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CONVERGENCE AND STABILITY ANALYSIS FOR MODIFIED RUNGE-KUTTA METHODS IN THE NUMERICAL TREATMENT OF SECOND KIND VOLTERRA INTEGRAL EQUATIONS

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Convergence and stability analysis for modified Runge-Kutta methods in the numerical treatment of second kind Volterra integral equations *)

by

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ABSTRACT

In this paper modified and conventional Runge-Kutta methods for second kind Volterra integral equations are discussed in a uniform way. The modification presented takes into account the residual of the previous step with the aim of improving the stability behaviour. A general convergence theorem is given which establishes that the modified methods may loose one order of accuracy. Furthermore, the stability behaviour of the methods is analyzed and explicit stability results are derived. It transpires that every A-stable Runge-Kutta method for ordinary differential equations generates mixed methods which can be made A-stable by a suitable modification.

KEY WORDS & PHRASES: *Numerical analysis, Volterra integral equations of the second kind, Runge-Kutta methods, convergence and stability*

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1. INTRODUCTION

1.1. Classical Runge-Kutta methods

For the numerical solution of Volterra integral equations of the second kind

$$(1.1)\qquad f(x) = g(x) + \int_0^x K(x,y,f(y))dy, \qquad x \geq 0,$$

we shall consider Runge-Kutta methods of the form

$$f_{n+1}^{(i)} = \tilde{F}_n(x_n+\theta_i h) + h \sum_{\ell=1}^{m} a_{i\ell}K(x_n+d_{i\ell}h, x_n+c_\ell h, f_{n+1}^{(\ell)}),$$

$$(1.2a)\qquad i = 1(1)m,\ n = 0,1,\ldots$$

$$f_{n+1} = f_{n+1}^{(m)}, \qquad \theta_m = c_m = 1.$$

Here, $x_n = nh$ and f_n is a numerical approximation to $f(x_n)$. The function $\tilde{F}_n(x)$ is a discretization of

$$F_n(x) := g(x) + \int_0^{x_n} K(x,y,f(y))dy,$$

defined by

$$(1.2b)\qquad \tilde{F}_n(x) := g(x) + h \sum_{j=0}^{n} \sum_{\ell=1}^{m} w_{nj}^{(\ell)} K(x, x_j^{(\ell)}, f_j^{(\ell)}), \qquad n \geq 0,$$

where $x_j^{(\ell)}$ denotes the point $x_{j-1} + c_\ell h$, and where $w_{nj}^{(\ell)}$ are suitable quadrature weights with $w_{00}^{(\ell)} = 0$, $\ell = 1(1)m$ (i.e. $\tilde{F}_0(x) = g(x)$). We define $f_0^{(m)} = f(0) = g(0)$, and adopt the convention that $w_{n0}^{(\ell)} = 0$ for $\ell = 1,2,\ldots,m-1$, so that the terms involving the undefined values $f_0^{(1)},\ldots,f_0^{(m-1)}$ (which we carry along only for notational convenience) vanish in (1.2b).

We shall refer to (1.2a) as the *forward (Runge-Kutta) step* and to (1.2b) as the *lag term*.

The Runge-Kutta parameters θ_i, $a_{i\ell}$, $d_{i\ell}$ and c_ℓ are determined by accuracy conditions (cf. [8] and the references therein; see also [13], where a more general class of methods with c_ℓ replaced by $c_{i\ell}$ is treated).

Depending on the choice of the parameters in the forward step two important classes of methods can be distinguished: the choice $d_{i\ell} = c_i$, $\theta_i = c_i$ yields methods of *Pouzet type* whereas for $d_{i\ell} = d_\ell$, $\theta_i = c_i$ we obtain methods of *Bel'tyukov type* (see [7] and [4]). In our analysis we consider the general methods defined by (1.2a) and some suitable lag term of the form (1.2b).

A division into subclasses can be given depending on the choice of the quadrature weights in the lag term (1.2b). Here, we give three important classes considered in the literature:

$$\text{(1.3a)} \qquad \tilde{F}_n(x) = g(x) + h \sum_{j=1}^{n} \sum_{\ell=1}^{m} a_{m\ell} K(x, x_j^{(\ell)}, f_j^{(\ell)}),$$

$$\text{(1.3b)} \qquad \tilde{F}_n(x) = g(x) + h \sum_{j=1}^{n} \sum_{\ell=1}^{m} \hat{a}_{m\ell} K(x, x_j^{(\ell)}, f_j^{(\ell)}),$$

$$\text{(1.3c)} \qquad \tilde{F}_n(x) = g(x) + h \sum_{j=0}^{n} w_{nj} K(x, x_j, f_j).$$

The choice (1.3a) can be used in combination with a forward step of Pouzet-type, and then yields an *extended Pouzet method*. Note that the quadrature weights in the lag term (1.3a) are the Runge-Kutta parameters $a_{m\ell}$ of the forward step. As a consequence of this connection, extended Pouzet methods have the property that

$$\text{(1.4)} \qquad f_n = \tilde{F}_n(x_n).$$

In contrast to extended methods, lag terms of the form (1.3b) or (1.3c) (in which the quadrature weights have no relation to the forward step) yield the so-called *mixed Runge-Kutta methods*. Note that for (1.3b) the lag term uses intermediate approximations $f_j^{(\ell)}$, whereas for (1.3c) only values f_j (i.e. approximations at the step points $x_j = jh$) are used.

1.2. Modified Runge-Kutta methods

This paper is primarily concerned with the stability behaviour of the methods (1.2a - b). In our analysis we follow the approach based on some test equation as a model problem, e.g. the *basic test equation* [1,6]

$$(1.5) \qquad f(x) = g(x) + \lambda \int_0^x f(y)dy.$$

It can be shown (cf. (3.4)) that such an analysis leads to recurrence relations of the form

$$(1.6) \qquad f_{n+1} = R(h\lambda)\tilde{I}_n + \text{inhomogeneous term},$$

where $\tilde{I}_n = \tilde{F}_n(x) - g(x)$ is independent of x, and where $R(h\lambda)$ is a rational function of $h\lambda$ whose coefficients are functions of the Runge-Kutta parameters. For extended Pouzet methods we have, using (1.4), $f_{n+1} = R(h\lambda)f_n$ + inh. term, which is the recurrence relation of a Runge-Kutta method for ODEs. For mixed methods $\tilde{I}_n \neq f_n - g_n$, and the stability behaviour is influenced by the lag term. In order to eliminate the effect of the lag term, VAN DER HOUWEN [13, 14] proposed a modification of the scheme (1.2a-b) by replacing $\tilde{F}_n(x)$ with $\tilde{F}^*_n(x)$ defined as

$$(1.7) \qquad \tilde{F}^*_n(x) = \tilde{F}_n(x) + \gamma(x)(f_n - \tilde{F}_n(x_n)),$$

where $\gamma(x_n + \theta_i h) = \gamma_i \in [0,1]$. The form (1.7) is motivated by the fact that for $\gamma(x) \equiv 1$, the relation (1.6) changes to $f_{n+1} = R(h\lambda)f_n$ + inh. term, *irrespective of the choice of the lag term.* An additional advantage of the formulation (1.7) is that for Runge-Kutta methods where one or more of the θ_i's vanish, the choice $\gamma(x_n) = 1$ and $\gamma(x) = 0$ for $x \neq x_n$ yields Runge-Kutta methods in which it is not necessary to evaluate the lag term $\tilde{F}_n(x)$ at $x = x_n$. The first examples of such methods can be found in BEL'TYUKOV [7] (see also [13] and [1]). In the latter reference this type of methods was termed *economized versions* of the Runge-Kutta method. Note that $\gamma(x) \equiv 0$ yields the unmodified method (1.2a-b). Observe that $f_n - \tilde{F}_n(x_n)$ in (1.7) can be regarded as a residual which measures the amount by which f_n fails to equal $\tilde{F}_n(x_n)$. Therefore $\gamma(x)(f_n - \tilde{F}_n(x_n))$ is called a (weighted) residual correction to $\tilde{F}_n(x)$.

In this paper we use the terminology given in definitions 1.1 and 1.2.

DEFINITION 1.1. A method based on (1.2a) with the (unmodified) lag term $\tilde{F}_n(x)$ defined by (1.2b) is an *unmodified* (or *classical, standard*) *Runge-*

Kutta method.

DEFINITION 1.2. A method based on (1.2a) with the lag term $\tilde{F}_n(x)$ replaced by the (modified) lag term $\tilde{F}_n^*(x)$ given in (1.7) is a (γ-)*modified Runge-Kutta method*.

In Section 3, we present the stability analysis of the modified Runge-Kutta methods described above, with respect to a convolution test equation (equation (3.1)), and in Section 4 stability results are given both for the basic test equation and this convolution equation.

Firstly, however, the effect of the modification (1.7) on the rate of convergence is investigated in Section 2. It turns out that the provable order of accuracy may be reduced by 1 if $\gamma_m = 1$; this is the price paid for an improved stability behaviour.

This paper is developed from the institute report [14]; it contains a more general convergence result and stability theorems for the basic test equation. We also derive the stability polynomials for a larger class of quadrature rules (cf. Section 3.3.2).

2. CONVERGENCE

In this section we prove the convergence of the Runge-Kutta methods (1.2a) modified according to (1.7). In the convergence proof we need the *local error* of the numerical method: let $\hat{f}_{n+1}^{(i)}$ $(i = 1,\dots,m)$ be the solution of (1.2a - b), (1.7) if we substitute $f(x_n)$ for f_n and $F_n(x)$ for $\tilde{F}_n(x)$ (which implies that $\tilde{F}_n^*(x) = F_n(x)$); then we define the local error $T_n^{(i)}(h)$ at $x_n + c_i h$ by

$$(2.1) \qquad T_n^{(i)}(h) := f(x_n + c_i h) - \hat{f}_{n+1}^{(i)}.$$

Furthermore, we define the global error $e_{n+1}^{(i)}$

$$(2.2) \qquad e_{n+1}^{(i)} := |f(x_n + c_i h) - f_{n+1}^{(i)}|,$$

the quadrature error $E_n(x,h)$ for the interval $[0,x_n]$

$$(2.3)\qquad E_n(x,h) := \int_0^{x_n} K(x,y,f(y))dy - h\sum_{j=0}^{n}\sum_{\ell=1}^{m} w_{nj}^{(\ell)}K(x,x_j^{(\ell)},f(x_j^{(\ell)}))$$

and the function $D_n(x,h)$

$$D_n(x,h) = \begin{cases} 0 & \text{if } x = x_n \\ (E_n(x,h)-E_n(x_n,h))/(x-x_n) & \text{if } x \neq x_n. \end{cases}$$

In the convergence theorem we shall need the vectors $\vec{e}_{n+1}$ and $\vec{T}_n(h)$ whose components are respectively given by $e_{n+1}^{(\ell)}$ and $T_n^{(\ell)}(h)$, where ℓ runs through the set of integers L defined by

$$L = \{1,2,\ldots,m\}\backslash\{\ell \mid w_{nj}^{(\ell)} = 0 \text{ for all n and j}\}.$$

In other words, if $\ell \notin L$ then, for all j, the values $f_j^{(\ell)}$ are not used in the lag term. For mixed RK methods of the form (1.3c), $L = \{m\}$, whereas for extended Pouzet methods $L = \{\ell \mid a_{m\ell} \neq 0\}$. For a vector $\vec{v}$ with components $v^{(\ell)}$, $\ell \in L$ we define the maximum norm $\|\;\|_\infty$

$$(2.4)\qquad \|\vec{v}\|_\infty := \max_{\ell\in L} |v^{(\ell)}|.$$

We shall also use the following lemmas.

