLICIT EQUATIONS

In an implementation of the Runge-Kutta method, the implicit equations (2.2) have to be solved by some iteration process, in which one may apply various strategies. BURRAGE, BUTCHER and CHIPMAN [2] perform fixed point iteration for non-stiff and Newton iteration for stiff problems, carrying out either a specified number of iterations or iterating to convergence. Alternatives are e.g. iterated defect correction (FRANK and UEBERHUBER [6], BUTCHER [3]) or Rosenbrock-type methods (KAPS and WANNER [9]). In the implemented Runge-Kutta methods one is faced with the problem whether to reevaluate the Jacobian matrix or to carry on with an old approximation, and when to break off the iterations. For the sake of efficiency, one will be inclined to perform a few iterations only and to evaluate the Jacobian matrix not too frequently, so that the equations (2.2) are not solved exactly.

Now, let Y_1,Y_2,\ldots,Y_s denote the exact solution of (2.2), and Z_1,Z_2,\ldots,Z_s the solution obtained by some iteration method. We define the iteration errors ϵ_i by

(3.1)
$$Z_i = y_{n-1} + h \sum_{j=1}^{s} a_{ij} f(x_{n-1} + hc_j, Z_j) + \epsilon_i, \quad i = 1, 2, ..., s.$$

In order to simplify the notation we introduce

(3.2)
$$k_{i}^{*} = hf(x_{n-1} + hc_{i}, Y_{i}), \qquad i = 1, 2, ..., s,$$
$$k_{i}^{*} = hf(x_{n-1} + hc_{i}, Z_{i}), \qquad i = 1, 2, ..., s.$$

We remark that the equations (2.2) can be written in the mathematical equivalent form

(3.3)
$$k_{i} = hf(x_{n-1} + hc_{i}, y_{n-1} + \sum_{j=1}^{s} a_{ij}k_{j}), \quad i = 1, 2, ..., s$$

$$y_{n} = y_{n-1} + \sum_{j=1}^{s} b_{j}k_{j}.$$

The defect iteration errors in the numerical solution of (2.2) and (3.3) are related, provided that the matrix A is non-singular. For example, let δ_i , $i=1,2,\ldots,s$ be the solution of $\sum_{j=1}^{S}a_{ij}\delta_j=\epsilon_i$, $i=1,2,\ldots,s$. Substitution of (3.1) in (3.2) and using the relation between δ_i and ϵ_i , $i=1,2,\ldots,s$, yields

$$k_{i}^{*} = hf(x_{n-1}^{+hc}, y_{n-1}^{+} + \sum_{j=1}^{s} a_{ij}(k_{j}^{*} + \delta_{j}^{*})), \quad i = 1, 2, ..., s,$$

so the defect errors in (3.3) upon substitution of $k_i^* + \delta_i$ for k_i are given by δ_i , i = 1, 2, ..., s.

When A is singular, it is generally not possible to obtain an approximate solution to (3.3) from a solution of (3.1). However, no useful algebraically stable method with singular A is known to the authors. Therefore, we will restrict ourselves to formulation (2.2) and assume that the numerical solution satisfies (3.1). We note that small values of ϵ_i , $i=1,2,\ldots,s$, not necessarily imply that the differences between the exact solutions Y and k and the numerical approximations Z_i and Z_i and Z_i are small, too. We will derive bounds on these differences in the next section. Moreover, we investigate the influence of the iteration errors on the approximation to y

at the point $x_n = x_{n-1} + h$.

4. ERROR BOUNDS

Let Y_i, Z_i, k_i^*, k_i and ϵ_i , i = 1, 2, ..., s, be defined as in the previous section, and z_n denote the numerical approximation at x_n

(4.1)
$$z_n = y_{n-1} + \sum_{j=1}^{s} b_j k_j^*$$

Let the differences between the numerical and exact solutions of the non-linear systems (2.2) and (3.2) be given by

$$v_{i} = Z_{i} - Y_{i}, \quad i = 1, 2, ..., s,$$

$$w_{i} = k_{i}^{*} - k_{i}, \quad i = 1, 2, ..., s,$$

$$v = z_{n} - y_{n}.$$

Now, for any positive matrix $D = diag(d_1, ..., d_s)$ we may define a norm $\| \|_D$ and an inner-product $[,]_D$ for sequences $W = (w_1, w_2, ..., w_s)^T$ and $V = (v_1, v_2, ..., v_s)^T$ by

