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A SPECIAL CLASS OF MULTISTEP RUNGE-KUTTA METHODS WITH EXTENDED REAL STABILITY INTERVAL

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A special class of multistep Runge-Kutta methods with extended real stability interval *)

by

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ABSTRACT

A special class of k-step Runge-Kutta methods is investigated which is generated by (nonlinear) Chebyshev iteration (Richardson iteration) of an implicit linear multistep method. By terminating the iteration process after (say) m iterations, a family of k-step, m-stage Runge-Kutta method is obtained of which the real stability interval can be derived for general values of k and m by a special application of the boundary locus method. The real stability boundary is maximized by choosing suitable values for the coefficients in the generating k-step method. The considerations are mainly restricted to second order methods. Examples are given for k = 1,2,3 and 4, and a few numerical experiments are reported with a nonlinear parabolic initial boundary value problem.

KEY WORDS & PHRASES: *Numerical Analysis, parabolic initial-boundary value problems, multistep Runge-Kutta methods, stability*

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*) This report will be submitted for publication elsewhere.

1. INTRODUCTION

In various papers [2,3,4,7,9,10,11] k-step Runge-Kutta methods were derived with extended intervals of stability for the integration of the system of ODE's

$$\frac{dy}{dt} = f(y), \quad y(t_0) = y_0. \tag{1.1}$$

These stability intervals are as large as cm^2 where c is some constant depending on k and the order of consistency and m is the number of stages in the Runge-Kutta formula. In the class of second order methods the maximal (normalized) stability constant c so far obtained is approximately .65 for k = 1, 1.19 for k = 2 and 2.32 for k = 3. The coefficients of these stabilized methods are known in analytical form for all m (for k = 1 it is known that methods exist with a stability constant $c \cong .82$ but the coefficients are not defined in a closed analytical form and have to be computed by numerical methods [3,9]). The derivations of the methods reported in the papers mentioned above become increasingly complicated if k increases and, in fact, for k > 3 stabilized methods have not yet been derived.

It is the purpose of this paper to present for general values of both k and m a straightforward derivation of stabilized Runge-Kutta methods which possess stability intervals of magnitude cm^2. Formally, our starting point is an implicit linear multistep method. The solution of the implicit relations is approximated by performing m Chebyshev type interations (nonlinear Richardson method). This process may be interpreted as a multistep, m-stage Runge-Kutta method. The order equations for this special class of methods are simple linear equations for the coefficients of the generating multistep method. Since not all coefficients are determined by the order equations, the remaining ones are used for maximizing the stability interval. By applying the boundary locus method the derivation of the maximal intervals is rather straightforward for all k and m.

Within the class of second order methods of the type described above we have found examples where the (normalized) stability constant c equals .81 for k = 1, 1.39 for k = 2, 2.22 for k = 3 and 3.14 for k = 4.

In the application of the methods one should provide an estimate of the spectral radius of $\partial f/\partial y$ (such an estimate is required by all explicit integration methods). An estimate of the smallest (absolute) eigenvalue of $\partial f/\partial y$ is not required. By a few numerical experiments we will show that the analysis is confirmed in actual computation.

2. SPECIFICATION OF THE CLASS OF METHODS

Let equation (1.1) be integrated by a linear multistep method, then the numerical solution at $t = t_{n+1}$ satisfies the equation

$$
\text{(2.1)}\qquad
\begin{aligned}
&y - b_0\tau f(y) = \Sigma_n, \quad b_0 \neq 0,\\
&\Sigma_n = \sum_{\ell=1}^{k} [a_\ell y_{n+1-\ell} + b_\ell \tau f(y_{n+1-\ell})],
\end{aligned}
$$

where $\tau = t_{n+1} - t_n$ and y_n denotes the numerical solution at t_n. This implicit relation is solved by the Richardson type process (nonlinear Chebyshev iteration [1])

$$
\text{(2.2)}\qquad
\begin{aligned}
&y_{n+1}^{(0)} = y_n, \quad y_{n+1}^{(1)} = y_n + \lambda_0[y_n - b_0\tau f(y_n) - \Sigma_n],\\
&y_{n+1}^{(j+1)} = \mu_j y_{n+1}^{(j)} + (1-\mu_j)y_{n+1}^{(j-1)} + \mu_j\lambda_0[y_{n+1}^{(j)} - b_0\tau f(y_{n+1}^{(j)}) - \Sigma_n],\\
&\qquad\qquad j = 1,2,\ldots,m-1,\\
&y_{n+1} = y_{n+1}^{(m)},
\end{aligned}
$$