LEMMA 2.1. *Let the sequence* $\{\varepsilon_n\}_{n=0}^{\infty}$ $(\varepsilon_n \geq 0)$ *satisfy the inequality*

$$\varepsilon_{n+1} - C_1\varepsilon_n \leq C_2 \sum_{j=0}^{n} \delta_j + M_n$$

where M_j *and* δ_j *and the constants* C_1 *and* C_2 *are non-negative. Then*

$$\varepsilon_{n+1} \leq C_2 \frac{C_1^{n+1}-1}{C_1-1} \sum_{j=0}^{n} \delta_j + C_1^{n+1}\varepsilon_0 + \frac{C_1^{n+1}-1}{C_1-1} \max_{j\leq n} M_j$$

PROOF. Multiply the inequality for ε_{n+1-i} by C_1^i and take the summation for $i = 0$ to n. □

LEMMA 2.2. *Let the sequence* $\{\varepsilon_n\}_{n=0}^{\infty}$ $(\varepsilon_n \geq 0)$ *satisfy the inequality*

$$\varepsilon_{n+1} \le hC_3 \sum_{j=0}^{n} \varepsilon_j + C_4,$$

where C_3 *and* C_4 *are non-negative constants. Then, for* h *sufficiently small and* $(n+1)h = x$,

$$\varepsilon_{n+1} \le (hC_3\varepsilon_0 + C_4)\exp(C_3 x).$$

PROOF. See e.g. BAKER [4, p. 926]. □

We now state the convergence theorem

THEOREM 2.1. *Let the function* $K(x,y,f)$ *satisfy the Lipschitz condition*

$$|K(x,y,f) - \alpha K(x_n,y,f) - K(x,y,f^*) + \alpha K(x_n,y,f^*)|$$

$$\le L\{1-\alpha+\alpha|x-x_n|\}|f-f^*|,$$

where L *is a constant and* $\alpha \in [0,1]$. *Then as* $h \to 0$, *while* $(n+1)h$ *remains fixed,*

$$(2.5)\qquad \|\vec{e}_{n+1}\|_\infty \le A \underset{j\le n,1\le i\le m}{\text{maximum}} \{|E_j(x_j+\theta_i h,h)|, \frac{h|D_j(x_j+\theta_i h,h)|}{1-\gamma_m + Ch}\} +$$

$$+ B \max_{j\le n} \{\|\vec{T}_j(h)\|_\infty, \frac{|T_j^{(m)}(h)|}{1-\gamma_m + Ch}\}$$

where A, B *and* C *are (bounded) constants.*

PROOF. From (2.1) and (2.2) it follows that

$$(2.6)\qquad e_{n+1}^{(i)} \le \hat{e}_{n+1}^{(i)} + |T_n^{(i)}(h)|,$$

where $\hat{e}_{n+1}^{(i)} := |f_{n+1}^{(i)} - \hat{f}_{n+1}^{(i)}|$. From the definition of $f_{n+1}^{(i)}$ and $\hat{f}_{n+1}^{(i)}$ and the Lipschitz condition on K with $\alpha = 0$ it follows that

$$(2.7)\qquad \hat{e}_{n+1}^{(i)} \le \Delta F_n(x_n + \theta_i h) + h\bar{a}L \sum_{\ell=1}^{m} \hat{e}_{n+1}^{(\ell)},$$

where $\Delta F_n(x) = |\tilde{F}_n^*(x) - F_n(x)|$ and $\bar{a} = \max_{i,\ell} |a_{i\ell}|$. From (2.7) we derive

$$\hat{e}_{n+1}^{(i)} \le \Delta F_n(x_n+\theta_i h) + hA_1 \max_{1\le\ell\le m} \Delta F_n(x_n+\theta_\ell h), \quad A_1 = \frac{\bar{a}Lm}{1-hm\bar{a}L}. \tag{2.8}$$

If we introduce the notation $F_n^+(x) = g(x) + h \sum\sum w_{nj}^{(\ell)} K(x,x_j^{(\ell)},f(x_j^{(\ell)}))$, then $E_n(x,h) = F_n(x) - F_n^+(x)$ and

$$\Delta F_n(x) = |\gamma(x)\{f_n - f(x_n)\} + \{\tilde{F}_n(x) - \gamma(x)\tilde{F}_n(x_n)\}$$

$$- \{F_n^+(x) - \gamma(x)F_n^+(x_n)\} - \{E_n(x,h) - \gamma(x)E_n(x_n,h)\}|.$$

Writing $e_n = |f_n - f(x_n)|$ we obtain

$$\Delta F_n(x) \le \gamma(x)e_n + h \sum_{j=0}^{n} \sum_{\ell=1}^{m} |w_{nj}^{(\ell)}| \cdot |K(x,x_j^{(\ell)},f_j^{(\ell)})$$

$$- \gamma(x)K(x_n,x_j^{(\ell)},f_j^{(\ell)}) - K(x,x_j^{(\ell)},f(x_j^{(\ell)}))$$

$$+ \gamma(x)K(x_n,x_j^{(\ell)},f(x_j^{(\ell)}))| + |E_n(x,h) - \gamma(x)E_n(x_n,h)|.$$

By using the Lipschitz condition on K with $\alpha = \gamma(x_n + \theta_i h) = \gamma_i$, and writing

$$\bar{x}_{n+1}^{(i)} = x_n + \theta_i h, \quad W = \max_{n,j,\ell} |w_{nj}^{(\ell)}|, \quad \gamma = \max_i \gamma_i, \quad \theta = \max_i |\theta_i|,$$

we obtain

$$\begin{aligned} \Delta F_n(x_n+\theta_i h) &\le \gamma_i e_n + hLW\{1-\gamma_i+\gamma\theta h\} \sum_{j=0}^{n} \|\vec{e}_j\|_\infty + \\ &+ (1-\gamma_i)|E_n(\bar{x}_{n+1}^{(i)},h)| + \gamma\theta h|D_n(\bar{x}_{n+1}^{(i)},h)|. \end{aligned} \tag{2.9}$$

Substitution of (2.9) in (2.8), and then (2.8) in (2.6) yields

$$\begin{aligned} e_{n+1}^{(i)} &\le \{\gamma_i + hA_1\gamma\}e_n + \{hLW[1-\gamma_i+\gamma\theta h] + h^2LWA_1[1+\gamma\theta h]\} \sum_{j=0}^{n} \|\vec{e}_j\|_\infty \\ &+ [1-\gamma_i+hA_1]|\bar{E}_n(x_n,h)| + [1+hA_1]\gamma\theta h|\bar{D}_n(x_n,h)| + |T_n^{(i)}(h)|, \end{aligned} \tag{2.10}$$

where $|\bar{E}_n(x_n,h)| = \max_i |E_n(\bar{x}_{n+1}^{(i)},h)|$, $|\bar{D}_n(x_n,h)| = \max_i |D_n(\bar{x}_{n+1}^{(i)},h)|$.

For i = m, (2.10) has the form

$$e_{n+1} = e_{n+1}^{(m)} \le A_2 e_n + A_3 \sum_{j=0}^{n} \|\vec{e}_j\|_\infty + A_4|\bar{E}_n(x_n,h)| + A_5 h|\bar{D}_n(x_n,h)| + |T_n^{(m)}(h)|, \tag{2.11}$$

where, as $h \to 0$, $A_5 = \mathcal{O}(1)$ and

$$A_2 = 1+hA_1\gamma, \quad A_1 \ne 0, \quad A_3 = \mathcal{O}(h^2), \quad A_4 = \mathcal{O}(h), \quad \text{if } \gamma_m = 1$$

or

$$A_2 < 1, \quad A_3 = \mathcal{O}(h), \quad A_4 = \mathcal{O}(1), \quad \text{if } \gamma_m < 1.$$

Application of Lemma 2.1 yields the inequality

$$e_{n+1} \le hA_5 \sum_{j=0}^{n} \|\vec{e}_j\|_\infty + A_6 e_0 + \frac{A_7}{1-\gamma_m+\mathcal{O}(h)} h \max_{j\le n} |\bar{D}_j(x_j,h)| + A_8 \max_{j\le n} |\bar{E}_j(x_j,h)| + \frac{A_9}{1-\gamma_m+\mathcal{O}(h)} \max_{j\le n} |T_j^{(m)}(h)|, \tag{2.12}$$

where the constants A_i are uniformly bounded. Substitute the inequality (2.12) for e_n into (2.10) to obtain

$$e_{n+1}^{(i)} \le hA_{10} \sum_{j=0}^{n} \|\vec{e}_j\|_\infty + A_{11}e_0 + A_{12} \max_{j\le n} |\bar{E}_j(x_j,h)| + \frac{A_{13}}{1-\gamma_m+\mathcal{O}(h)} h \max_{j\le n} |\bar{D}_j(x_j,h)| + \frac{A_{14}}{1-\gamma_m+\mathcal{O}(h)} \max_{j\le n-1} |T_j^{(m)}(h)| + |T_n^{(i)}(h)|. \tag{2.13}$$

From (2.13) it is easily verified that

$$\|\vec{e}_{n+1}\|_\infty \le hA_{10} \sum_{j=0}^{n} \|\vec{e}_j\|_\infty + A_{11}e_0 + A_{12} \max_{j\le n} |\bar{E}_j(x_j,h)|$$

$$(2.14) \qquad + \frac{A_{13}}{1-\gamma_m+\mathcal{O}(h)} h \max_{j\le n} |\bar{D}_j(x_j,h)|$$

$$+ \frac{A_{14}}{1-\gamma_m+\mathcal{O}(h)} \max_{j\le n-1} |T_j^{(m)}(h)| + \|\vec{T}_n(h)\|_\infty .$$

Application of Lemma 2.2 yields the result (2.5). □

The condition on K required in this theorem is satisfied if, for example, K and K_x satisfy Lipschitz conditions with respect to f. We then may write

$$|K(x,y,f)-\alpha K(x_n,y,f)-K(x,y,f^*)+\alpha K(x_n,y,f^*)|$$

$$= |(1-\alpha)[K(x,y,f)-K(x,y,f^*)] + \alpha \int_{x_n}^{x} K_x(t,y,f)dt - \alpha \int_{x_n}^{x} K_x(t,y,f^*)dt|$$

$$\le (1-\alpha)L_1|f-f^*| + \alpha|x-x_n|L_2|f-f^*|$$

from which the condition in the theorem is immediate.