(4.3)
$$[v,w]_D = \sum_{i=1}^{s} d_i < v_i, w_i > .$$

LEMMA 4.1. Let (2.1) be an algebraically stable method, $f: \mathbb{R}^{N+1} \to \mathbb{R}^N$ satisfy (1.2) and the numerical approximations satisfy (3.1). Define $\varepsilon = (\varepsilon_1, \dots, \varepsilon_s)^T$. Then,

PROOF. (Confer [1], theorem 2.2). Using (3.1)-(3.2) we have

(4.5)
$$v_i = \varepsilon_i + \sum_{j=1}^{s} a_{ij} w_j, \quad i = 1, 2, ..., s,$$

(4.6)
$$v = \sum_{j=1}^{s} b_{j} w_{j}$$
.

The squared norm of v is

$$\|\mathbf{v}\|^2 = \sum_{i=1}^{s} \sum_{j=1}^{s} b_i b_j < \mathbf{w}_i, \mathbf{w}_j > = \sum_{i=1}^{s} \sum_{j=1}^{s} (b_i a_{i,j} + b_j a_{i,j} - \mathbf{m}_{i,j}) < \mathbf{w}_i, \mathbf{w}_j > ,$$

where m_{ij} are the elements of the symmetric matrix M given by (2.3). Substitution of the inner products of (4.5) and w_{ij} yields

$$\|v\|^2 = -\sum_{i=1}^{s} \sum_{j=1}^{s} m_{ij} \langle w_i, w_j \rangle + 2\sum_{i=1}^{s} b_i \langle v_i, w_i \rangle - 2\sum_{i=1}^{s} b_i \langle \varepsilon_i, w_i \rangle.$$

Algebraic stability implies that M is nonnegative definite, so that the first term is non-positive. Moreover, B = diag(b₁,b₂,...,b_s) is nonnegative and $\langle v_i,w_i \rangle = \langle Z_i - Y_i, hf(x_{n+1}+hc_i,Z_i)-hf(x_{n-1}+hc_i,Y_i) \rangle \leq 0$ according to the assumptions. Thus

$$\| \mathbf{v} \|^2 \le -2 \sum_{i=1}^{s} b_i < \epsilon_i, \mathbf{w}_i > = -2[\epsilon, \mathbf{W}]_B \le 2\|\epsilon\|_B \|\mathbf{W}\|_B.$$

LEMMA 4.2. Let $f: \mathbb{R}^{N+1} \to \mathbb{R}^N$ be continuous and satisfy (1.2). Let B be positive diagonal, $\widetilde{A} = B^{\frac{1}{2}}AB^{-\frac{1}{2}}$ and assume that $\widetilde{A} + \widetilde{A}^T$ is positive. Then, the system (2.2) has a unique solution $Y = (Y_1, \ldots, Y_s)^T$ and for any numerical approximation satisfying (3.1) the following error bound holds

(4.7)
$$\|\mathbf{W}\|_{\mathbf{B}} \leq \|\mathbf{\varepsilon}\|_{\mathbf{B}} \left\{ \frac{1}{2} \lambda_{\min} (\widetilde{\mathbf{A}} + \widetilde{\mathbf{A}}^{\mathrm{T}}) \right\}^{-1}.$$

<u>PROOF</u>. Following [8] we define the function $\mathbb{F}: \mathbb{R}^{Ns} \to \mathbb{R}^{Ns}$ by

$$\mathbb{F}(Y) = h(f(x_{n-1} + c_1h, Y_1), f(x_{n-1} + c_2h, Y_2), \dots, f(x_{n-1} + c_sh, Y_s))^T$$

and

$$\mathbb{A} = \mathbb{A} \otimes \mathbb{I}_{\mathbb{N}}$$

where I_N is the N × N identity matrix and \otimes stands for the Kronecker product. Let $1 = (1,1,\ldots,1)^T$ be a vector of dimension s. Then the system (2.2) can be written as the equation

