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INTERNAL S-STABILITY FOR GENERALIZED RUNGE-KUTTA METHODS

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Internal S-stability for generalized Runge-Kutta methods

by

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ABSTRACT

In a previous report the *S-stability* for *generalized Runge-Kutta methods* was investigated. In this report the concept of *internal S-stability* is introduced. Internal S-stability is concerned with the stability behaviour of approximations at intermediate points from the step-interval, while S-stability is only concerned with the approximation at the endpoint of the step-interval. In order to illustrate the relevance of the new concept of stability, numerical results are presented of an A-stable, an S-stable, and an internally S-stable method, applied to four stiff, nonlinear problems from literature.

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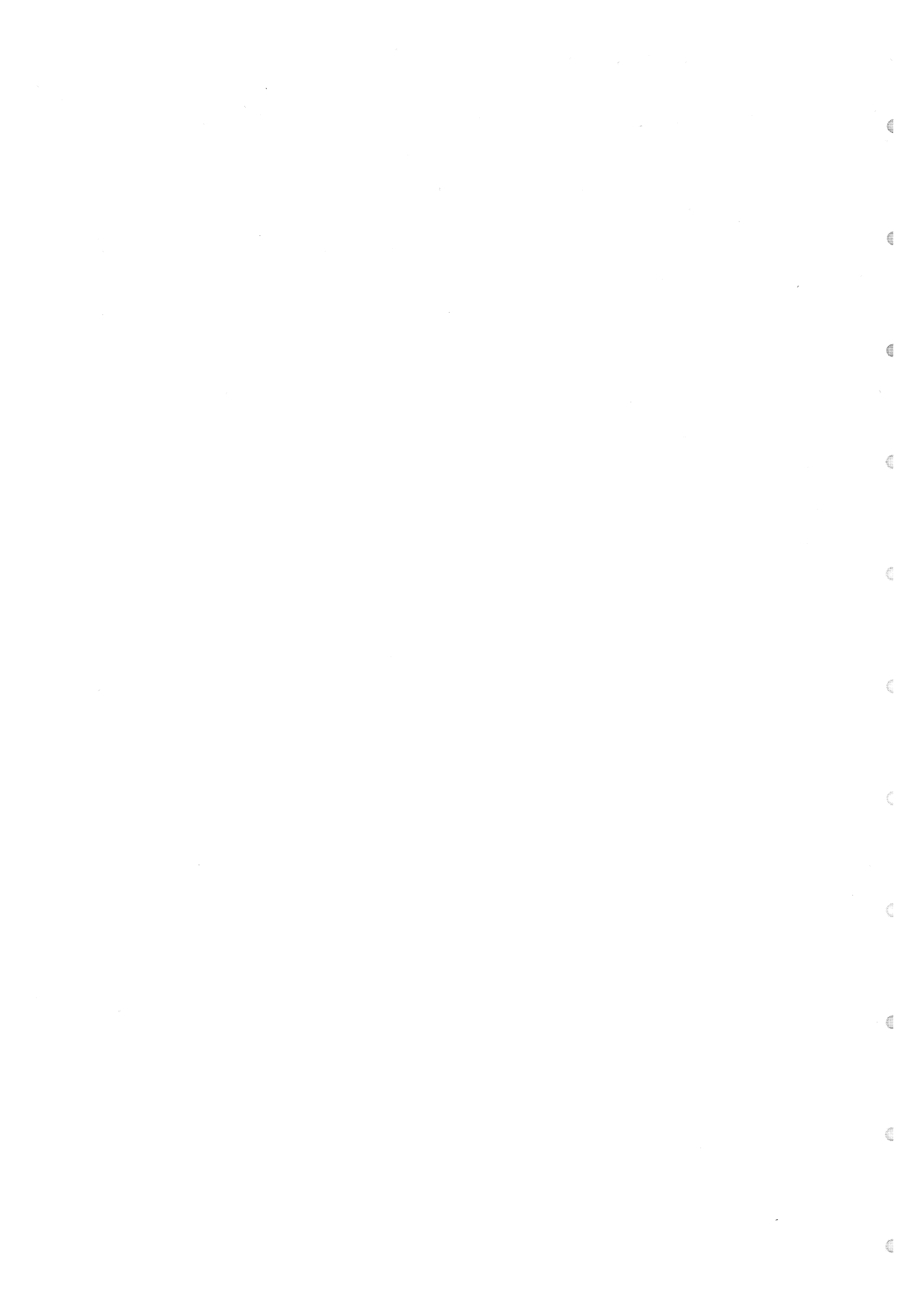
1. INTRODUCTION

Let

(1.1) $y' = f(x,y)$

represent a set of stiff differential equations, subject to the initial condition

(1.2) $y = y_0$ at $x = x_0$.