Furthermore, we shall now discuss the error bound (2.5) in more detail. If $\gamma_m < 1$, then $1-\gamma_m+\mathcal{O}(h) = \mathcal{O}(1)$ and in this case

$$\max_{1\le i\le m} h|D_j(x_j+\theta_i h,h)| \le 2 \max_{1\le i\le m} |E_j(x_j+\theta_i h,h)|,$$

so that we can express (2.5) in terms of the quadrature errors $E_j(x,h)$ and local truncation errors only.

If $\gamma_m = 1$, however, then $1-\gamma_m+\mathcal{O}(h) = \mathcal{O}(h)$ and the left-hand side of (2.5) contains expressions of the form $D_j(x_j+\theta_i h,h)$ and $\mathcal{O}(h^{-1})T_j^{(m)}(h)$. For most quadrature formulae, however, it can be shown that $D_n(x,h)$ (which was defined as $(E_n(x,h)-E_n(x_n,h))/(x-x_n)$ has the same order of accuracy as $E_n(x,h)$, provided that the kernel is sufficiently smooth.

A disadvantage of the introduction of the modification (1.7) with $\gamma_m = 1$ in a given Runge-Kutta method is the possibility of loosing an order of accuracy. This can be seen by the following heuristic argument.

Let us assume that $|E_j(x,h)| = \mathcal{O}(h^q)$, $|T_j^{(m)}(h)| = \mathcal{O}(h^{p+1})$ and $\|\vec{T}_j(h)\|_\infty = \mathcal{O}(h^{r+1})$ then $\|\vec{e}_{n+1}\|_\infty = \mathcal{O}(h^q) + \mathcal{O}(h^{p+1}) + \mathcal{O}(h^{r+1})$ if $\gamma_m < 1$ and $\|\vec{e}_{n+1}\|_\infty = \mathcal{O}(h^q) + \mathcal{O}(h^p) + \mathcal{O}(h^{r+1})$ if $\gamma_m = 1$. If the lag term (1.3c) is used, then $\|\vec{T}_j(h)\|_\infty = |T_j^{(m)}(h)|$ and hence $r = p$. Therefore an order of accuracy is lost if $\gamma_m = 1$ and $p+1 \le q$. This result is corroborated by the numerical examples in Section 5.

3. STABILITY

Various equations of the form (1.1) have been taken as test equations in the study of numerical stability. The test kernel $K = \lambda f$ was proposed by MAYERS [17] in 1962 and only recently (1977) was an x-dependent kernel which essentially behaves as $K = (a+bx)f$ investigated [13]. A rather general class of separable kernels $K = \sum A_i(x)B_i(y,f)$ for the study of stability was first proposed in [15] where also polynomial convolution kernels are discussed. The most simple example of such convolution equations is given by

$$(3.1) \qquad f(x) = g(x) + \int_0^x (\lambda+\mu(x-y))f(y)\,dy, \qquad \lambda,\mu \in \mathbb{R}.$$

The papers mentioned above deal with a rather restricted class of methods. Extensions to more general classes of methods have been presented in a number of recent papers ([6], [5], [1] and [2]).

In this paper we consider the linear equation (3.1) since consideration of this equation is sufficient to enable us to establish some promising stability properties of the modified methods, in comparison with conventional (unmodified) methods.

Application to (3.1) of the γ-modified Runge-Kutta method ((1.2) with $\tilde{F}_n^*(x)$ for $\tilde{F}_n(x)$) yields the equations

$$(3.2a)\qquad f_{n+1}^{(i)} = g(x_n + \theta_i h) - \gamma_i g(x_n) + \gamma_i f_n + (1-\gamma_i)\tilde{I}_n + h\mu\theta_i\tilde{G}_n + \sum_{\ell=1}^{m} a_{i\ell}\{h\lambda + h^2\mu(d_{i\ell} - c_\ell)\}f_{n+1}^{(\ell)},$$

where we have defined

$$(3.2b)\qquad \tilde{I}_n \ (= \tilde{I}_n(x_n)) := h \sum_{j=0}^{n}\sum_{\ell=1}^{m} w_{nj}^{(\ell)}\{\lambda + \mu(x_n - x_{j-1} - c_\ell h)\}f_j^{(\ell)},$$

$$(3.2c)\qquad \tilde{G}_n := h \sum_{j=0}^{n}\sum_{\ell=1}^{m} w_{nj}^{(\ell)} f_j^{(\ell)}.$$

Let $\vec{\varepsilon} = [1,\ldots,1]^T$, $\vec{\gamma} = [\gamma_1,\ldots,\gamma_m]^T$, $\vec{\theta} = [\theta_1,\ldots,\theta_m]^T$ and let A_0 and A_1 denote the matrices whose entries in the i-th row and ℓ-th column are $a_{i\ell}$ and $a_{i\ell}(d_{i\ell}-c_\ell)$, respectively, and define, with $M = (I - h\lambda A_0 - h^2\mu A_1)^{-1}$

$$(3.3)\qquad R_i = \vec{\varepsilon}_i^T M\vec{\varepsilon},\quad S_i = \vec{\varepsilon}_i^T M\vec{\theta},\quad U_i = \vec{\varepsilon}_i^T M\vec{\gamma},\quad V_i = R_i - U_i,\quad i = 1(1)m.$$

Thus, R_i, S_i, U_i and V_i are rational functions in the variables $h\lambda$ and $h^2\mu$. It is then easily verified that we may write (3.2a) in the form

$$(3.4)\qquad f_{n+1}^{(i)} = h\mu S_i\tilde{G}_n + U_i f_n + V_i\tilde{I}_n + \text{inh. term.}$$

In particular, we have for i = m

$$(3.5)\qquad f_{n+1} = h\mu S_m\tilde{G}_n + U_m f_n + V_m\tilde{I}_n + \text{inh. term.}$$

Notice that for $\vec{\gamma} = \gamma\vec{\varepsilon}$ (i.e. $\gamma_i = \gamma$ for all i, i = 1(1)m) (3.4) reduces to

$$(3.4')\qquad f_{n+1}^{(i)} = \gamma R_i f_n + (1-\gamma)R_i\tilde{I}_n + h\mu S_i\tilde{G}_n + \text{inh. term}$$

where R_i and S_i, defined in (3.3), are *independent of* γ.

Relation (3.5) describes how the forward step (characterized by S_m, U_m and V_m), the lag term (i.e. $\tilde{I}_n$ and $\tilde{G}_n$), and f_n influence the value f_{n+1}. In the following we shall consider different lag terms in which the weights $w_{nj}^{(\ell)}$ display a special structure. Due to this structure it is possible to derive coupled difference equations for values f_n, $\tilde{I}_n$ and $\tilde{G}_n$. From these difference equations $\tilde{G}_n$ and $\tilde{I}_n$ can be eliminated yielding a difference equation in terms of f_n-values only. (These are the components we are usually interested in, and stability of such a relation is called "full step stability" in [1].) This elimination step is described in the following Lemma.

LEMMA 3.1. *Let* $\{\vec{z}_n\}_{n=0}^{\infty}$ $(\vec{z}_n = [z_n^{(1)},\dots,z_n^{(M)}]^T)$ *satisfy the system of difference equations with constant coefficients*

$$(3.6) \qquad \sum_{j=1}^{M} \tau_{ij}(E)z_{n+1-k}^{(j)} = g_{n+1}^{(i)}, \qquad i = 1(1)M,$$

where τ_{ij} *is a polynomial of degree at most* k, *and where* E *denotes the forward shift operator. Then each component* $\{z_n^{(i)}\}_{n=0}^{\infty}$ *satisfies a difference equation of the form*

$$(3.7) \qquad \hat{\tau}(E)z_{n+1-kM}^{(i)} = \hat{g}_{n+1}^{(i)}, \qquad i = 1(1)M,$$

where $\hat{g}_{n+1}^{(i)}$ *has the form* $\sum\sigma_{ij}(E)g_{n+1}^{(j)}$ *for some polynomial* σ_{ij} *and*

$$(3.8) \qquad \hat{\tau}(E) = \det(\tau_{ij}(E)).$$

PROOF. The proof is based essentially on a formal application of an elimination process. It is perhaps best illustrated for $M = 2$. For $M = 2$ the system reads (with n replaced by $n-k$)

$$\tau_{11}(E)z_{n+1-2k}^{(1)} + \tau_{12}(E)z_{n+1-2k}^{(2)} = g_{n+1-k}^{(1)},$$

$$\tau_{21}(E)z_{n+1-2k}^{(1)} + \tau_{22}(E)z_{n+1-2k}^{(2)} = g_{n+1-k}^{(2)}.$$

In order to eliminate $\{z_n^{(2)}\}$ we apply $\tau_{22}(E)$ to the first equation, and $\tau_{12}(E$ to the second, and subtract to obtain

$$\{\tau_{22}(E)\tau_{11}(E) - \tau_{12}(E)\tau_{21}(E)\}z_{n+1-2k}^{(1)} = \tau_{22}(E)g_{n+1-k}^{(1)} - \tau_{12}(E)g_{n+1-k}^{(2)}$$

which is of the form (3.7). A general proof arises on writing $T(E) = [\tau_{ij}(E)]$, $\Sigma(E) = [\sigma_{ij}(E)]$ and defining $\Sigma(E) := \mathrm{adj}(T(E))$, the classical adjoint. Then $\Sigma(E)T(E) = \hat{\tau}(E)I$ and (3.7) may be deduced from (3.6). □

A caveat in the interpretation of Lemma 3.1 is appropriate, since if $\hat{\tau}(E)$ and $\sigma_{ij}(E)$, $j = 1,\ldots,M$, have common factors then (3.7) is a recurrence of higher order than necessary, and its characteristic equation has unwanted roots.