(4.8)
$$Y = (1 \otimes I_N)y_{n+1} + AF(Y).$$

Existence. At first we observe that the positivity of \widetilde{A} + \widetilde{A}^T implies that \widetilde{A} is regular and hence A and A are regular too. Consequently we may define the function $G(Y) = A^{-1}(Y-(1\otimes I_N)y_{n+1})-F(Y)$. We calculate for arbitrary Y and \widetilde{Y}

$$\begin{bmatrix} G(\widetilde{Y}) - G(Y), \widetilde{Y} - Y \end{bmatrix}_{B} = \begin{bmatrix} A^{-1}(\widetilde{Y} - Y), \widetilde{Y} - Y \end{bmatrix}_{B} - \begin{bmatrix} \mathbb{F}(\widetilde{Y}) - \mathbb{F}(Y), \widetilde{Y} - Y \end{bmatrix}_{B} \geq$$

$$\geq \begin{bmatrix} A^{-1}(\widetilde{Y} - Y), \widetilde{Y} - Y \end{bmatrix}_{B},$$

because of condition (1.2) and the definition of the inner product $[,]_B$. Now, introduce $V = A^{-1}(\widetilde{Y}-Y)$. Evaluation of the inner product yields

$$\begin{split} (\star) & \qquad \left[\mathbb{V}_{\bullet} \mathbb{A} \ \mathbb{V} \right]_{B} \ = \ \mathbb{V}^{T} (\mathbb{B} \otimes \mathbb{I}_{N}) \mathbb{A} \mathbb{V} \ = \ \mathbb{V}^{T} (\mathbb{B} \mathbb{A} \otimes \mathbb{I}_{N}) \mathbb{V} \ = \\ & \qquad = \ \mathbb{V}^{T} (\frac{1}{2} (\mathbb{B} \mathbb{A} + \mathbb{A}^{T} \mathbb{B}) \otimes \mathbb{I}_{N}) \mathbb{V} \ = \ \mathbb{V}^{T} (\mathbb{B}^{\frac{1}{2}} \otimes \mathbb{I}_{N}) (\frac{1}{2} (\widetilde{\mathbb{A}} + \widetilde{\mathbb{A}}^{T}) \otimes \mathbb{I}_{N}) (\mathbb{B}^{\frac{1}{2}} \otimes \mathbb{I}_{N}) \mathbb{V} \ \geq \\ & \qquad \geq \ \frac{1}{2} \lambda_{\min} \{ (\widetilde{\mathbb{A}} + \widetilde{\mathbb{A}}^{T}) \otimes \mathbb{I}_{N} \} [\mathbb{V}_{\bullet} \mathbb{V}_{B}] \ = \ \frac{1}{2} \lambda_{\min} (\widetilde{\mathbb{A}} + \widetilde{\mathbb{A}}^{T}) [\mathbb{V}_{\bullet} \mathbb{V}_{B}]_{B} . \end{split}$$

Moreover, $\|AV\|_{B} \le \|A\|_{B} \|V\|_{B}$. Using these results we obtain

$$[G(\widetilde{Y})-G(Y),\widetilde{Y}-Y]_{B} \geq \frac{1}{2}\lambda_{\min}(\widetilde{A}+\widetilde{A}^{T}) \frac{\|\widetilde{Y}-Y\|_{B}^{2}}{\|A\|_{B}^{2}},$$

so G is uniformly monotone, because the constant $\frac{1}{2}\lambda_{\min}(A+A^T)\|A\|_B^{-2}$ is positive, and according to the uniform monotonicity theorem formulated in [10,p.167] G has a zero.