(2.2)

where

$$
\text{(2.3)}\qquad
\begin{aligned}
&\mu_j = 2w_0 \frac{T_j(w_0)}{T_{j+1}(w_0)}, \quad \lambda_0 = \frac{w_1}{w_0},\\
&w_0 = \frac{2}{b_0\beta(1-\alpha)} + \frac{1+\alpha}{1-\alpha}, \quad w_1 = \frac{-2}{b_0\beta(1-\alpha)}.
\end{aligned}
$$

Here, α and β are free parameters and $T_j(w)$ is the Chebyshev polynomial of degree j in w. The result y_{n+1} can be considered as the numerical approximation at $t = t_{n+1}$ obtained by a *k-step, m-stage Runge-Kutta method.* The numerical scheme (2.2) - (2.3) will be called a *Runge-Kutta-Richardson method* (or briefly *RKR method*). In fact, in the subsequent analysis we will consider (2.2) as a Runge-Kutta method and not as an iteration method for solving the implicit relations (2.1).

It will be assumed that $w_0 \geq 1$ and $w_1 < 0$, i.e.

(2.4) $$-\frac{1}{b_0\beta} \leq \alpha < 1, \quad \beta > 0, \quad b_0 > 0.$$

The parameter β will appear to be the stability boundary of the RKR method. In actual applications this parameter will be chosen according to

(2.5) $$\beta = \tau \cdot \text{(spectral radius of } \partial f/\partial y).$$

3. CONSISTENCY

3.1 The local error of the RKR method

It is convenient to define the polynomials

(3.1) $$\begin{aligned} P_j(z) &= T_j^{-1}(w_0)T_j(w_0 + w_1 - w_1b_0z), \\ \rho(z) &= -\sum_{\ell=0}^{k} a_\ell z^{k-\ell}, \quad a_0 = -1, \\ \sigma(z) &= \sum_{\ell=0}^{k} b_\ell z^{k-\ell}. \end{aligned}$$

Let $y_\ell = y(t_\ell)$ for $\ell \leq n$ where $y(t)$ is the exact solution of (1.1) through the point (t_n, y_n). The RKR method (2.2) - (2.3) can then be written in the form

(3.2) $$\begin{aligned} y_{n+1}^{(0)} - y_n &= 0 , \\ y_{n+1}^{(1)} - y_n &= \lambda_0 r , \end{aligned}$$

$$y_{n+1}^{(j+1)} - y_n = \mu_j[1 + \lambda_0 - \lambda_0 b_0 \tau \frac{\partial f}{\partial y}][y_{n+1}^{(j)} - y_n]$$

$$+ (1 - \mu_j)[y_{n+1}^{(j-1)} - y_n]$$

$$+ \mu_j \lambda_0 [r + b_0 \tau \mathcal{O}(\| y_{n+1}^{(j)} - y_n \|^2)],$$

where $\partial f/\partial y$ is evaluated at t_n, r is sort of a residual term defined by

$$r = y_n - \sum_n - b_0 \tau f(y_n), \tag{3.3}$$

and where the order constant is uniformly bounded for all τ, α and β provided that $\partial f/\partial y$ satisfies a Lipschitz condition in y.

We will use the following lemma for deriving an expression for the local error $y_{n+1} - y(t_{n+1})$.