An important corollary is:

<u>COROLLARY</u>. *Let the vector* $\{\vec{z}_n\}_{n=0}^{\infty}$ *satisfy the system of difference equations* (3.6), *and let* $\{z_n^{(i)}\}_{n=0}^{\infty}$ *satisfy the scalar difference equation* (3.7). *Then the characteristic equations associated with these difference equations are identical.* □

This corollary tells us that the values $z_{n+1-k}^{(i)}$ satisfy a stable recurrence relation (3.7) if $\hat{\tau}(E)$ is a Schur polynomial. (We observe that one should check whether (3.7) is of sufficiently low order.)

Returning to the equation (3.5) we shall now derive the difference equations for $\tilde{I}_n$ and $\tilde{G}_n$ for three different choices of the lag term. Application of the Corollary then yields the characteristic equation associated with the difference equation satisfied by $\{f_n\}_{n=0}^{\infty}$. For a discussion of the characteristic equation as a tool in the stability analysis for integral equations we refer to [6].

3.1. <u>Extended Pouzet methods</u>

In this case $f_n = \tilde{I}_n + g_n$ so that (3.4) yields

$$f_{n+1}^{(i)} = R_i f_n + h\mu S_i \tilde{G}_n + \text{inh. term} \tag{3.9}$$

where R_i is independent of $\vec{\gamma}$! In addition, we have, in view of (1.3a), that

$$\tilde{G}_{n+1} - \tilde{G}_n = h \sum_{\ell=1}^{m} a_{m\ell} f_{n+1}^{(\ell)} = \text{(using (3.9))}$$

$$= hR_m^* f_n + h^2 \mu S_m^* \tilde{G}_n + \text{inh. term}$$

where $R_m^* = \sum_{\ell=1}^m a_{m\ell}R_\ell$ and $S_m^* = \sum_{\ell=1}^m a_{m\ell}S_\ell$. Taking i = m in (3.9) we arrive at the equations

$$(3.10)\qquad \begin{aligned} f_{n+1} &= R_m f_n + h\mu S_m \tilde{G}_n + \text{inh. term} \\ \tilde{G}_{n+1} - \tilde{G}_n &= hR_m^* f_n + h^2\mu S_m^* \tilde{G}_n + \text{inh. term.} \end{aligned}$$

From these equations $\tilde{G}_n$ can be eliminated to obtain a difference equation in terms of f_n only, whose characteristic equation is, after application of Lemma 3.1 given by

$$(3.11)\qquad \zeta^2 - (R_m + 1 + h^2\mu S_m^*)\zeta + \{R_m + h^2\mu(R_m S_m^* - R_m^* S_m)\} = 0.$$

3.2. Mixed Runge-Kutta methods using intermediate values $f_j^{(\ell)}$ in the lag term

In this case the lag term is defined by (1.3b). We derive the following difference equation for $\tilde{G}_n$.

$$(3.12)\qquad \begin{aligned} \tilde{G}_{n+1} - \tilde{G}_n &= h \sum_{\ell=1}^m \hat{a}_{m\ell} f_{n+1}^{(\ell)} = \text{(using (3.4))} \\ &= h\hat{U}_m f_n + h\hat{V}_m \tilde{I}_n + h^2\mu\hat{S}_m \tilde{G}_n + \text{inh. term,} \end{aligned}$$

where $\hat{U}_m = \sum \hat{a}_{m\ell} U_\ell$ and similar definitions for $\hat{V}_m$ and $\hat{S}_m$. For $\tilde{I}_n$ we derive

$$(3.13)\qquad \begin{aligned} \tilde{I}_{n+1} - \tilde{I}_n &= h\mu\tilde{G}_n + h \sum_{\ell=1}^m \hat{a}_{m\ell}\{\lambda + \mu h(1-c_\ell)\} f_{n+1}^{(\ell)} \\ &= h\mu\tilde{G}_n + h\tilde{U}_m f_n + h\tilde{V}_m \tilde{I}_n + h^2\mu\tilde{S}_m \tilde{G}_n + \text{inh. term} \end{aligned}$$

where $\tilde{U}_m = \sum \hat{a}_{m\ell}\{\lambda + \mu h(1-c_\ell)\}U_\ell$ and similar definitions for $\tilde{V}_m$ and $\tilde{S}_m$. The difference equations (3.12) and (3.13) together with (3.5) yield a system of difference equations, and the characteristic equation of the difference equation satisfied by $\{f_n\}$ can be found by application of Lemma 3.1 (with M = 3).

3.3. Mixed Runge-Kutta methods using only values f_j in the lag term

3.3.1. $\{\rho,\sigma\}$-reducible quadrature rules

The lag term is now defined by (1.3c) so that the expressions (3.2b) and (3.2c) become

$$\tilde{I}_n = h \sum_{j=0}^{n} w_{nj}[\lambda+\mu(x_n-x_j)]f_j$$

$$\tilde{G}_n = h \sum_{j=0}^{n} w_{nj}f_j.$$

For the present we assume that the quadrature formulae based upon the weights w_{nj} are (ρ,σ)-reducible (see [19]), i.e. we assume that

$$(3.14) \qquad \sum_{r=0}^{k} a_r w_{n-r,j} = \begin{cases} 0 & \text{for } j = 0(1)n-k-1, \\ b_{n-j} & \text{for } j = n-k(1)n. \end{cases}$$

where a_r and b_r are the coefficients of a LMS method for ODEs, and where $\rho(\zeta) = \sum a_r\zeta^{k-r}$ and $\sigma(\zeta) = \sum b_r\zeta^{k-r}$. With this assumption we can derive the difference equations

$$(3.15a) \qquad \sum_{r=0}^{k} a_r\tilde{G}_{n+1-r} = h \sum_{r=0}^{k} b_r f_{n+1-r}$$

$$(3.15b) \qquad \sum_{r=0}^{k} a_r\tilde{I}_{n+1-r} = \sum_{r=0}^{k} b_r\{h\lambda + r\,h^2\mu\}f_{n+1-r} - h\mu \sum_{r=0}^{k} r a_r\tilde{G}_{n+1-r}$$

Application of Lemma 3.1 to (3.15a-b) together with (3.5) yields the characteristic equation

$$(3.16) \qquad \begin{aligned} &\zeta^{k-1}\{\rho^2(\zeta)(\zeta - U_m) - h\lambda V_m\rho(\zeta)\sigma(\zeta) \\ &\quad - h^2\mu V_m[\rho(\zeta)\sigma_1(\zeta) - \rho_1(\zeta)\sigma(\zeta)] - h^2\mu S_m\rho(\zeta)\sigma(\zeta)\} = 0 \end{aligned}$$

where $\rho_1(\zeta) = \sum r a_r\zeta^{k-r}$ and $\sigma_1(\zeta) = \sum r b_r\zeta^{k-r}$. For the special case that $\vec{\gamma} = \vec{\varepsilon}$ (i.e. $\gamma_i = 1$ for $i = 1(1)m$) $V_i \equiv 0$ and (3.16) reduces to

$$(3.16') \qquad \zeta^{k-1}\rho(\zeta)\{\rho(\zeta)(\zeta - U_m) - h^2\mu S_m\sigma(\zeta)\} = 0.$$

We observe that for this special case the equation (3.16') has a factor $\rho(\zeta)$ The presence of this factor is a consequence of the generality of the analysis, and it indicates that the analysis can be simplified to obtain (3.16') without the factor $\rho(\zeta)$. In order to see this we look at (3.5) and observe that we do not need the recurrence relation (3.15b) for $\tilde{I}_n$ since $V_m = 0$. Application of Lemma 3.1 to (3.5) and (3.15a) then yields (3.16') without the factor $\rho(\zeta)$.

3.3.2. Block-reducible quadrature rules

In Section 3.3.1 we assumed the (ρ,σ)-reducibility of the quadrature rules. We now extend these results by considering quadrature rules which are block-reducible. That is, we assume that the weights w_{nj} can be partitioned into matrices V_{nj} (with $V_{nj} = 0$ for $j > n$) such that

$$(3.17) \qquad \sum_{r=0}^{k} A_r V_{n-r,j} = \begin{cases} 0 & j = 0(1)n-k-1, \\ B_{n-j} & j = n-k(1)n, \end{cases}$$

where A_r and B_r are fixed matrices (with $\sum_{r=0}^{k} A_r \vec{\varepsilon} = \vec{0}$; see [1], where examples are also given).

We further restrict attention to the case where each matrix A_r is diagonal ($A_0 = I$). It may be noted that all the quadrature rules considered in [6] have weights which can be partitioned so that $A_0 = I$, $A_1 = -I$, $A_r = 0$, $r = 2(1)k$. We suppose that the matrices A_r and B_r are of order M and we write

$$(3.18) \qquad \vec{\psi}_n = [f_{nM+1}, f_{nM+2}, \ldots, f_{nM+M}]^T, \qquad f_{nM+r} \simeq f(x_{nM+r}),$$

so that, for example, the quadrature method applied to (1.5) yields vectors $\vec{\psi}_n$ satisfying $\vec{\psi}_n = \vec{g}_n + h\lambda \sum_{j=0}^{n} V_{nj}\vec{\psi}_j$.

We shall employ the following lemma.