A basic difficulty in the numerical solution of stiff, non-linear systems, is the requirement of stability. In order to analyse the numerical difficulties that are encountered when solving such systems with implicit one-step methods, PROTHERO & ROBINSON [7] propose the scalar test-model

(1.3) $y' = g'(x) + \delta(y - g(x))$, $\delta \in \mathbb{C}$, $\text{Re}(\delta) < 0$,

where g is an arbitrary function with bounded derivative. They analyse the stability of numerical approximations to the solution $y \equiv g$ of equation (1.3) and derive necessary and sufficient conditions for such stability, which is termed *S-stability*. They also analyse the accuracy of numerical approximations to the solution $y \equiv g$, by considering the asymptotic form of the local truncation error for

(1.4) $h\text{Re}(\delta) \to -\infty$ and $h \to 0$,

where h denotes an integration stepsize. Herewith, they propose the concept of stiff-accuracy.

In VERWER [11], we have applied the ideas of Prothero and Robinson to *generalized Runge-Kutta methods*. We have derived necessary and sufficient conditions for the coefficient functions, to obtain the S-stability property. This property has been shown to be of practical relevance for our class of methods. When applied to stiff, *non-linear* systems, S-stable methods

are more reliable than A-stable methods.

We also considered the asymptotic form of the local truncation error, with respect to the solution $y \equiv g$ of (1.3), in the limit (1.4). It is of importance to note that our definition of stiff-accuracy differs from that given by Prothero and Robinson. Following a suggestion of PROTHERO [8], it is more convenient to use the term stiff-consistency instead of stiff-accuracy for our methods.

In VERWER [11], we suggested to develop formulas for which the asymptotic error mentioned above, is minimized. Until now this has not been shown to be of great practical relevance for our methods, when applied to stiff, non-linear systems. A more realistic approach to improve our S-stable methods is discussed in this report.

With the derivation of the test-model (1.3) we neglect the dependence of the Jacobian upon x on each step-interval. In order to predict the stability and accuracy behaviour of an integration method for stiff, non-linear systems, it is more realistic to consider test-models in which a *variable Jacobian* occurs. However, for most integration methods, and certainly for ours, it is impracticable to do this (see also LAMBERT & SIGURDSSON [5]). To get round this difficulty, we propose for our class of methods the concept of *internal S-stability*, which is stronger than S-stability. Internal S-stability imposes conditions on approximations at *intermediate points* from the step-interval, while S-stability is only concerned with the approximation at the endpoint of the step-interval. Thus, in a certain sense, this form of stability takes into account a variable Jacobian matrix. In the last section of this report we shall present some numerical examples which illustrate the relevance of the various stability concepts.

2. PRELIMINARIES

Let h_n denote the steplength $h_n = x_{n+1} - x_n$, and let y_n denote the numerical approximation to the analytical solution $y(x)$ of system (1.1) at $x = x_n$. Let J_n denote the Jacobian matrix of system (1.1) at the point (x_n, y_n). Further, define

(2.1) $\Lambda_{j,\ell}$, $j = 0,\ldots, m$; $\ell = 0,\ldots,j-1$,

to be rational functions with real coefficients. Then, the generalized Runge-Kutta method is defined by

$$(2.2) \qquad y_{n+1} = y_n + \sum_{j=0}^{m-1} \Lambda_{m,j}(h_n J_n)k_n^{(j)},$$

$$(2.3) \qquad k_n^{(j)} = h_n f(x_n + \mu_j h_n, y_n + \sum_{\ell=0}^{j-1} \Lambda_{j,\ell}(h_n J_n)k_n^{(\ell)}),$$

where the parameters μ_j are given by

$$(2.4) \qquad \mu_j = \sum_{\ell=0}^{j-1} \Lambda_{j,\ell}(0).$$

By means of (2.4), we also define the parameter μ_m, and shall always assume that $\mu_m = 1$. This means that the scheme has always order of consistency $p \geq 1$. For convenience, it is also assumed that $\mu_j \neq \mu_k$ if $j \neq k$, $j,k = 0,\ldots,m-1$. Results can be easily extended to the case of equal parameters.