LEMMA 3.1. *The recurrence relation*

$$v_{j+1} = \mu_j(1 + \lambda_0 - \lambda_0 b_0 z)v_j + (1 - \mu_j)v_{j-1} + \mu_j \lambda_0 u_1$$

is satisfied by the function

$$v_j = (1 - b_0 z)^{-1}[P_j(z) - 1]u_1 + P_j(z)u_2$$

for every vector pair (u_1, u_2). □

PROOF. The proof follows easily from the recurrence relation for the polynomials $P_j(z)$, i.e.

$$P_{j+1}(z) = \mu_j(1 + \lambda_0 - \lambda_0 b_0 z)P_j(z) + (1 - \mu_j)P_{j-1}(z). \tag{3.4}$$

□

Let us write

$$y_{n+1}^{(j)} - y_n = [I - b_0 \tau \frac{\partial f}{\partial y}]^{-1}[P_j(\tau \frac{\partial f}{\partial y}) - I]r \tag{3.5}$$

$$+ \lambda_0 b_0 \tau \varepsilon_j,$$

where ε_j is some function yet to be determined. On substitution into (3.2) and application of lemma 3.1 with $u_1 = r$, $u_2 = 0$ and $z = \tau\, \partial f/\partial y$ we find that ε_j satisfies the recurrence relation

$$\text{(3.6)} \qquad \begin{aligned} &\varepsilon_0 = \varepsilon_1 = 0, \\ &\varepsilon_{j+1} = \mu_j(1+\lambda_0-\lambda_0 b_0 \tau \frac{\partial f}{\partial y})\varepsilon_j + (1-\mu_j)\varepsilon_{j-1} + \mu_j \mathcal{O}(\| y_{n+1}^{(j)} - y_n \|^2). \end{aligned}$$

In order to obtain an explicit expression for the local error

$$\text{(3.7)} \qquad y_{n+1} - y(t_{n+1}) = y_{n+1}^{(m)} - \exp(\tau \frac{d}{dt}) y(t) \Big|_{t = t_n}$$

we need an expression for the vector r. From its definition (3.3) and using the polynomials $\rho(z)$ and $\sigma(z)$ we obtain

$$\text{(3.3')} \qquad \begin{aligned} r = {} & [1-\exp(\tau \frac{d}{dt}) + \exp((1-k)\tau \frac{d}{dt})\rho(\exp\,(\tau \frac{d}{dt}))]y(t)\Big|_{t_n} \\ & - \tau \frac{d}{dt}[b_0 + \exp((1-k)\tau \frac{d}{dt})\sigma(\exp(\tau \frac{d}{dt})) - b_0 \exp(\tau \frac{d}{dt})]y(t)\Big|_{t_n} \end{aligned}$$

or compactly

$$\text{(3.8a)} \qquad r = \phi(\tau \frac{d}{dt}) y(t)\Big|_{t_n}$$

where

$$\text{(3.86)} \qquad \phi(z) = (1-e^z)(1-b_0 z) + e^{(1-k)z}[\rho(e^z) - z\sigma(e^z)].$$

Furthermore, we define the polynomial (note that $P_m(1/b_0) = 1$)

$$\text{(3.9)} \qquad Q_m(z) = \frac{P_m(z) - 1}{1 - b_0 z}\,.$$

In section 4.2 we will see that $Q_m(z)$ also plays a rôle in the stability analysis. The following theorem expresses the local error in terms of the functions $\phi(z)$ and $Q_m(z)$.

<u>THEOREM 3.1</u>. *If* $\phi(0) = 0$ *then the local error can be expressed as*

$$(3.7') \qquad y_{n+1}-y(t_{n+1}) = [Q_m(\tau \frac{\partial f}{\partial y})\ \phi(\tau \frac{d}{dt}) + I - \exp(\tau \frac{d}{dt})]y(t)\Big|_{t=t_n}$$

$$- \frac{2b_0\tau^3}{2+(1+\alpha)b_0\beta}\ c_m(\tau,\alpha,\beta),$$

where $c_m(\tau,\alpha,\beta)$ *is uniformly bounded for all* τ, α *and* β. □

<u>PROOF</u>. Substitution of (3.8a) into (3.5) and using (2.3) and (3.7) yields (3.7') if the function c is understood to be

$$\tau^{-2}\varepsilon_m.$$

We now show that this function is uniformly bounded in τ, α and β if $\phi(0) = 0$. We deduce from (3.5) that

$$y^{(j)}_{n+1} - y_n = d_j\ \tau + \lambda_0 b_0\ \tau\ \varepsilon_j$$

with d_j uniformly bounded in (τ,α,β). Substitution into (3.6) and writing

$$\varepsilon_j = c_j\tau^2$$

yields for c_j

$$c_0 = c_1 = 0,$$

$$c_{j+1} = \mu_j[1 + \lambda_0 - \lambda_0 b_0\tau \frac{\partial f}{\partial y}]c_j + (1-\mu_j)c_{j-1}$$

$$+ \mu_j\ \mathcal{O}(\|d_j + \lambda_0 b_0\varepsilon_j\|^2).$$

Recalling that the order constant is uniformly bounded with respect to (τ,α,β) we conclude that c_j is also uniformly bounded and therefore the function $c_m = c_m(\tau,\alpha,\beta)$. □