LEMMA 3.2. *Let the assumptions of this section prevail and suppose that*

$$(3.19) \qquad \vec{\sigma}_n = h \sum_{j=0}^{n} [V_{nj} * K^{\#}_{n-j}]\vec{\psi}_j,$$

where $*$ denotes the Schur (or pointwise) product[†] *and* $K^{\#}_{n-j}$ *is the matrix with entries* $\Lambda_0 + \Lambda_1((n-j)Mh + (\ell-m)h)$ *in the* (ℓ,m)*-th position* $(\ell,m = 1,2,\ldots,M)$. *Then*

$$(3.20)\qquad \sum_{r,s=0}^{k} A_s A_r \vec{\sigma}_{n-r-s} = h \sum_{r,s=0}^{k} A_s [B_r * K^{\#}_{r-s}] \vec{\psi}_{n-r-s}.$$

PROOF. Writing (3.19) in more explicit form we have

$$\vec{\sigma}_n = h\Lambda_0 \sum_{j=0}^{n} V_{nj}\vec{\psi}_j + h^2\Lambda_1 \sum_{j=0}^{n} (n-j)MV_{nj}\vec{\psi}_j + h^2\Lambda_1 \sum_{j=0}^{n} (DV_{nj} - V_{nj}D)\vec{\psi}_j,$$

where $D = \mathrm{diag}(1,2,\ldots,M)$. We now find, employing (3.17), that

$$\begin{aligned}(3.21)\qquad \sum_{r=0}^{k} A_r\vec{\sigma}_{n-r} &= h\Lambda_0 \sum_{r=0}^{k} B_r\vec{\psi}_{n-r} + h^2\Lambda_1 \sum_{j=0}^{n}\sum_{r=0}^{k} (n-j)MA_rV_{n-r,j}\vec{\psi}_j \\ &\quad - h^2\Lambda_1 \sum_{j=0}^{n}\sum_{r=0}^{k} rMA_rV_{n-r,j}\vec{\psi}_j \\ &\quad + h^2\Lambda_1 \sum_{j=0}^{n}\sum_{r=0}^{k} A_r(DV_{n-r,j}-V_{n-r,j}D)\vec{\psi}_j \\ &= h\Lambda_0 \sum_{r=0}^{k} B_r\vec{\psi}_{n-r} + h^2\Lambda_1 \sum_{r=0}^{k} rMB_r\vec{\psi}_{n-r} \\ &\quad - h^2\Lambda_1 \sum_{j=0}^{n}\sum_{r=0}^{k} rMA_rV_{n-r,j}\vec{\psi}_j \\ &\quad + h^2\Lambda_1 \sum_{r=0}^{k} (DB_r - B_rD)\vec{\psi}_{n-r}.\end{aligned}$$

Here, we have used the fact that the matrices A_r are diagonal and hence commute with D. Applying $\sum A_s$ to successive equations (3.21) yields

†) We define the Schur product $A*B$ of the matrices $[a_{ij}]$ and $[b_{ij}]$ as the matrix $[a_{ij}b_{ij}]$.

$$\sum_{r,s=0}^{k} A_s A_r \vec{\sigma}_{n-r-s} = h\Lambda_0 \sum_{r,s=0}^{k} A_s B_r \vec{\psi}_{n-r-s} + h^2\Lambda_1 \sum_{r,s=0}^{k} A_s B_r rM\vec{\psi}_{n-r-s}$$

$$- h^2\Lambda_1 \sum_{r,s=0}^{k} rMA_r B_s \vec{\psi}_{n-r-s}$$

$$+ h^2\Lambda_1 \sum_{r,s=0}^{k} A_s (DB_r - B_r D)\vec{\psi}_{n-r-s},$$

which, when expressed in terms of $K^{\#}_{r-s}$, is the required result. □

Establishing our notation and the above lemma has been preliminary to our task. We return to equation (3.5) from which we deduce, in terms of (3.18)

$$(3.22) \qquad \begin{bmatrix} f_{nM+2} \\ \vdots \\ f_{nM+M+1} \end{bmatrix} = h\mu S_m \begin{bmatrix} \tilde{G}_{nM+1} \\ \vdots \\ \tilde{G}_{nM+M} \end{bmatrix} + V_m \begin{bmatrix} \tilde{I}_{nM+1} \\ \vdots \\ \tilde{I}_{nM+M} \end{bmatrix} + U_m \vec{\psi}_n .$$

We designate the left-hand side vector in (3.22) by $\vec{\phi}_n$, and the sum of the first two terms on the right-hand side by $\vec{\sigma}_n$ so that (3.22) becomes

$$(3.22') \qquad \vec{\phi}_n = \vec{\sigma}_n + U_m \vec{\psi}_n .$$

Moreover, if we take $\Lambda_0 = h\mu S_m + \lambda V_m$ and $\Lambda_1 = V_m \mu$ then $\vec{\sigma}_n$ coincides with (3.19) in the statement of Lemma 3.2. Taking these values of Λ_0 and Λ_1 in the definition of $K^{\#}_{r-s}$ we have, from (3.20)

$$\sum_{r,s=0}^{k} A_s A_r \vec{\sigma}_{n-r-s} = h \sum_{r,s=0}^{k} A_s [B_r * K^{\#}_{r-s}] \vec{\psi}_{n-r-s} .$$

In consequence, from (3.22')

$$(3.23) \qquad \sum_{r,s=0}^{k} A_s A_r \vec{\phi}_{n-r-s} = h \sum_{r,s=0}^{k} A_s [B_r * K^{\#}_{r-s}] \vec{\psi}_{n-r-s} + U_m \sum_{r,s=0}^{k} A_s A_r \vec{\psi}_{n-r-s}$$

It remains to observe that if

$$(3.24)\qquad J = \begin{bmatrix} 0 & \cdots & & 0 \\ 1 & \ddots & & \vdots \\ & \ddots & \ddots & \vdots \\ 0 & & 1 & 0 \end{bmatrix}, \qquad J^{\#} = \begin{bmatrix} 0 & \cdots & 0 & 1 \\ \vdots & & \vdots & 0 \\ \vdots & & \vdots & \vdots \\ 0 & \cdots & 0 & 0 \end{bmatrix}$$

then

$$(3.25)\qquad \vec{\psi}_n = J\vec{\phi}_n + J^{\#}\vec{\phi}_{n-1}$$

and that substitution of (3.25) in (3.23) yields a recurrence relation for the vectors $\vec{\phi}_n$. Thus we have shown that the vectors $\vec{\phi}_n = [f_{nM+2}, f_{nM+3}, \ldots$ $\ldots, f_{nM+M+1}]^T$, satisfy, under the assumptions of Lemma 3.2, a recurrence relation whose characteristic equation is given by

$$(3.26)\qquad \det[\sum_{s=0}^{k} A_s \sum_{r=0}^{k} \{A_r\zeta - [hB_r * K^{\#}_{r-s} + U_m A_r][J\zeta + J^{\#}]\}\zeta^{2k-r-s}] = 0.$$

Note that for $M = 1$ the result (3.16) is obtained as a special case of (3.26) on writing $K^{\#}_{r-s} = (h\mu S_m + \lambda V_m) + \mu V_m(r-s)h$, $A_r = a_r$, $B_r = b_r$ and defining $J = (0)$ and $J^{\#} = (1)$.

3.4. The special case $\mu = 0$ and $\gamma_i = \gamma$

If $\mu = 0$ the convolution test equation reduces to the basic test equation (1.5). In this case the characteristic equations derived in the previous §§, can be factorized, which indicates that the analysis can be simplified (in fact, we do not need the recurrence relations for $\tilde{G}_n$). Furthermore, we assume that $\vec{\gamma} = \gamma\vec{\varepsilon}$ so that we can use (3.4') with $R_i = \vec{\varepsilon}_i^T(I - h\lambda A_0)^{-1}\vec{\varepsilon}$; in particular $R_m(h\lambda)$ represents the amplification factor of the RK-method for ODEs (see e.g. [16]). Below we give the characteristic equations associated with the three classes of methods discussed in the previous §§. These characteristic equations with $\gamma = 0$ can also be found in [1]. For the extended Pouzet methods we obtain

$$(3.27)\qquad \zeta - R_m = 0,$$

and for the mixed methods of §3.2.

$$(3.28)\qquad \zeta^2 - (1+\gamma R_m + (1-\gamma)h\lambda \sum_{\ell=1}^{m} \hat{a}_{m\ell}R_\ell)\zeta + \gamma R_m.$$

The mixed methods of §3.3 yield

$$(3.29)\qquad (\zeta - \gamma R_m)\rho(\zeta) - h\lambda(1-\gamma)R_m\sigma(\zeta) = 0.$$

Note that for $\gamma = 1$, (3.28) and (3.29) can be simplified to yield (3.27). In the next section we shall analyze the equation (3.29) for $\gamma \neq 1$.

4. STABILITY RESULTS

4.1. Results for the basic test equation

In analogy with the stability theory for ODEs, a numerical method for (1.1) is said to be *A-stable* if, when applied to (1.5) with $g(x)$ constant, the solution f_n tends to zero as $n \to \infty$ for all values of the step size h and for all $\lambda \in \mathbb{C}$ with Re $\lambda < 0$. It is easily seen that A-stability is equivalent to asymptotic stability of the discrete scheme when Re$(h\lambda) < 0$ and is obtained precisely when the zeros of the characteristic polynomial are within the unit circle. We shall call the method *weakly A-stable* if these zeros are on the unit disk, those on the boundary being simple roots. The following theorem gives us an important result for the modified methods with $\vec{\gamma} = \vec{\varepsilon}$ already mentioned in the introduction.

THEOREM 4.1. *Consider a general Runge-Kutta method* (1.2a-b) *which is modified according to* (1.7) *with* $\gamma_i = 1$ $(i = 1,\dots,m)$. *Then the method is (weakly) A-stable if and only if the generating Runge-Kutta method defining the forward part is (weakly) A-stable for ordinary differential equations.*

PROOF. From relation (3.4') which holds for a general lag term (1.2b), the result of the theorem is readily seen. Here, weak A-stability for ordinary differential equations is defined in a similar manner as above. □

The next theorem states necessary conditions for A-stability in the weak sense.

THEOREM 4.2. *Consider a mixed Runge-Kutta method* (1.2a-b) *which employs* (ρ,σ)-*reducible quadrature formulae for the lag term* (1.3c), *and which is modified according to* (1.7) *with* $\gamma_i = \gamma$, $(i = 1,2,\dots,m)$, $\gamma \in [0,1)$. *Let the amplification factor* $R_m(z) = P(z)/Q(z)$, *where* P *and* Q *are polynomials, and where* $z = h\lambda$. *Then necessary conditions for weak* A-*stability are*

(i) $|R_m(z)| = \mathcal{O}(1/|z|)$ *as* $|z| \to \infty$,

(ii) $Q(z)$ *has no zeros in the half plane* $\mathrm{Re}\, z \le 0$,

(iii) $P(z)$ *has no zeros in the half plane* $\mathrm{Re}\, z < 0$.