In the form (2.2)-(2.3), Runge-Kutta formulas are usually presented in the literature. By putting

$$k_n^{(j)} = h_n f(x_n + \mu_j h_n, y_{n+1}^{(j)}), \qquad j = 0,\ldots,m-1,$$

(2.5)

$$y_{n+1} = y_{n+1}^{(m)},$$

the Runge-Kutta scheme assumes the form

$$y_{n+1}^{(0)} = y_n,$$

$$(2.6) \qquad y_{n+1}^{(j)} = y_n + h_n \sum_{\ell=0}^{j-1} \Lambda_{j,\ell}(h_n J_n) f(x_n + \mu_\ell h_n, y_{n+1}^{(\ell)}), \qquad j = 1,\ldots,m,$$

$$y_{n+1} = y_{n+1}^{(m)}.$$

In this paper we shall use representation (2.6). Formula (2.6) may be formally characterized by the $(m+1)*(m+1)$ matrix

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$$
(2.7) \qquad \Lambda = \begin{bmatrix} 0 & 0 & . & . & . & . & & 0 \\ \Lambda_{1,0} & 0 & . & . & . & . & & 0 \\ \Lambda_{2,0} & \Lambda_{2,1} & & & & & & . \\ . & . & . & & & & & . \\ . & . & & . & & & & . \\ . & . & & & . & & & . \\ . & . & & & & . & & . \\ \Lambda_{m,0} & \Lambda_{m,1} & . & . & . & & \Lambda_{m,m-1} & 0 \end{bmatrix} \qquad .
$$

In the next section we need the elements of the inverse of the matrix $I - z\Lambda(z)$. In order to determine these elements, we introduce the functions

$$
(2.8) \qquad \sigma_{j,k,\ell} = \sum \Lambda_{i_{k+1},i_k} \Lambda_{i_k,i_{k-1}} \cdots \Lambda_{i_2,i_1} \Lambda_{i_1,i_0} ,
$$

where the summation runs over all $(k+2)$-tuples $(i_{k+1},i_k,\ldots,i_0)$, which satisfy: $j = i_{k+1} > i_k > \ldots > i_1 > i_0 = \ell$. Then, by means of elementary matrix algebra, it is easily proved that the inverse of the matrix

$$
(2.9) \qquad I - z\Lambda(z),
$$

is given by

$$
(2.10) \qquad \eta(z) = \begin{bmatrix} 1 & 0 & 0 & . & . & . & 0 \\ \eta_{1,0}(z) & 1 & 0 & . & . & . & 0 \\ \eta_{2,0}(z) & \eta_{2,1}(z) & 1 & & & & . \\ . & . & . & & & & . \\ . & . & & . & & & . \\ . & . & & & . & & 0 \\ \eta_{m,0}(z) & \eta_{m,1}(z) & . & . & . & \eta_{m,m-1}(z) & 1 \end{bmatrix} ,
$$

where

$$(2.11) \qquad \eta_{j,\ell}(z) = \sum_{k=0}^{j-1-\ell} z^{k+1} \sigma_{j,k,\ell}(z).$$

In this paper we pay no special attention to rational approximations to the exponential. For all properties and definitions which are used the reader is referred to LAMBERT [4]. We will, however, give one definition: Let R be A-acceptable, then R is said to be strongly A-acceptable if, in addition,

$$(2.12) \qquad \lim_{\mathrm{Re}(z) \to -\infty} |R(z)| < 1.$$

3. INTERNAL S-STABILITY

In VERWER [11] we have studied the S-stability- and stiff-consistency properties of the generalized Runge-Kutta method. To that end we had to neglect the dependence of the Jacobian upon x on each step-interval $[x_n, x_n + h_n]$. In order to predict the stability and accuracy behaviour of a generalized Runge-Kutta method when applied to a stiff, non-linear system, it is more realistic to consider test-equations in which a variable Jacobian occurs. However, for integration schemes of the Runge-Kutta type (2.6) it is impracticable to perform such an analysis (see also Lambert & Sigurdsson [5]).

To get round this difficulty we propose, for generalized Runge-Kutta methods, the concept of internal S-stability, which is stronger than S-stability. In a certain sense, this form of stability takes into account a variable Jacobian matrix.

Internal S-stability imposes more conditions on the rational functions $\Lambda_{j,\ell}$ than S-stability. As a consequence, it will often occur that the conditions for internal S-stability will only hold if $|\arg(-\delta)| < \alpha, \alpha \in (0, \frac{\pi}{2})$. Therefore, it is more convenient to discuss internal $S(\alpha)$-stability rather than internal S-stability.

From formulas (2.4-(2.6) we see that the intermediate vectors

$y_{n+1}^{(j)}$, $j = 1,\ldots,m-1$, are first order consistent approximations at the intermediate points $x_n + \mu_j h_n$. Because method (2.6) is generally applied to stiff, non-linear systems, it is of importance to relate the stiffness of the equation also with the intermediate approximations $y_{n+1}^{(j)}$, $j = 1,\ldots,m-1$. Until now, the stiffness has only been related to the approximation $y_{n+1} = y_{n+1}^{(m)}$.