Uniqueness. Let Y be a solution of (2.2) and $Z = (Z_1, Z_2, ..., Z_s)^T$ be a solution of (3.1). Let v_i, w_i , i = 1, 2, ..., s be defined as in the previous lemma, and define $V = (v_1, v_2, ..., v_s)^T$, $W = (w_1, w_2, ..., w_s)^T$. Then, according to (4.5)

$$(4.8) \qquad V = \varepsilon + AW$$

so using (*) we obtain the estimate

$$\frac{1}{2}\lambda_{\min}(\widetilde{A}+\widetilde{A}^{T})\|\mathbf{W}\|_{B}^{2}\leq\left[\mathbf{A}\mathbf{W},\mathbf{W}\right]_{B}=\left[\mathbf{V},\mathbf{W}\right]_{B}-\left[\boldsymbol{\varepsilon},\mathbf{W}\right]_{B}\leq\left\|\boldsymbol{\varepsilon}\right\|_{B}\|\mathbf{W}\|_{B}.$$

The uniqueness is an immediate consequence of this error bound: $\|\epsilon\|_B = 0$ implies that $\|W\|_B = 0$ and hence $\|V\|_B = 0$. \square

REMARK. Obviously the solution of the implicit equations (2.2) does not depend on the weights b_i , i = 1,2,...,s. Thus, lemma 2.2 remains valid if we replace B by an arbitrary diagonal matrix. We did use the matrix B in our formulation in order to have the same inner products as in lemma 3.1 and because algebraic stability implies that \widetilde{A} + \widetilde{A}^T is non-negative, so that the requirement of positivity is only a slightly stronger condition. However, for an arbitrary positive matrix D the eigenvalues of $D^{\frac{1}{2}}AD^{-\frac{1}{2}} + D^{-\frac{1}{2}}A^{T}D^{\frac{1}{2}}$ may be negative (see example 4.3). Finally, we remark that HUNSDORFER and SPIJKER [8] did also use the matrix B in their theorem. Noting that algebraic stability and irreducibility imply that B is positive, we arrive at

COROLLARY 4.3. Let (2.1) be an irreducible, algebraically stable method, and suppose that $B^{\frac{1}{2}}AB^{-\frac{1}{2}} + B^{-\frac{1}{2}}A^TB^{\frac{1}{2}}$ is positive definite. Then, for any problem (1.1) satisfying (1.2) the error $v = z_n - y_n$ is bounded by

(4.9)
$$\|v\| \leq 2\{\lambda_{\min}(B^{\frac{1}{2}}AB^{-\frac{1}{2}}+B^{-\frac{1}{2}}A^{T}B^{\frac{1}{2}})\}^{-\frac{1}{2}}\|\varepsilon\|_{B},$$

where ε denotes the defect errors given by (3.1).

We conclude with some examples of algebraically stable methods. The first two satisfy the conditions of the lemmata, the third one fulfills the requirements of lemma 4.2 after B is replaced by a diagonal D. The last method does not satisfie these conditions for any diagonal D and system (3.1) is shown to have no solution for some particular dissipative equation.

EXAMPLE 4.1. The two-stage Lobatto IIIC method given by

$$\begin{array}{c|cccc}
0 & \frac{1}{2} & -\frac{1}{2} \\
1 & \frac{1}{2} & \frac{1}{2} \\
\hline
& \frac{1}{2} & \frac{1}{2}
\end{array}$$

Moreover, $A + A^{\perp} = B^2AB^{-\frac{1}{2}} + B^{-\frac{1}{2}}A^{\perp}B^{\frac{1}{2}} = A + A^{\perp} = \frac{1}{2}I$. Thus, according to corollary 4.3, $\|\mathbf{v}\| \le 2\sqrt{2}\|\mathbf{e}\|_{B}$.

EXAMPLE 4.2. The two-stage Radau IIA method given by

M is given by $\frac{1}{16} \binom{1}{-1}$, so the method is algebraically stable. $B^{\frac{1}{2}}AB^{-\frac{1}{2}} + B^{-\frac{1}{2}}A^{T}B^{\frac{1}{2}} \text{ equals } \frac{1}{6} \binom{5}{\sqrt{3}}$, which matrix has the eigenvalues $\frac{1}{3}$ and 1, so the error estimate (4.9) becomes $\|\mathbf{v}\| \leq 2\sqrt{3} \|\mathbf{e}\|_{\mathbf{R}}$.