PROOF. Observe first that the coefficient of ζ^{k+1} in equation (3.29) is independent of z. If $R_m(z)$ or $zR_m(z)$ is unbounded, then the polynomial (3.29) has at least one unbounded coefficient. This implies that (3.29) has at least one unbounded root. This proves (i) and (ii). Next we prove (iii). We observe that the zeros $\zeta_1(z),\dots,\zeta_{k+1}(z)$ of (3.29) can be interpreted as the values of an algebraic function. Let $P(z_0) = 0$ with $\mathrm{Re}\, z_0 < 0$. Then $R_m(z_0) = 0$ and (3.29) reduces to $\zeta\rho(\zeta) = 0$ which has a root $\zeta_1(z_0) = 1$. Now $\zeta_1(z)$ is a branch of an algebraic function which is analytic in a neighbourhood of z_0. Let $C_\varepsilon = \{z \mid |z-z_0| \le \varepsilon\}$ be a small circle around the point z_0, which is contained entirely in the left half plane $\mathrm{Re}\, z < 0$. Application of the maximum principle for analytic functions yields that $|\zeta_1(z)| > 1$ for some z with $|z-z_0| = \varepsilon$ or that $\zeta_1(z)$ must reduce to a constant (= 1) on C_ε. However, $\zeta_1(z) \equiv 1$ on C_ε implies that $R_m(z) \equiv 0$ on C_ε which is not true. Hence, we have shown that there exists a point z with $\mathrm{Re}\, z < 0$ such that (3.29) has a root greater than unity which implies that the method cannot be A-stable. □

The following Corollary is a consequence of the condition (iii) in Theorem 4.2 and indicates that high-order mixed Runge-Kutta methods cannot be A-stable.

COROLLARY. *Consider the methods treated in Theorem* 4.2. *Let the amplification factor* $R_m(z)$ *be* A-*acceptable and a* p-*th order approximation to* exp(z). *Then the method is not* A-*stable for* $p \ge 3$.

PROOF. The order star associated with $R_m(z)$ has at least $[(p+1)/2] - 1$ bounded dual fingers in the left-hand plane $\mathrm{Re}\, z < 0$ (see the proof of Theorem 5 of WANNER et al. [20]). This implies (see Proposition 4 in [20]) that $R_m(z)$

has at least $[(p+1)/2] - 1$ zeros in the left-half plane. Therefore condition (iii) of Theorem 4.2 is violated. □

Let us now consider the case that λ assumes only real values. A numerical method is said to be weakly A_0-*stable* if, when applied to (1.5) with $g(x)$ constant, the solution f_n remains bounded as $n \to \infty$ for all values of the stepsize h and all $\lambda \in \mathbb{R}$ with $\lambda \le 0$. This condition is equivalent to stability of the discrete scheme when $\mathrm{Re}(h\lambda) \le 0$.

THEOREM 4.3. *Consider the methods treated in Theorem 4.2. Let the amplification factor* $R_m(x) = P(x)/Q(x)$ *with* $P(0) = Q(0) = 1$ *and* $x = h\lambda \in \mathbb{R}^-$. *Then necessary conditions for weak* A_0*-stability are*

(i) $|R_m(x)| = \mathcal{O}(1/|x|)$ *as* $|x| \to \infty$.

(ii) $Q(x)$ *has no zeros for* $x \le 0$.

(iii) $P(x)$ *does not change sign for* $x \le 0$, *i.e.* $P(x) \ge 0$.

PROOF. The proof for (i) and (ii) is the same as for Theorem 4.2. For (iii) we reason as follows. Since $Q(x) > 0$ on $(-\infty,0)$ and $P(0) = 1$, we know that $P(x) \ge 0$ if $P(x)$ does not change sign on $(-\infty,0)$. Suppose that $R_m(x)$ changes sign at $x = x_0$ with $x_0 < 0$. Then $R_m(x)$ has a zero at $x = x_0$, and if μ is the multiplicity of that zero then μ is odd. Since $R_m(x_0) = 0$, the equation (3.29) reduces to $\zeta\rho(\zeta) = 0$ which has a root $\zeta = 1$. By (repeated) differentiation of (3.29) with respect to $h\lambda$, and using the fact that $R_m(x_0) = \ldots = R_m^{(\mu-1)}(x_0) = 0$, $R_m^{(\mu)}(x_0) \ne 0$, we derive that

$$\zeta(x) = \zeta(x_0) + \frac{1}{\mu!}(x-x_0)^{\mu}(1-\gamma)x_0R_m^{(\mu)}(x_0) + \mathcal{O}((x-x_0)^{\mu+1}).$$

Since $\zeta(x_0) = 1$, $R_m^{(\mu)}(x_0) \ne 0$ and μ odd, we can always find an x sufficiently close to x_0 such that $\zeta(x) > 1$, which implies that the method cannot be A_0-stable. □

We conclude this section on the basic test equation by listing the stability boundaries of a number of mixed Runge-Kutta methods (the stability boundary β is defined by the interval $-\beta \le h\lambda \le 0$ where the characteristic roots $\zeta(h\lambda)$ are on the unit disk, those on the unit circle being simple roots). In Table 4.1 the lag terms in these methods are defined by specifying the characteristic polynomials $\{\rho,\sigma\}$, and in Table 4.2 we give the vector $\vec{\theta}$ and the matrices A_0, A_1 associated with the Runge-Kutta parts used. Deriving the functions U_m, V_m and S_m defined according to (3.3), and substitution of $\{\rho,\sigma\}$ and $\{U_m,V_m,S_m\}$ into (3.16) yields the characteristic equation

Table 4.1. Lag terms defined by $\{\rho,\sigma\}$

	k	$\rho(\zeta)$	$\sigma(\zeta)$
third order Gregory rule [4]	2	$\zeta(\zeta-1)$	$(5\zeta^2+8\zeta-1)/12$
trapezoidal rule	1	$\zeta-1$	$(\zeta+1)/2$
third order backward differentiation formula [19]	3	$(11\zeta^3-18\zeta^2+9\zeta-2)/11$	$6\zeta^3/11$

of the various mixed Runge-Kutta methods. In Table 4.3 the stability boundaries for the basic test equation are listed for $\vec{\gamma} = \vec{0}$, $\vec{\gamma} = \vec{\varepsilon}_1$ and $\vec{\gamma} = \vec{\varepsilon}$, respectively. We also include the stability boundaries when the lag term is combined with the one-step Runge-Kutta part defined by the forward and backward Euler formula and the trapezoidal rule. (In the following a particular Runge-Kutta method will be indicated by specifying first the lag term and then the Runge-Kutta part.)

From the data of Table 4.3, the stabilizing effect of $\vec{\gamma} = \vec{\varepsilon}$ is evident. It should be remarked, however, that the $\vec{\gamma} = \vec{\varepsilon}_1$ version of the method may have a smaller stability boundary. (Recall that if $\vec{\gamma} = \vec{\varepsilon}_1$ the methods in Table 4.3 are economized, except for the Nørsett formula where $\theta_1 \neq 0$ (see Table 4.2).)

The result $\beta(\vec{0}) = 2$ obtained for the trapezoidal rule when *mixed with the repeated trapezoidal rule for the lag term,* is surprising at first sight because it is well-known that the trapezoidal rule when used as a *direct quadrature method* is A-stable (see e.g. [6]). Although both representations will produce the same numerical solution if exact arithmetic is used, different numerical solutions are obtained in the actual computation on a finite precision computer. In Table 4.4 this is illustrated for the integral equation

(4.1) $$f(x) = 1 + 100x + e^{-x}\sin x - \int_0^x [100 + e^{-x}\cos(yf(y))]f(y)\,dy$$

with the exact solution $f(x) \equiv 1$.

Table 4.2. Runge-Kutta parts defined by $\vec{\theta}$, A_0 and A_1

	$\vec{\theta}$	A_0	A_1
Third order Bel'tyukov [9, p.148]	$\begin{pmatrix} 0 \\ 1 \\ 1/3 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1/9 & 2/9 & 0 & 0 \\ 0 & 1/4 & 3/4 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 0 \\ 1/18 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 \end{pmatrix}$
Third order Newton-Cotes [14]	$\begin{pmatrix} 0 \\ 1/2 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 1/4 & 1/4 & 0 \\ 1/6 & 2/3 & 1/6 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 1/8 & 0 & 0 \\ 1/6 & 1/3 & 0 \end{pmatrix}$
Third order Nørsett [11, p.150]	$\frac{1}{6}\begin{pmatrix} 3+\sqrt{3} \\ 3-\sqrt{3} \\ 6 \end{pmatrix}$	$\frac{1}{6}\begin{pmatrix} 3+\sqrt{3} & 0 & 0 \\ -2\sqrt{3} & 3+\sqrt{3} & 0 \\ 3 & 3 & 0 \end{pmatrix}$	$\frac{1}{36}\begin{pmatrix} 0 & 0 & 0 \\ 12 & 0 & 0 \\ 9-3\sqrt{3} & 9+3\sqrt{3} & 0 \end{pmatrix}$

Table 4.3. Stability boundaries $\beta(\vec{\gamma})$ for $\vec{\gamma} = \vec{0}$, $\vec{\gamma} = \vec{\varepsilon}_1$ and $\vec{\gamma} = \vec{\varepsilon}$

Runge-Kutta part	LAG TERM Trap. Rule $\beta(\vec{0})$	Trap. Rule $\beta(\vec{\varepsilon}_1)$	Trap. Rule $\beta(\vec{\varepsilon})$	Gregory $\beta(\vec{0})$	Gregory $\beta(\vec{\varepsilon}_1)$	Gregory $\beta(\vec{\varepsilon})$	Backw. diff. $\beta(\vec{0})$	Backw. diff. $\beta(\vec{\varepsilon}_1)$	Backw. diff. $\beta(\vec{\varepsilon})$
Forward Euler	1	1	2	1	1.2	2	1	.9	2
Trap. Rule	2	∞	∞	2	∞	∞	2	6.6	∞
Backward Euler	∞	∞	∞	∞	∞	∞	∞	∞	∞
Bel'tyukov	1.6	1.3	2.5	1.6	1.3	2.5	1.6	1.3	2.5
Newton-Cotes	5.6	2.4	12	5.1	2.4	12	7.7	2.4	12
Nørsett	2.2	8.5	∞	2.2	4.8	∞	2.2	3.5	∞

Table 4.4. Numerical solution of (4.1) obtained on the CDC CYBER750 for h = 1/10.

x	Mixed Method (4.2)	Direct Method (4.3)
.2	1.000001...	1.000001...
1.0	.999998...	.999998...
1.6	.9996...	.999998...
1.9	.95...	.
2.0	.79...	.
2.1	-.04...	.
2.2	-4.2...	.
2.3	-25.1...	.
2.4	-129.8...	.999998...