From this theorem the order equations for first and second order consistency are easily derived in terms of the derivatives of $Q_m(z)$ and $\phi(z)$ at $z = 0$. In table 3.1 the error constants and order equations are listed.

It may be interesting to consider the case where β is so large that the last term in (3.7') is negligible. It is then possible to derive from (3.7') the order equations for higher orders of accuracy. The conditions for "third order accuracy" are also listed in table 3.1. Since in actual application the parameter β will be chosen according to (2.5) we usually have $\beta >> 1$.

In this paper it will be assumed that all methods satisfy the (zero-order) condition

$$(3.10) \qquad \phi(0) = \rho(1) = 0.$$

In example 3.1 we illustrate the use of table 3.1.

Table 3.1. Consistency conditions for the RKR scheme (2.2)-(2.3)

$$p = 1: C_0 = \phi(0) = 0; \; C_1 = Q_m(0)\phi'(0) - 1 = 0;$$

$$p = 2: C_2 = \tfrac{1}{2} Q_m(0)\phi''(0) + Q_m'(0)\phi'(0) - \tfrac{1}{2} = 0;$$

$$p \cong 3: \quad C_{31} = \frac{1}{6} Q_m(0)\phi'''(0) - \frac{1}{6} = 0, \qquad \beta >> 1$$

$$C_{32} = \frac{1}{2} [Q_m'(0)\phi''(0) + Q_m''(0)\phi'(0)] = 0.$$

EXAMPLE 3.1 Let (2.1) correspond to the consistent one-step formula

$$b_1 = 1 - b_0, \quad \rho(z) = z - 1, \quad \sigma(z) = b_0 z + 1 - b_0,$$

then

$$\phi(z) = -z.$$

By virtue of table 3.1 we have *first order consistency* if $Q_m(0) = -1$, i.e.

$$P_m(0) = 0.$$

This can be achieved by choosing

$$\alpha = \frac{\cos\frac{\pi}{2m} - 1}{\cos\frac{\pi}{2m} + 1} .$$

Second order consistency is also possible if b_0 satisfies the relation

$$(b_0 - \tfrac{1}{2})T_m(w_0) = \frac{m(1 + \cos\frac{\pi}{2m})}{\beta \sin\frac{\pi}{2m}} .$$

Methods of the above type were consider in [5] in connection with multigrid methods for parabolic differential equations. □

This example shows that starting with a *first order* consistent linear multistep method, a *second order* RKR method can be obtained by a suitable choice of the coefficient b_0. Conversely, a second order one-step RKR method is not possible if we would have started with the (second order) trapezoidal rule. Therefore, in the following sections we do not not assume a priori consistency of the generating linear multistep methods.

3.2. Solution of the order equations

In this subsection we solve the order equations for p = 2 and express the error constants C_{31} and C_{32} in terms of the coefficients a_ℓ and b_ℓ, and the parameters w_0 and w_1.

From the definition of $\phi(z)$ it follows that

$$\phi(0) = -\sum a_\ell,\quad \phi'(0) = -1 - \sum (1-\ell)a_\ell - \sum b_\ell,$$

$$\phi''(0) = 2b_0 - 1 - \sum (1-\ell)^2 a_\ell - 2\sum (1-\ell)b_\ell, \tag{3.11a}$$

$$\phi'''(0) = 3b_0 - 1 - \sum (1-\ell)^3 a_\ell - 3\sum (1-\ell)^2 b_\ell,$$

where all summations run from $\ell = 0$ until $\ell = k$. Furthermore, from the definition of $Q_m(z)$ we derive