We shall consider the test-equation (1.3). To begin with, we introduce the abbreviations

$$r_{n+1}^{(j)} = g'(x_n+\mu_j h_n) - \delta g(x_n+\mu_j h_n), \qquad j = 0,\ldots,m-1,$$

(3.2)

$$g_{n+1}^{(j)} = g(x_n+\mu_j h_n), \qquad j = 0,\ldots,m.$$

Furthermore, we define the m+1-vectors

$$\vec{r}_{n+1} = [r_{n+1}^{(0)},\ldots,r_{n+1}^{(m-1)}, \ 0]^T,$$

(3.3)
$$\vec{g}_{n+1} = [g_{n+1}^{(0)},\ldots,g_{n+1}^{(m)}]^T,$$

$$\vec{e} = [1,\ldots,1]^T.$$

Observe that in our notation $g_{n+1}^{(0)} = g(x_n)$. Finally, for scalar equations, we define the m+1-vector

(3.4)
$$\vec{y}_{n+1} = [y_{n+1}^{(0)},\ldots,y_{n+1}^{(m)}]^T.$$

When applied to (1.3), the Runge-Kutta method (2.6) yields the relation

(3.5)
$$\vec{y}_{n+1} = (I-z\Lambda(z))^{-1}y_n\vec{e} + z^{-1}((I-z\Lambda(z))^{-1}-I)h_n\vec{r}_{n+1},$$

where $z = h_n$ (compare VERWER [11]).

Next, we define the errors

$$(3.6) \qquad \varepsilon_{n+1}^{(j)} = y_{n+1}^{(j)} - g_{n+1}^{(j)}, \qquad j = 0,\ldots,m,$$

and the error-vector

$$(3.9) \qquad \vec{\varepsilon}_{n+1} = \vec{y}_{n+1} - \vec{g}_{n+1}.$$

The concept of $S(\alpha)$-stability is concerned with the error $\varepsilon_{n+1}^{(m)}$. We shall now define the concept of internal $S(\alpha)$-stability, which is concerned with the errors $\varepsilon_{n+1}^{(j)}$, $j = 1,\ldots,m$. For our class of methods, internal $S(\alpha)$-stability is a stronger form of stability than $S(\alpha)$-stability.

DEFINITION 3.1. The generalized Runge-Kutta method is said to be *internally* $S(\alpha)$-stable, if for a differential equation of the form (1.3) and for any real constant $\delta_0 < 0$, there exists an $h_0 > 0$ such that

$$(3.8) \qquad |\varepsilon_{n+1}^{(j)}| < |\varepsilon_{n+1}^{(0)}|, \qquad j = 1,\ldots,m,$$

for all stepsizes $0 < h_n < h_0$ and all δ with $\mathrm{Re}(\delta) \le \delta_0$, and $|\arg(-\delta)| < \alpha$.

REMARK 3.1. An important effect of internal S-stability is that at each stage of the scheme the stiff components in the numerical solution are suppressed. This property is of importance, as in general we are dealing with non-linear systems. In such a situation, the Jacobian matrix varies over the step-interval. In case of linear systems, the effect of internal S-stability is that at each stage rounding errors are suppressed.

Let us derive the difference equation which governs the internal $S(\alpha)$-stability. It follows from (3.5) that

$$(3.9) \qquad \vec{\varepsilon}_{n+1} = (I-z\Lambda(z))^{-1} y_n \vec{e} + z^{-1}((I-z\Lambda(z))^{-1}-I)h_n \vec{r}_{n+1} - \vec{g}_{n+1}.$$

Now it is easy to see that the dependence of $\vec{\varepsilon}_{n+1}$ upon $\varepsilon_{n+1}^{(0)}$ is governed by the error-equation

$$(3.10) \quad \vec{\epsilon}_{n+1} = (I-z\Lambda(z))^{-1}\vec{e}\ \epsilon_{n+1}^{(0)} + h_n[z^{-1}((I-z\Lambda(z))^{-1}-I)\vec{r}_{n+1} +$$

$$+ ((I-z\Lambda(z))^{-1}\vec{e}\ g_{n+1}^{(0)} - \vec{g}_{n+1})/h_n].$$

In order to be able to use results from the $S(\alpha)$-stability theory, we write (3.10) in a component-wise representation. By means of (2.10)-(2.11), the j-th component, $R^{(j)}(z)$ say, of the vector $(I-z\Lambda(z))^{-1}\vec{e}$, can be written as

$$(3.11) \quad R^{(j)}(z) = 1 + \sum_{\ell=0}^{j-1} \sum_{k=0}^{j-1-\ell} \sigma_{j,k,\ell}(z)z^{k+1}, \quad j = 0,\ldots,m.$$