We recall that the "mixed" representation reads

$$(4.2)\qquad \begin{aligned} f_{n+1}^{(1)} &= g(x_n) + h \sum_{j=0}^{n}{}'' K(x_n, x_j, f_j) \\ f_{n+1} &= g(x_{n+1}) + h \sum_{j=0}^{n}{}'' K(x_{n+1}, x_j, f_j) \\ &\quad + \frac{1}{2} h[K(x_{n+1}, x_n, f_{n+1}^{(1)}) + K(x_{n+1}, x_{n+1}, f_{n+1})] \end{aligned}$$

and the "direct" representation simply

$$(4.3)\qquad f_{n+1} = g(x_{n+1}) + h \sum_{j=0}^{n+1}{}'' K(x_{n+1}, x_j, f_j).$$

According to Table 4.3 and Table 4.4 as well, the direct representation is stable, whereas the mixed version (4.2) is unstable for this stepsize (the same phenomenon occurs for the basic test equation).

4.2. Stability plots for the linear convolution equation

For the convolution equation (3.1) the stability regions (that region in the $(h\lambda, h^2\mu)$-plane where the characteristic equation has its roots on the unit disk with simple roots on the unit circle) were computed for a number

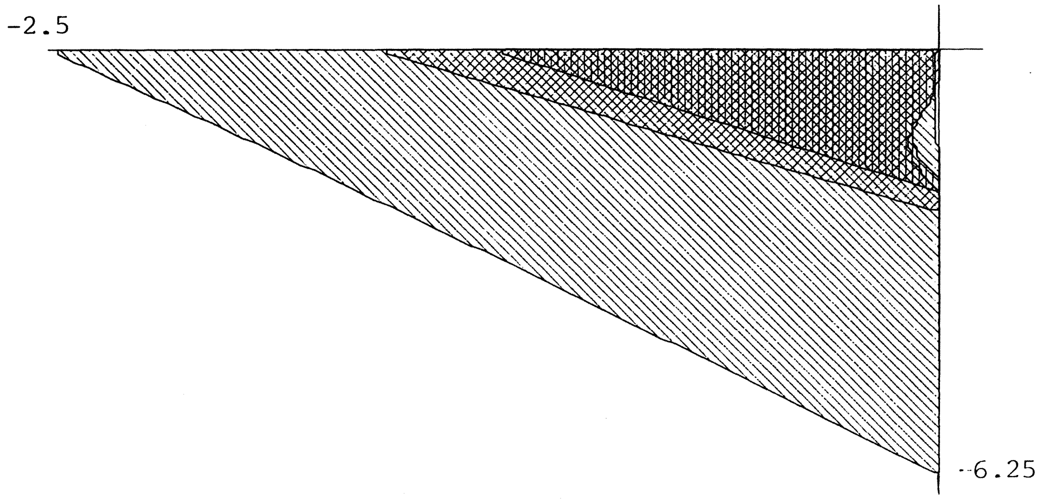

Figure 4.1. Gregory-Bel'tyukov

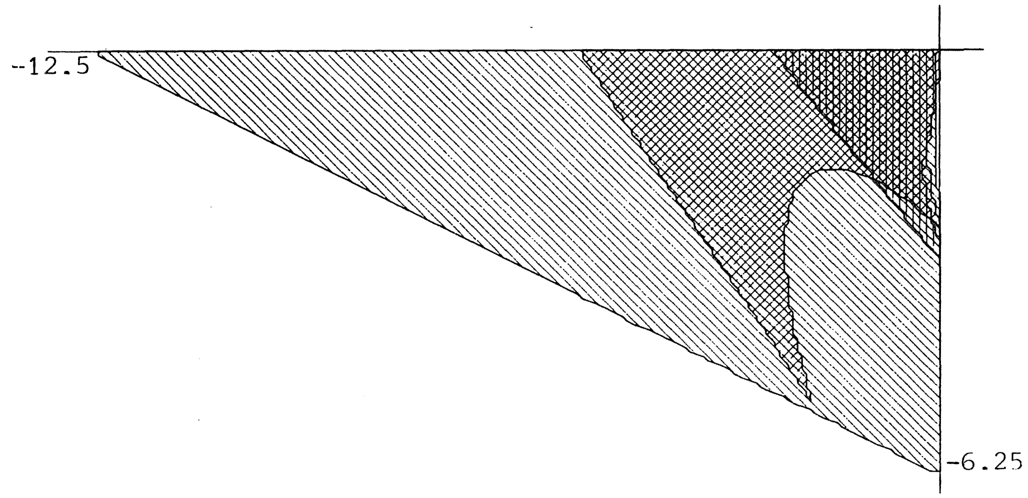

Figure 4.3. Gregory-Newton Cotes

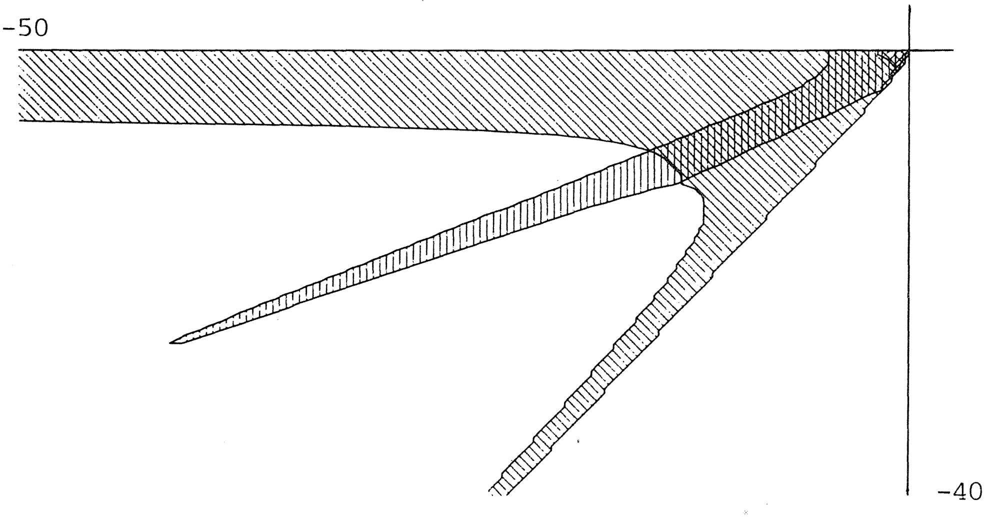

Figure 4.5. Gregory-Nørsett

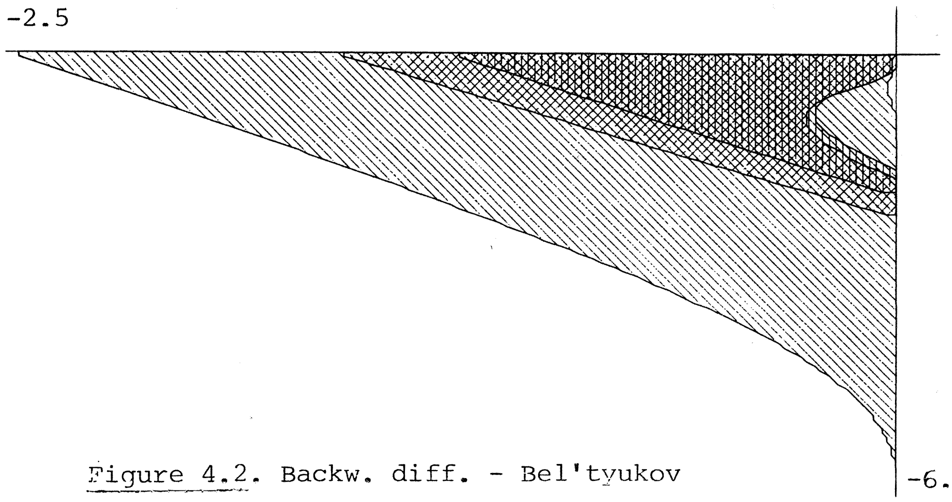

Figure 4.2. Backw. diff. - Bel'tyukov

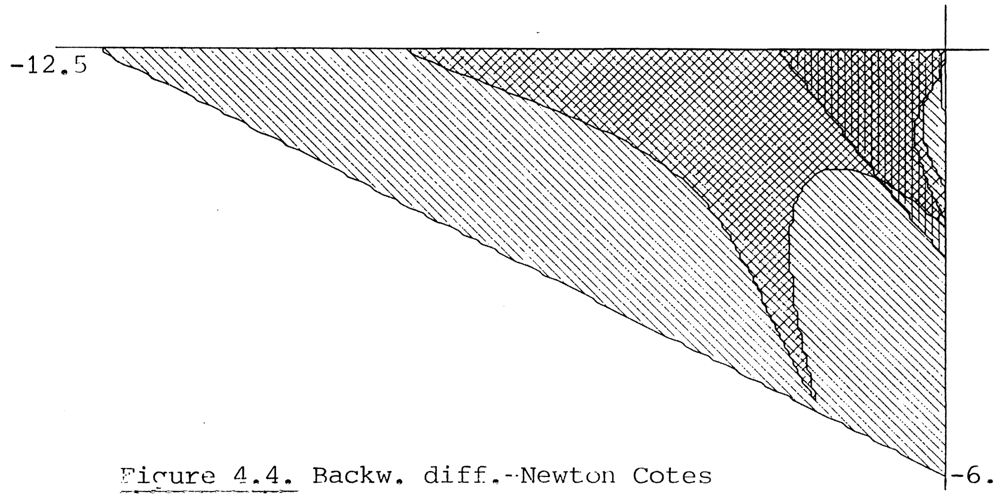

Figure 4.4. Backw. diff.-Newton Cotes

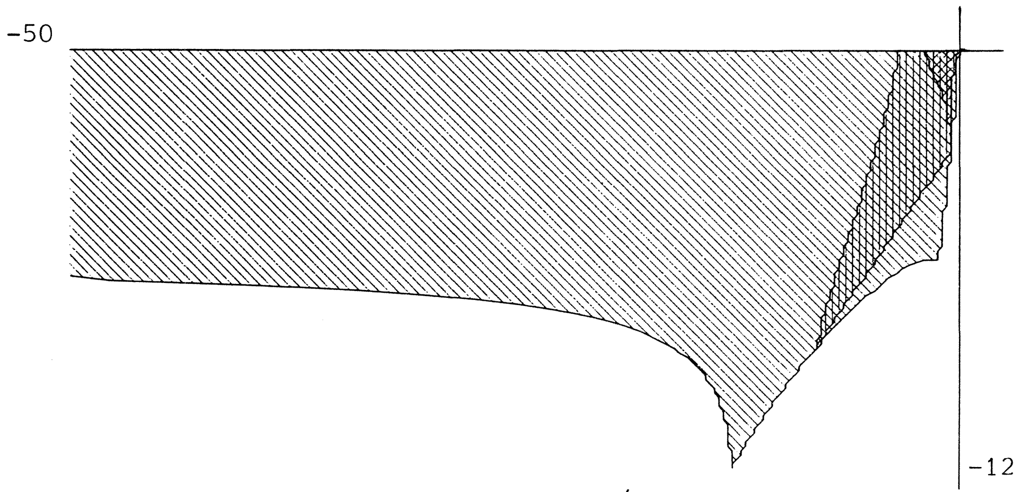

Figure 4.6. Backw. diff. - Nørsett

of mixed Runge-Kutta methods specified in the Tables 4.1 and 4.2. In the figures 4.1 - 4.6 these regions are given for $\vec{\gamma} = \vec{0}$ (///), $\vec{\gamma} = \vec{\varepsilon}_1$ (|||) and for $\vec{\gamma} = \vec{\varepsilon}$ (\\\). The values given in these figures refer to the part of the $(h\lambda, h^2\mu)$-plane to which the stability plots are restricted.