$$Q_m(0) = \frac{T_m(w_0+w_1)}{T_m(w_0)} - 1,$$

(3.11b) $$Q'_m(0) = b_0\, \tilde{Q}'_m(0),\quad \tilde{Q}'_m(0) = \frac{T_m(w_0+w_1)-T_m(w_0)-w_1T'_m(w_0+w_1)}{T_m(w_0)},$$

$$Q''_m(0) = b_0^2\, \tilde{Q}''_m(0),\quad \tilde{Q}''_m(0) = \frac{w_1^2}{[1-(w_0+w_1)^2]T_m(w_0)}\,[(w_0+w_1)T'_m(w_0+w_1) - m^2T_m(w_0+w_1)] + 2\,\tilde{Q}'_m(0).$$

Assuming that appropriate values for the parameters w_0 and w_1 (see below) are given we can compute $Q_m(0)$, $\tilde{Q}'_m(0)$ and $\tilde{Q}''_m(0)$, and solve the order equations in terms of the coefficients a_ℓ and b_ℓ. For that purpose we write them in the form

$$p = 1:\quad \phi(0) = 0,\quad \phi'(0) = \frac{1}{Q_m(0)}$$

$$p = 2:\quad \phi''(0) = \frac{Q_m(0) - 2b_0\tilde{Q}'_m(0)}{Q_m^2(0)}$$

with the error constants

(3.12) $$C_{31} = \frac{1}{6}\,[Q_m(0)\phi'''(0)-1],$$

$$C_{32} = b_0\,\frac{\tilde{Q}'_m(0)[Q_m(0) - 2b_0\tilde{Q}'_m(0)] + b_0\tilde{Q}''_m(0)Q_m(0)}{2Q_m^2(0)}\;.$$

Substitution of (3.11) yields *first order consistency* if

(3.13a) $$a_1 = 1 - \sum_{\ell=2}^{k} a_\ell,\quad b_1 = -\sum_{\ell=2}^{k}\,[(1-\ell)a_\ell + b_\ell] - b_0 - \frac{1}{Q_m(0)},$$

where b_0 and a_ℓ, b_ℓ with $\ell \geq 2$ are still free parameters (note that $a_0 = -1$). *Second order consistency* is obtained if

$$(3.13b) \qquad b_0 = \frac{Q_m(0)}{2\tilde{Q}_m'(0)} [1 + Q_m(0) \sum_{\ell=2}^{k} (1-\ell)((1-\ell)a_\ell + 2b_\ell)]$$

leaving a_ℓ and b_ℓ, $\ell \geq 2$, as free parameters. The error constants are easily evaluated by substitution of the coefficients a_ℓ and b_ℓ. For $k \geq 2$ it is possible to make them zero by replacing (3.13b) by the equivalent condition

$$(3.13'b) \qquad a_2 = \frac{2b_0\tilde{Q}_m'(0) - Q_m(0)}{Q_m^2(0)} + 2b_2 - \sum_{\ell=3}^{k} (1-\ell)((1-\ell)a_\ell + 2b_\ell)$$

and defining b_0 and b_2 according to

$$b_0 = \frac{Q_m(0)\ \tilde{Q}_m'(0)}{2\tilde{Q}_m'^2(0) - Q_m(0)\tilde{Q}_m''(0)},$$

(3.13c)

$$b_2 = 2\,\frac{b_0\tilde{Q}_m'(0) - Q_m(0)}{Q_m^2(0)}$$

$$- \sum_{\ell=3}^{k} (1-\ell)[(1-\ell)(2-\ell)a_\ell + (5-3\ell)b_\ell],$$

to obtain *third order consistency as* $\beta \to \infty$.

In this paper we investigate the case where $Q_m(0)$, $Q_m'(0)$ and $Q_m''(0)$ are more or less independent of m as $m \gg 1$. This is achieved by choosing

$$(3.14) \qquad \alpha = -\,tg^2\,\frac{\theta}{2m}, \qquad \beta = cm^2,$$

where θ and c are constants. (c will be called the *stability constant*). Furthermore, we want to satisfy condition (2.17) once and for all. Substitution of (3.14) into (2.4) yields

(3.15) $$c \le \frac{1}{m^2 b_0 tg^2 \frac{\theta}{2m}} \cong \frac{4}{b_0\theta^2} \quad \text{as } m \gg 1$$

so that (3.15), and therefore (2.4), is satisfied if we put

(3.16a) $$c = \frac{4}{b_0(\theta^2+\varepsilon^2)},$$

where ε is a small real constant, and if we choose m sufficiently large, i.e.