In the same way, the j-th component of the vector $\vec{T}_{n+1} = z^{-1}((I-z\Lambda(z))^{-1}-I)\vec{r}_{n+1}$, can be written as

$$(3.12) \quad T_{n+1}^{(j)} = \sum_{\ell=0}^{j-1} T_{\ell,j}(z)r_{n+1}^{(\ell)} ,$$

where

$$(3.13) \quad T_{\ell,j}(z) = \sum_{k=0}^{j-1-\ell} \sigma_{j,k,\ell}(z)z^k.$$

The component-wise representation of (3.10) thus reads

$$(3.14) \quad \epsilon_{n+1}^{(j)} = R^{(j)}(z)\ \epsilon_{n+1}^{(0)} + d_n^{(j)} ,$$

where

$$(3.15) \quad d_n^{(j)} = h_n T_{n+1}^{(j)} + R^{(j)}(z)\ g_{n+1}^{(0)} - g_{n+1}^{(j)}, \quad j = 0,\ldots,m.$$

Observe that $R^{(m)}$ represents the *stability function* of the integration method. The rational functions $R^{(j)}$, $j = 1,\ldots,m-1$, may be considered as stability functions for the intermediate approximations $y_{n+1}^{(j)}$. The function $R^{(j)}$ is a rational approximation to the exponential $\exp(\mu_j z)$, of at least order one. Thus, for these functions the usual definitions are applicable.

Following the same method of proof, as given in VERWER [11], p.16, we now arrive at the following result.

THEOREM 3.1. *The m-point, generalized Runge-Kutta method is internally* $S(\alpha)$*-stable, if and only if*

(a) *The stability functions* $R^{(j)}$, $j = 1,\ldots,m$, *are strongly* $A(\alpha)$*-acceptable,*

(b) *A constant* $\bar{h} > 0$ *exists, such that* $d_n^{(j)}/h_n$, $j = 1,\ldots,m$, *is uniformly bounded on* $\{(h_n,z)|h_n \in (0,h], |\arg(-z)| < \alpha\}$.

By means of this theorem, we are able to prove a result which gives necessary and sufficient conditions for the rational functions.

THEOREM 3.2. *The m-point, generalized Runge-Kutta method is internally* $S(\alpha)$*-stable, if and only if*

(a) *The stability functions* $R^{(j)}$, $j = 1,\ldots,m$ *are strongly* $A(\alpha)$*-acceptable,*

(b) *The rational functions* $T_{\ell,j}$, $j = 1,\ldots,m$; $\ell = 0,\ldots,j-1$, *have a zero at infinity.*

PROOF. Necessity: for each $j = 1,\ldots,m$, $d_n^{(j)}$ reads

$$(3.16) \qquad d_n^{(j)} = h_n \sum_{\ell=0}^{j-1} T_{\ell,j}(z)[g'(x_n+\mu_\ell h_n) - \delta g(x_n+\mu_\ell h_n)] +$$
$$R^{(j)}(z)\, g_{n+1}^{(0)} - g_{n+1}^{(j)}.$$

According to theorem 3.1, a constant $\bar{h} > 0$ exists, such that $d_n^{(j)}/h_n$, $j = 1,\ldots,m$, is uniformly bounded on $\{(h_n,z)|h_n \in (0,\bar{h}], |\arg(-\delta)| < \alpha\}$. By means of expression (3.16), the necessity of assertion (b) is now easily established. The necessity of assertion (a) follows immediately from the necessity of assertion (a) of theorem 3.1.

Sufficiency: According to assertion (b), the functions $z\, T_{\ell,j}(z)$, $j = 1,\ldots,m$; $\ell = 0,\ldots,j-1$, are uniformly bounded on $\{z|\mathrm{Re}(z) < 0\}$. Thus, in order to prove the uniform boundedness of $d_n^{(j)}/h_n$, $j = 1,\ldots,m$, on a region $\{(h_n,z)|h_n \in (0,\bar{h}],\bar{h} > 0, |\arg(-z)| < \alpha\}$, it is sufficient to prove that $d_n^{(j)}/h_n$ is bounded for any fixed z, $\mathrm{Re}(z) < 0$, as $h_n \to 0$. By expanding $g(x)$ and $g'(x)$ about x_n, $d_n^{(j)}$ may be formally expanded as

$$(3.17) \quad d_n^{(j)} = [R^{(j)}(z) - z \sum_{\ell=0}^{j-1} T_{\ell,j}(z) - 1]g(x_n) +$$

$$+ \sum_{k=1}^{\infty} \left[\sum_{\ell=0}^{j-1} T_{\ell,j}(z)(k\mu_\ell^{k-1} - z\mu_\ell^k) - \mu_j^k \right] \frac{h_n^k g^{(k)}(x_n)}{k!} \quad,$$