EXAMPLE 4.3. The two-stage diagonally implicit method

$$\begin{array}{c|cccc}
\lambda & \lambda & 0 \\
1-\lambda & 1-2\lambda & \lambda \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}$$

is algebraically stable iff $\lambda \geq \frac{1}{4}$ (see [1]). The eigenvalues μ of $B^{\frac{1}{2}}AB^{-\frac{1}{2}}+B^{-\frac{1}{2}}A^TB^{\frac{1}{2}}=\widetilde{A}+\widetilde{A}^T$ are obtained from the equation $(\mu-2\lambda)^2-(1-2\lambda)^2=0$. Hence, we have the estimates for the error

$$\| \mathbf{v} \| \leq \begin{cases} 2 \| \boldsymbol{\varepsilon} \|_{B} / \sqrt{4 \lambda - 1}, & \frac{1}{4} < \lambda < \frac{1}{2} \\ 2 \| \boldsymbol{\varepsilon} \|_{B}, & \lambda > \frac{1}{2}. \end{cases}$$

This bound is not very satisfactory for values of λ close to $\frac{1}{4}$. However, if we take in stead of B a suitable diagonal matrix D = diag(1,d²), according to the remark after lemma 4.2, we obtain a better estimate. The eigenvalues of $D^{\frac{1}{2}}AD^{-\frac{1}{2}} + D^{-\frac{1}{2}}A^{T}D^{\frac{1}{2}}$ are $2\lambda \pm d(1-2\lambda)$, so lemma (4.2) yields the estimate

$$\|W\|_{D} \leq 2\|\varepsilon\|_{D} \frac{1}{2\lambda(1+d)-d}, \quad \tfrac{1}{4} \leq \lambda < \tfrac{1}{2}, \quad 0 < d < \tfrac{2\lambda}{1-2\lambda} \ .$$

Using the relation between the B and D norms,

$$\sqrt{2} \min(1,d) \| \cdot \|_{B} \le \| \cdot \|_{D} \le \sqrt{2} \max(1,d) \| \cdot \|_{B}$$

and taking the optimal value for d, we obtain

$$\|\mathbf{W}\|_{\mathbf{B}} \leq 2\|\mathbf{\varepsilon}\|_{\mathbf{B}} \frac{1-2\lambda}{\lambda^{2}}, \qquad \frac{1}{4} \leq \lambda \leq \frac{1}{3},$$

$$\|\mathbf{v}\| \leq 2\|\mathbf{\varepsilon}\|_{\mathbf{B}} \left\{\frac{1-2\lambda}{\lambda^{2}}\right\}^{\frac{1}{2}}, \quad \frac{1}{4} \leq \lambda \leq \frac{1}{3}.$$

For values of λ outside the interval $[\frac{1}{4},\frac{1}{3}]$ the choice D = B turns out to yield the best estimates.

EXAMPLE 4.4. The three-stage Lobatto method of order 4 given by

A straightforward calculation yields $M = (\frac{1}{6}, -\frac{1}{3}, \frac{1}{6})^T (\frac{1}{6}, -\frac{1}{3}, \frac{1}{6})$; thus M is nonnegative. The matrix $\widetilde{A} + \widetilde{A}^T$ is singular, because it is given by $B^{-\frac{1}{2}}(M+bb^T)B^{-\frac{1}{2}}$ and $M + bb^T$ has rank two. Thus we cannot apply Lemma 4.2 directly. When we try $D = diag(p^2, 4, q^{-2})$, we obtain for $D^{\frac{1}{2}}AD^{-\frac{1}{2}} + D^{-\frac{1}{2}}A^TD^{\frac{1}{2}}$ the eigenvalue equation

$$-\mu^{3} + \frac{3}{2}\mu^{2} - \frac{1}{36}\mu \left\{24 - c_{p}^{2} - c_{q}^{2} - c_{pq}^{2}\right\} + \frac{1}{216}\left\{20 - 2c_{p}^{2} - 2c_{q}^{2} - 5c_{pq}^{2} + 2c_{p}c_{q}c_{pq}\right\} = 0,$$

where $C_p = \frac{2}{p} - p$, $C_q = \frac{2}{q} - q$ and $C_{pq} = pq + \frac{1}{pq}$. All eigenvalues are real and they lie on the positive axis if: the coefficients of the characteristic polynomial have alternating signs. However, as $C_{pq} \ge 2$, one easily verifies that these conditions can not be satisfied. In fact, only the case p = q = 1 yields non-negative eigenvalues, although one of these equals zero.