(3.16b) $$m \ge m_0 \cong \theta\{[120(1+\frac{\varepsilon^2}{\theta^2})^{\frac{1}{2}} - 95]^{\frac{1}{2}} - 5\}^{-\frac{1}{2}} \quad \text{as } \varepsilon \ll 1.$$

The relations (3.14) and (3.16) will be assumed to be satisfied throughout this paper.

We are now in a position to derive expressions for $Q_m(0)$, $\tilde{Q}'_m(0)$ $\tilde{Q}''_m(0)$. Using the relations

(3.17) $$w_0 = \cos\frac{\theta}{m} + \frac{\theta^2+\varepsilon^2}{2m^2(1+tg^2\frac{\theta}{2m})}, \quad w_1 = -\frac{\theta^2+\varepsilon^2}{2m^2(1+tg^2\frac{\theta}{2m})}$$

we find on substitution into (3.12) that

$$Q_m(0) = \frac{\cos\theta}{T_m(w_0)} - 1 \cong \frac{\cos\theta}{\cosh\varepsilon} - 1 \quad \text{as } m \gg 1$$

$$\tilde{Q}'_m(0) = \frac{\cos\theta}{T_m(w_0)} - 1 - \frac{mw_1 \sin\theta}{\sin\frac{\theta}{m} T_m(w_0)}$$

(3.12b) $$\cong \frac{\cos\theta}{\cosh\varepsilon} - 1 + \frac{(\theta^2+\varepsilon^2)\sin\theta}{2\,\theta\cosh\varepsilon} \quad \text{as } m \gg 1,$$

$$\tilde{Q}''_m(0) = (\frac{w_1\cos\theta/m}{\sin^2\theta/m} - 2)\frac{mw_1\sin\theta}{\sin\frac{\theta}{m} T_m(w_0)} - 2 + (2 - \frac{m^2w_1^2}{\sin^2\theta/m})\frac{\cos\theta}{T_m(w_0)}$$

$$\cong \frac{(5\theta^2+\varepsilon^2)(\theta^2+\varepsilon^2)\sin\theta}{4\theta^3\cosh\varepsilon} - 2 + \frac{[8\theta^2-(\theta^2+\varepsilon^2)^2]\cos\theta}{4\theta^2\cosh\varepsilon}$$

as $m \gg 1$.

The consistency conditions (3.13) can now be solved in a straightforward way. It should be remarked, however, that in the case of vanishing error constants C_{3j} the coefficient b_0 defined by (3.13c) has to be positive in order to satisfy condition (2.4). Let us consider the expression for b_0 as $m \to \infty$. Substitution of (3.11b') yields

$$(3.13c') \qquad b_0 = \frac{2\,\theta^2\eta\,[\frac{\sin\theta}{\theta} - \eta]}{\eta[(\theta^2+\varepsilon^2)\cos\theta + (3\theta^2-\varepsilon^2)\,\frac{\sin\theta}{\theta}] - 4\sin^2\theta} \quad \text{as } m \to \infty\,,$$

where we have written $\eta = 2(\cosh\varepsilon - \cos\theta)/(\theta^2+\varepsilon^2)$. A straightforward calculation yields

$$\theta = 0:\quad b_0 = \frac{2\eta(1-\eta)}{(4 - \frac{1}{3}\varepsilon^2)\eta - 4} \cong \frac{10}{\varepsilon^2} \quad \text{as } \varepsilon \ll 1,$$

$$\theta = \pi:\quad b_0 = \frac{4\pi^2(\cosh\varepsilon + 1)}{(\pi^2+\varepsilon^2)^2} \cong \frac{8}{\pi^2} \quad \text{as } \varepsilon \ll 1\,.$$

From these expressions it may be expected that b_0 is also positive for finite values of m.