for $h_n \to 0$. From relations (3.11) and (3.13), it follows that

$$(3.18) \quad R^{(j)}(z) - z \sum_{\ell=0}^{j-1} T_{\ell,j}(z) - 1 = 0.$$

As a result (3.17) is reduced to

$$(3.19) \quad d_n^{(j)} = \sum_{k=1}^{\infty} \left[\sum_{\ell=0}^{j-1} T_{\ell,j}(z)(k\mu_\ell^{k-1} - z\mu_\ell^k) - \mu_j^k \right] \frac{h_n^k g^{(k)}(x_n)}{k!} \quad,$$

which implies that $d_n^{(j)}/h_n$ is bounded for any fixed z, Re(z) < 0, as $h_n \to 0$. Consequently, the sufficiency of assertion (b) is established. The sufficiency of assertion (a) is trivial. $\square$

EXAMPLE 3.1. As an example, we give the rational functions that are needed in order to establish internal S(α)-stability for the two-point scheme

$$(3.20) \quad y_{n+1} = y_n + h_n \Lambda_{2,0}(h_n J_n) f(x_n, y_n) +$$

$$h_n \Lambda_{2,1}(h_n J_n) f(x_n + \mu_1 h_n, y_n + h_n \Lambda_{1,0}(h_n J_n) f(x_n, y_n)).$$

The functions are

$$(3.21) \quad R^{(1)}(z) = 1 + \Lambda_{1,0}(z)z,$$

$$R^{(2)}(z) = 1 + (\Lambda_{2,0}(z) + \Lambda_{2,1}(z))z + \Lambda_{2,1}(z)\Lambda_{1,0}(z)z^2,$$

and

$$T_{0,1}(z) = \Lambda_{1,0}(z),$$

$$(3.22) \quad T_{0,2}(z) = \Lambda_{2,0}(z) + \Lambda_{2,1}(z)\Lambda_{1,0}(z)z,$$

$$T_{1,2}(z) = \Lambda_{2,1}(z).$$

REMARK 3.2. A sufficient condition for assertion (b) of theorem 3.2, is that $\Lambda_{j,\ell}$, $j = 1,\ldots,m$; $\ell = 0,\ldots,j-1$, has a zero at infinity. This follows easily from definition (3.13).

REMARK 3.3. It should also be remarked that the conditions for internal S-stability for an m-point scheme may be found more directly by successively writing down the S-stability conditions for a k-point scheme, for $k = 1,2,\ldots,m$. In order to present a more self-contained discussion of the stability problem, we have given the above derivation.

REMARK 3.4. In case of equal parameters μ_j, $j = 0,\ldots,m-1$, assertion (b) of theorem 3.2 can be easily modified by reordering relevant terms in expression (3.16).

4. NUMERICAL EXAMPLES

In order to demonstrate the relevance of the various stability concepts we have discussed, i.e., $A(\alpha)$-stability, $S(\alpha)$-stability and internal $S(\alpha)$-stability, we shall apply three schemes to four stiff, non-linear problems from literature. The problems are also discussed by ENRIGHT et al [2].

They read:

I.   (BJUREL et al [1]).

$$y_1' = y_3 - 100 y_1 y_2,$$

$$y_2' = y_3 + 2y_4 - 100\ y_1 y_2 - 2.10^4 y_2^2,$$

$$y_3' = 100\ y_1 y_2 - y_3,$$

$$y_4' = 10^4 y_2^2 - y_4,$$

$$y_1(0) = y_2(0) = 1,\ y_3(0) = y_4(0) = 0,\ 0 \leq x \leq 20,$$

reference solution at $x = 20$:

$$y_1 = 0.6397604446, \quad y_2 = 0.5630850708_{10}-2,$$

$$y_3 = 0.3602395553, \quad y_4 = 0.3170647969.$$

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II. (LINIGER & WILLOUGHBY [6]).

$y_1' = 0.01 - (1+(y_1+1000)(y_1+1))(0.01+y_1+y_2)$,

$y_2' = 0.01 - (1+y_2^2)(0.01+y_1+y_2)$,

$y_1(0) = y_2(0) = 0$, $0 \leq x \leq 10$,

reference solution at x = 10:

$y_1 = - 0.10975436$, $y_2 = 0.09977678$.

III. (GEAR [3]).

$y_1' = - 0.013y_2 - 1000y_1y_2 - 2500y_1y_3$,

$y_2' = - 0.013y_2 - 1000y_1y_2$,

$y_3' = - 2500y_1y_3$,

$y_1(0) = 0$, $y_2(0) = y_3(0) = 1$, $0 \leq x \leq 10$,

reference solution at x = 10:

$y_1 = - 0.325_{10}-5$, $y_2 = 0.90916832$,

$y_3 = 0.10908284_{10}1$.