Now we construct a class of dissipative equations for which the errors

between the exact solution of (2.2) Y and the numerical approximation Z may become arbitrarily large even if the defect errors ε_i , i = 1,2,3, are very small.

Define the function $f:\mathbb{R}^2\to\mathbb{R}$ by f(x,y)=-K(x)y, where $K(x_{n-1})=K(x_{n-1}+h)=K(K>0)$ and $K(x_{n-1}+h)=0$. Then Y is the solution of

$$Y = 1y_{n-1} + A diag(-hK, 0, -hK)Y.$$

Let Z be the exact solution of

$$Z = 1y_{n-1} + A \operatorname{diag}(-hK, 0, -hK)Z + (\epsilon_1, 0, -\epsilon_1)^T$$
.

Then the difference Z - Y equals $(\epsilon_1, -\frac{1}{4}hK\epsilon_1, -\epsilon_1)^T$ and this may increase beyond all bounds if we choose K large enough.

EXAMPLE 4.5. HUNSDORFER and SPIJKER [8] constructed the fourth order algebraically stable method

and a dissipative equation for which system (2.2) does not have a solution. Indeed, we verify that lemma 4.2 is not applicable. Let D be diag(p²,q²,1), and v the vector (p(α + β), q($-\alpha$ + β), $-\beta$)^T, where α and β are arbitrary constants. Then we calculate the quadratic form $v^T(D^{\frac{1}{2}}AD^{-\frac{1}{2}}+D^{-\frac{1}{2}}A^TD^{\frac{1}{2}})v=(p^2-q^2)(\frac{1}{3}\sqrt{6\alpha^2-\sqrt{6}\beta^2})+\frac{2}{3}\sqrt{6\alpha\beta}(1-p^2-q^2).$ Obviously we can choose α and β in such a way that this form is negative, unless $p^2=q^2=\frac{1}{2}$. Thus, $\lambda_{\min}(D^{\frac{1}{2}}AD^{-\frac{1}{2}}+D^{-\frac{1}{2}}A^TD^{\frac{1}{2}})\leq 0$, and equality occurs for D = B.

Acknowledgement

The author is very grateful to Dr. J. Verwer for his useful comments.

REFERENCES

- [1] BURRAGE, K. and J.C. BUTCHER, Stability criteria for implicit Runge-Kutta methods, SIAM J. Num. An. 16(1979), pp.46-57.
- [2] BURRAGE, K., J.C. BUTCHER and F.H. CHIPMAN, Stride: Stable Runge-Kutta integrator for differential equations, Computational Mathematics, Report No. 19, University of Auckland, 1979.
- [3] BUTCHER, J.C., Some implementation schemes for implicit Runge-Kutta methods, Proceedings of Dundee Conference in Numerical Analysis, 1979.
- [4] DAHLQUIST, G., G-stability is equivalent to A-stability, BIT 18(1978), pp.384-401.
- [5] DAHLQUIST, G. and R. JELTSCH, Generalized disks of contractivity for explicit and implicit Runge-Kutta methods, TRITA-NA Report 7906, Stockholm, 1979.
- [6] FRANK, R. and C.W. UEBERHUBER, Iterated defect correction for the efficient solution of stiff systems of ordinary differential equations, BIT 17(1977), pp.146-159.
- [7] HUNSDORFER, W.H. and M.N. SPIJKER, A note on B-stability of Runge-Kutta methods, Numer. Math. 36(1981), pp.319-331.
- [8] HUNSDORFER, W.H. and M.N. SPIJKER, On the existence of solutions to the algebraic equations in implicit Runge-Kutta methods, Report no. 81-49, University of Leiden, 1981.
- [9] KAPS, P. and G. WANNER, A study of Rosenbrock-type methods of high order, Numer. Math. 38 (1981), pp.279-298.
- [10] ORTEGA, J.M. and W.C. RHEINBOLDT, Iterative solution of nonlinear equations in several variables, New York, Academic Press, 1970.
- [11] VERWER, J.G., On the practical value of the notion of BN-stability, BIT 21 (1981), pp.355-361.