In these figures we see that except for the Gregory-Nørsett method (Fig. 4.5) *the stability regions corresponding to* $\vec{\gamma} = \vec{\varepsilon}$ *contain those corresponding to the standard method* $(\vec{\gamma} = \vec{0})$ *or to the economized version* $(\vec{\gamma} = \vec{\varepsilon}_1$ *and are considerably larger.* In figure 4.5 the $\vec{\gamma} = \vec{\varepsilon}_1$ method is stable where the modified method is not but this has no practical significance.

Furthermore, we may conclude that just as in Table 4.3 *the Runge-Kutta part mainly determines the magnitude of the stability region and the lag ter is less important.*

5. NUMERICAL EXPERIMENTS

In this section we report on numerical experiments with mixed Runge-Kutta methods and their modification employing residual corrections. The pur pose of these experiments is to verify the order of convergence expected fro Theorem 2.1, and to indicate the relevance of the stability results obtained in Section 3 and 4.

In the accuracy experiment, we have chosen the following mixed Runge-Kutta method of Pouzet type, where the forward step is given by the two-stag third order Radau formula (see LAPIDUS and SEINFELD [16, p.62]).

$$\vec{\theta} = [0,2/3,1]^T, \qquad A_0 = \begin{bmatrix} 0 & 0 & 0 \\ 1/3 & 1/3 & 0 \\ 1/4 & 3/4 & 0 \end{bmatrix},$$

and where the lag term (1.3c) was computed by the Gregory-rules of order 4. For the classical $(\vec{\gamma} = \vec{0})$ and economized $(\vec{\gamma} = \vec{\varepsilon}_1)$ method the expected order of accuracy is $p = 4$, whereas for the modification with $\vec{\gamma} = \vec{\varepsilon}$ it is $p = 3$. For these choices of $\vec{\gamma}$ we have applied the method to the equation

$$(5.1) \qquad f(x) = g(x) - \int_0^x \frac{2}{(x-y+2)^2} f(y)\,dy, \qquad 0 \le x \le 2.$$

The kernel in the equation (5.1) occurs in the study of the reflection of sound pulses (see FRIEDLANDER [10]). In order to have the exact solution at hand, we have chosen $g(x) = 2 - 2/(x+2)$ which yields $f(x) \equiv 1$. We have integrated the problem (5.1) with stepsizes $h = 0.1, 0.05, 0.01$ and 0.005. In Table 5.1 the number of correct digits (defined by $cd = -{}^{10}\log$ absolute error) at $x = 2$ and the computed order p^* is listed ($p^* = [cd(h) - cd(2h)]/{}^{10}\log 2$). The results confirm the theoretical result given in Theorem 2.1. Notice that the economized version ($\vec{\gamma} = \vec{\varepsilon}_1$) yields the same results as the standard version ($\vec{\gamma} = \vec{0}$). The stabilized version is considerably less accurate in this non-stiff example.

In the following experiment we have applied the third order Nørsett formula mixed with the third order Gregory rule (see Section 4.1) to the integral equation (5.2):

Table 5.1. Number of correct digits at $x = 2$ and computed order for problem (5.1)

h	$\vec{\gamma} = \vec{0}$		$\vec{\gamma} = \vec{\varepsilon}_1$		$\vec{\gamma} = \vec{\varepsilon}$	
	cd	p^*	cd	p^*	cd	p^*
0.1	6.1		6.1		4.6	
		3.7		3.7		3.0
0.05	7.2		7.2		5.5	
		3.7		3.7		3.0
0.01	9.8		9.8		7.7	
		4.0		4.0		3.0
0.005	11.0		11.0		8.6	

(5.2) $$f(x) = g(x) - \int_0^x [16+(x-y)][1-0.01\exp(-x)\cos(yf(y))]f(y)\,dy.$$

With $g(x) = 1 + 16x + 1/2\, x^2 - 0.01\exp(-x)[1 - \cos x + 16\sin x]$ the exact solution of (5.2) is $f(x) \equiv 1$. The kernel in (5.2) deviates only slightly from our linear convolution test equation (3.1), and therefore, it is expected that the stability regions given in Fig. 4.5 can be used in a *quantitative manner* to predict stable or unstable behaviour. The problem (5.2) was integrated with stepsizes $h = 1/2, 1/4, 1/8, 1/16$ and $1/32$; the endpoint was $128h$. From Fig. 4.5 we expect the modified ($\vec{\gamma} = \vec{\varepsilon}$) method to be stable for all stepsizes considered and the classical ($\vec{\gamma} = \vec{0}$) version only for $h \neq 1/2, 1/4$. The truth is given in Table 5.2 where we have listed the number of correct digit at the endpoint xe = 128h. (An asterisk indicates that the absolute error is larger than 10^{+10}.) These results indicate that the modified method is reall

Table 5.2. The number of correct digits at xe = 128h for problem (5.2).

h	xe	$\vec{\gamma} = \vec{0}$	$\vec{\gamma} = \vec{\varepsilon}$
1/2	64	*	3.4
1/4	32	*	3.2
1/8	16	4.5	3.5
1/16	8	6.1	4.0
1/32	4	7.2	4.6

highly stable but also that its accuracy is rather modest. If one decides to base a computer program on the modified methods it seems desirable to have some strategy which makes an appropriate choice between the more accurate standard method (for nonstiff problems) and the more stable modified method (for stiff problems). However, to justify such a strategy one has to be sure that the behaviour shown in Table 5.2 is also typical of problems which do not resemble the model problem (3.1).

Our first "non-model" problem is a nonlinear convolution equation with increasing stiffness as x increases:

$$(5.3) \qquad f(x) = 17(\exp(x)-1) - \int_0^x (16+x-y)\exp(f(y))\,dy$$

with the exact solution f(x) = x. Applying the Gregory-Nørsett method, we obtained the results listed in the Tables 5.3 and 5.4 showing the higher accuracy of the standard method for small h and the increased stability of the modified method for larger values of h.

Our final problem is a nonlinear, non-convolution equation given by

$$(5.4) \qquad f(x) = [1+(1+x)\exp(-10x)]^{1/2} + \frac{\lambda}{10}(1+x)[10\ln(1+x)+1-\exp(-10x)] - \lambda\int_0^x \frac{1+x}{1+y} f^2(y)\,dy, \qquad 0 \le x \le 10.$$

Table 5.3. The number of correct digits for problem (5.3)

$\vec{\gamma} = \vec{0}$	x=.5	1.0	1.5	2.0	2.5	3.0	3.5
h = 1/4	0.9	-0.1	-1.2	*	*	*	*
1/8	1.4	0.4	0.5	*	*	*	*
1/16	2.7	1.8	0.6	0.2	-1.7	*	*
1/32	3.9	3.4	2.5	1.0	0.9	-0.9	*

Table 5.4. The number of correct digits for problem (5.3)

$\vec{\gamma} = \vec{\varepsilon}$	x=.5	1.0	1.5	2.0	2.5	3.0	3.5
1/4	0.9	0.7	0.5	0.3	0.0	-0.2	-0.4
1/8	1.6	1.4	1.1	0.9	0.7	0.4	0.2
1/16	2.3	2.0	1.8	1.5	1.3	1.0	0.8
1/32	3.1	2.7	2.4	2.2	1.9	1.7	1.4

with the exact solution $f(x) = [1+(1+x)\exp(-10x)]^{1/2}$. We considered the values $\lambda = 1$, 10 and 100 in order to make this problem increasingly stiff. For $\lambda = 10$, (5.4) is the frequently quoted equation of DE HOOG and WEISS [12]. In order to avoid the computation of the initial phase of the solution, we computed the integral over [0,1] exactly and started the integration at $x = 1$. The results obtained with the Gregory-Nørsett method are listed in Table 5.5 and indicate that the methods ($\vec{\gamma} = \vec{0}$ and $\vec{\gamma} = \vec{\varepsilon}$) have the same behaviour as in the case of convolution kernels.

Table 5.5. The number of correct digits at x = 10 for problem (5.4)

h	$\lambda = 1$		$\lambda = 10$		$\lambda = 100$	
	$\vec{\gamma}=\vec{0}$	$\vec{\gamma}=\vec{\varepsilon}$	$\vec{\gamma}=\vec{0}$	$\vec{\gamma}=\vec{\varepsilon}$	$\vec{\gamma}=\vec{0}$	$\vec{\gamma}=\vec{\varepsilon}$
1/2	3.6	3.3	*	1.8	*	*
1/4	4.8	4.0	*	2.6	*	*
1/8	6.0	4.8	*	3.2	*	*
1/16	7.1	5.6	5.3	3.9	*	2.7
1/32	8.2	6.5	6.6	4.7	*	3.3

6. EXTENSIONS

To conclude this work we indicate briefly some topics of further interes

Concerning *convergence*, it will be observed that the use of (1.3a) or (1.3b) may correspond to superconvergence in the values $f_{n+1} \equiv f_{n+1}^{(m)}$ which is not revealed by application of Theorem 2.1.

Concerning *stability*, we recall that it is possible to consider test equations of the form

$$(6.1) \qquad f(x) = g(x) + \int_0^x \{\sum_{r=0}^{R} \lambda_r (x-y)^r\} f(y)\,dy$$

in place of (3.1), or to extend consideration to non-convolution kernels in which there is polynomial dependence on x (cf. [2], [15] and [18]). In [2] certain unmodified methods have been analysed for the equation (6.1) and the present authors have adapted these results to include modified Runge-Kutta methods considered here. These extensions are in preparation and will be published in the near future [3].

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