IV. (ROBERTSON [9]).

$y_1' = 0.04 - 0.04(y_1+y_2) - y_1(3.10^7y_1+10^4y_2)$,

$y_2' = 3.10^7y_1^2$,

$y_1(0) = y_2(0) = 0$, $0 \leq x \leq 10$,

reference solution at x = 10:

$y_1 = 0.1623391063_{10}^{-4}$, $y_2 = 0.1586138424$.

The given problems all have real eigenvalues (see ENRIGHT et al [2]). Therefore, in the present section, we shall only be concerned with stability properties along the real axis ($\alpha=0$). We emphasize that the relevance of the stability concepts we have discussed, continuous to go on in case of non-real eigenvalues.

The three integration schemes to be considered, all have order of consistency equal to three. Only stability properties along the real axis shall be mentioned. The schemes use two stages. We shall characterize them as follows:

I.   (VAN DER HOUWEN [10]).

$$(4.1) \qquad \Lambda(z) = \begin{bmatrix} 0 & 0 & 0 \\ \dfrac{4}{3} \dfrac{R(z)-1-z}{z^2} & 0 & 0 \\ \dfrac{1}{3} & \dfrac{3}{4} & 0 \end{bmatrix} \quad ,$$

where

$$(4.2) \qquad R(z) = \frac{1 + \dfrac{1}{3} z}{1 - \dfrac{2}{3} z + \dfrac{1}{6} z^2} \quad .$$

This scheme is L(0)-stable, but not S(0)-stable, as the functions

$$(4.3) \qquad T_{0,2}(z) = \frac{1}{4} + \frac{R(z)-1-z}{z} \quad , \quad T_{1,2}(z) = \frac{3}{4}$$

have no zero at infinity.

II.   (VERWER [11]).

$$(4.4) \qquad \Lambda(z) = \begin{bmatrix} 0 & 0 & 0 \\ \dfrac{\dfrac{2}{3} - \dfrac{1}{3} z}{1 - \dfrac{7}{12} z + \dfrac{1}{12} z^2} & 0 & 0 \\ \dfrac{\dfrac{1}{4} - \dfrac{11}{24} z}{1 - \dfrac{7}{12} z + \dfrac{1}{12} z^2} & \dfrac{\dfrac{3}{4} - \dfrac{1}{8} z}{1 - \dfrac{7}{12} z + \dfrac{1}{12} z^2} & 0 \end{bmatrix} \quad .$$

This scheme is S(0)-stable, but not internally S(0)-stable, as the function

$$(4.5) \qquad R^{(1)}(z) = \frac{1 + \dfrac{1}{12} z - \dfrac{3}{12} z^2}{1 - \dfrac{7}{12} z + \dfrac{1}{12} z^2} \to -3 \text{ as } z \to -\infty.$$

The stability function $R^{(2)}$, i.e., the stability function of the scheme, is L(0)-acceptable, and reads

$$(4.6) \qquad R^{(2)}(z) = \frac{144 - 24z - 23z^2 - z^3}{(z-3)^2 (z-4)^2} \quad .$$

III.

$$(4.7) \qquad \Lambda(z) = \begin{bmatrix} 0 & 0 & 0 \\[2em] \dfrac{\dfrac{2}{3} - \dfrac{1}{8} z}{1 - \dfrac{29}{32} z + \dfrac{1}{8} z^2} & 0 & 0 \\[3em] \dfrac{\dfrac{1}{4} - \dfrac{1}{8} z}{1 - \dfrac{29}{32} z + \dfrac{1}{8} z^2} & \dfrac{\dfrac{3}{4} - \dfrac{25}{32} z}{1 - \dfrac{29}{32} z + \dfrac{1}{8} z^2} & 0 \end{bmatrix} .$$

This scheme is internally S(0)-stable. Both stability functions $R^{(1)}$ and $R^{(2)}$ are L(0)-acceptable, and read

$$(4.8) \qquad R^{(1)}(z) = \frac{1 - \dfrac{23}{96} z}{1 - \dfrac{29}{32} z + \dfrac{1}{8} z^2} ,$$

$$(4.9) \qquad R^{(2)}(z) = \frac{1 - \dfrac{13}{16} z - \dfrac{247}{1024} z^2 + \dfrac{323}{3072} z^3}{(1 - \dfrac{29}{32} z + \dfrac{1}{8} z^2)^2} .$$

Summarizing, method I is *L(0)-stable*, method II is *S(0)-stable*, and method III is *internally S(0)-stable*. We still have to observe that we have chosen these three methods only to illustrate the relevance of the new stability theory. In this section, it is not our intention to propose a new, third order generalized Runge-Kutta scheme.