Summarizing the results of this subsection, we may conclude that for any given pair (θ,ε) and all k a 2(k-1)-parameter family of second order RKR methods exist which satisfy the condition (2.4) if m satisfies (3.16b). Also, for all (θ,ε) such that the expression for b_0 in (3.13c) is positive and for $k \geq 2$ a 2(k-2)-parameter family of "almost" third order RKR methods exist which satisfy (2.4) if m satisfies (3.16b) and $\beta \gg 1$.

3.2 The approximation error

A necessary condition for convergence of the numerical solution to the exact solution of (1.1) is the convergence of the discrete scheme to the continuous problem as $\tau \to 0$. Let us write the RKR scheme (2.2)-(2.3) in the form

$$\tau L_\tau v = 0,$$

where v is an interpolating function v(t) such that $v(t_n) = y_n$, n = 0,1,... . The continuous problem (1.1) is written as

$$Ly \equiv \dot{y} - f(y) = 0.$$

Let y(t) be a function of sufficient differentiability, then by a similar derivation which led to (3.5) we find that

$$\text{(3.18)} \qquad L_\tau y = \tau^{-1}[y(t+\tau)-y(t) - Q_m(\tau \frac{\partial f}{\partial y})r(t) + O(\tau^3)] ,$$

where the quantity r(t) is of the form (cf. (3.3'))

$$r(t) = [1 - \exp(\tau \frac{d}{dt})+\exp((1-k)\tau \frac{d}{dt})\rho(\exp(\tau\frac{d}{dt}))]y(t)$$
$$- \tau\ \sigma(1)f(y(t)) - \tau^2[\sigma'(1)-b_0-(k-1)\sigma(1)]\frac{\partial f}{\partial y}(y(t))\dot{y}(t)+O(\tau^3).$$

THEOREM 3.2. *The RKR operator* L_τ *can be approximated by*

$$\text{(3.19)} \qquad L_\tau y = F\dot{y} - \tilde{C}_0 f(y) - \tau[\tilde{C}_1\ddot{y} + \tilde{C}_2 \frac{\partial f}{\partial y}\dot{y} + \tilde{C}_3 \frac{\partial f}{\partial y} f(y)] + O(\tau^2),$$

where

$$F = 1 - Q_m(0)[\rho'(1) - 1]$$
$$\tilde{C}_0 = - Q_m(0)\sigma(1)$$
$$\tilde{C}_1 = Q_m(0)[-\tfrac{1}{2}+(\tfrac{3}{2} - k)\rho'(1)+\tfrac{1}{2}\rho''(1)] - \tfrac{1}{2}$$
$$\tilde{C}_2 = Q'_m(0)[\rho'(1)-1]+Q_m(0)[(k-1)\sigma(1)+b_0-\sigma'(1)]$$
$$\tilde{C}_3 = -Q'_m(0)\sigma(1). \quad \square$$

PROOF. Taylor expansion of the right hand side of (3.18) and using $\rho(1) = 0$ leads straightforwardly to the result (3.19).

It is easily verified by means of table 3.1 and the definition of $\phi(z)$ that $\tilde{C}_0/F = 1$ iff $p \geq 1$.

Thus, the numerical scheme approximates the differential equation (1.1) iff it is consistent ($p \geq 1$). We will call the quantity ($p \geq 1$)

$$(3.20) \qquad A(t) = Ly - \frac{1}{F} L_\tau y = \frac{\tau}{F}(\tilde{C}_1 \ddot{y} + \tilde{C}_2 \frac{\partial f}{\partial y} \dot{y} + \tilde{C}_3 \frac{\partial f}{\partial y} f(y) + O(\tau)]$$

the *approximation error* of the numerical operator L_τ. In the following it is assumed that $p \geq 1$.

Evidently, the numerical scheme poorly approximates the differential equation (1.1) as the factor F becomes small. This leads us to the criterion to require the factor

$$(3.21) \qquad F = -Q_m(0)[\rho'(1)-1] + 1 = - Q_m(0)\sigma(1)$$

sufficiently far away from zero. F will be called the *normalizing factor*.