The methods were applied with the following simple step-size strategies: strategy A: h_n = if $x_0 \leq x \leq x_t$ then $h^{(1)}$ else $h^{(2)}$, where $h^{(1)} < < h^{(2)}$,

strategy B: $h_n = h$, i.e., a constant step-size.

These numbers will be specified with the tables. In these tables, we give for each j-th component the number of significant digits $sd_j = {}^{-10}\log$ (*absolute error*), at the endpoint of the given interval. The letter u refers to an unstable result. The calculations have been performed on a Cyber 73-26 computer.

Results for problem I: $h^{(1)} = 0.01$, $h^{(2)} = 0.1$, $x_t = 0.1$, $h = 0.1$.

strategy	A			B		
method	I	II	III	I	II	III
sd_1	u	u	11.4	u	u	0.4
sd_2	u	u	13.3	u	u	1.4
sd_3	u	u	11.0	u	u	0.1
sd_4	u	u	10.0	u	u	-1.3

Results for problem II: $h^{(1)} = 0.01$, $h^{(2)} = 0.1$, $x_t = 0.1$, $h = 0.1$.

strategy	A			B		
method	I	II	III	I	II	III
sd_1	6.6	5.4	6.6	u	4.0	5.6
sd_2	6.6	5.4	6.6	u	4.0	5.6

Results for problem III: $h^{(1)} = 0.05$, $h^{(2)} = 0.5$, $x_t = 0.5$, $h = 0.5$.

strategy	A			B		
method	I	II	III	I	II	III
sd_1	u	9.4	9.3	3.2	9.5	9.3
sd_2	u	6.8	8.4	2.4	4.8	8.3
sd_3	u	6.7	7.6	2.4	4.8	7.6

Results for problem IV: $h^{(1)} = 0.001$, $h^{(2)} = 0.1$, $x_t = 0.004$, $h = 0.05$.

strategy	A			B		
method	I	II	III	I	II	III
sd_1	7.9	10.3	9.7	u	u	4.9
sd_2	6.1	8.5	7.5	u	u	1.0

The results of these computations indicate that the stability proper-
ties, derived for the test-model (1.3), carry over to a certain extent to
non-linear systems. We observe that the internally stabilized formula III
is more reliable than the S-stable formula II. In general, internally sta-
bilized formulas may also be expected to be more accurate than the others.
Finally, we observe that the results of these computations clearly indicate
that S-stable methods are superior to A-stable methods.

REFERENCES

[1] BJUREL, G., G. DAHLQUIST, B. LINDBERG, S. LINDE & L. ODEN, *Survey of
       stiff ordinary differential equations,* Comp. Sc. Report NA 70.11,
       Royal Institute of Technology, Dept. of Information Processing,
       Stockholm, 1970.

[2] ENRIGHT, W.H., T.E. HULL & B. LINDBERG, *Comparing numerical methods
       for stiff systems of ODEs,* Techn. Report No. 69, Dept. of Comp.
       Sc., Univ. of Toronto, 1974.

[3] GEAR, C.W., *Numerical integration of stiff ordinary differential
       equations,* Report 221, Dept. of Comp. Sc., Univ. of Illinois,
       Urbana, 1967.

[4] LAMBERT, J.D., *Computational methods in ordinary differential equations,*
       John Wiley and Sons, London, 1973.

[5] LAMBERT J.D. & S.T. SIGURDSSON, *Multistep methods with variable matrix
       coefficients,* SIAM J. Numer. Anal. 9, pp. 715-733, 1972.

[6] LINIGER, W. & R.A. WILLOUGHBY, *Efficient numerical integration of stiff
       systems of ordinary differential equations,* Techn. Report
       RC-1970, IBM Thomas J. Watson Research Centre, Yorktown Heights,
       New York, 1967.

[7] PROTHERO, A. & A. ROBINSON, *On the stability and accuracy of one-step
       methods for solving stiff systems of ordinary differential
       equations,* Math. Comp. 28, pp. 145-162, 1974.

[8] PROTHERO, A., *Private communication.*

[9] ROBERTSON, H.H., *The solution of a set of reaction rate equations in numerical analysis,* ed. J. Walsh, Thompson Book Co., Washington, 1967.

[10] VAN DER HOUWEN, P.J., *One-step methods with adaptive stability functions for the integration of differential equations,* Lecture Notes in Mathematics 333, pp. 164-174, Springer-Verlag, Berlin, 1972.

[11] VERWER, J.G., *S-stability and stiff-accuracy for two classes of generalized integration methods,* Report NW 15/75, Mathematisch Centrum, Amsterdam, 1975.