We emphasize that so far the function y(t) in (3.19) is an arbitrary, sufficiently smooth function. In the special case where y is a solution of the differential equation $Ly = 0$ the approximation error A(t) differs from the local error discussed in the preceding section by a factor τF, so that by virtue of theorem 3.1

$$(3.22) \qquad A(t) = \frac{1}{F\tau}\{[Q_m(\tau \frac{\partial f}{\partial y}) \phi(\tau \frac{d}{dt}) + I - \exp(\tau \frac{d}{dt})]y(t)$$

$$- \frac{2b_0 \tau^3}{2+(1+\alpha)b_0\beta} \; c_m(\tau,\alpha,\beta)\} .$$

Although small values of the normalizing factor F will decrease the *accuracy* of the RKR method it does not necessarily lead to a less *efficient* formula. To see this we express the approximation error (3.22) in terms of the total number of evaluations of the right hand function f needed for integrating the interval [0,t]. Let p be the order of consistency then it follows from (3.22) that

$$A(t) \cong \frac{C(t)}{F} \tau^p \text{ as } \tau \to 0,$$

where C(t) is independent of τ. The number of f-evaluations is given by

$$N = m\,\frac{t}{\tau} = t\sqrt{\frac{\text{spectral radius}}{c\tau}}$$

with m constant and where we have assumed that the integration steps are defined by (2.5). Elimination of τ yields

$$\text{(3.22')} \qquad A(t) = \frac{C(t)}{c^p F}\,[\frac{t^2}{N^2}\cdot\text{spectral radius}]^p .$$

The function C(t) depends both on the integration formula and the problem at hand. For example, in the case of a second order RKR method we have

$$C(t) = C_{31}\,\dddot{y}\,(t) + C_{32}\,\frac{\partial f}{\partial y}\,\ddot{y}(t),$$

hence for a given problem and a given number of f-evaluations the accuracy of the numerical scheme is controlled by the expressions

$$\text{(3.23)} \qquad \frac{C_{3j}}{c^2 F}, \qquad j = 1,2.$$

This suggests to look for formulas with large values for the stability constant c and the normalizing factor F as well. In the next section where the stability constant is computed, we will see that usually stability can be obtained for large values of c provided, however, that F is small. This and in view of (3.22') leads us to define the *normalized stability constant*

$$\text{(3.24)} \qquad c^* = cF^{1/p}.$$

4. STABILITY

We will consider the *internal stability properties* of the class (2.2)-(2.3), that is the stability behaviour within a single integration step, and the *step stability* which deals with the accumulation of errors in a number of successive integration steps.

4.1. Internal stability

In view of the possibly large values of m we have to consider the amplification of errors within a single integration step. In first approximation these errors are described by the relation

(4.1) $$\Delta y_{n+1}^{(j+1)} = \mu_j[1+\lambda_0-\lambda_0 b_0 \tau \frac{\partial f}{\partial y}(y_n)]\Delta y_{n+1}^{(j)} + (1-\mu_j)\Delta y_{n+1}^{(j-1)},$$

where the $\Delta y_{n+1}^{(j)}$ are perturbations resulting from an initial perturbation $\Delta y_{n+1}^{(0)}$ of $y_{n+1}^{(0)}$. Applying lemma 3.1 with $u_1 = 0$ and $u_2 = \Delta y_{n+1}^{(0)}$ reveals that (4.1) is solved by

(4.2) $$\Delta y_{n+1}^{(j)} = P_j(\tau \frac{\partial f}{\partial y}(y_n))\Delta y_{n+1}^{(0)}.$$

We will call the scheme (2.2)-(2.3) *internally stable* if the eigenvalues of the matrix $P_j(\tau\, \partial f/\partial y)$ are on the unit disk for $j = 1,2,\ldots,m$. Thus,

(4.3) $$|P_j(z)| \leq 1 \text{ for } z \in \tau\Delta, \qquad j = 1,2,\ldots,m,$$

where Δ denotes the (negative) spectrum of $\frac{\partial f}{\partial y}$ at t_n. From the definition of $P_j(z)$ it follows that (4.3) is satisfied if (2.4) is satisfied.

4.2. Step stability

The stability in subsequent integration steps can be described by the variational equation

(4.4) $$\Delta y_{n+1} = \mu_{m-1}[1+\lambda_0-\lambda_0 b_0 \tau \frac{\partial f}{\partial y}(y_n)]\Delta y_{n+1}^{(m-1)}$$

$$+ (1-\mu_{m-1})\Delta y_{n+1}^{(m-2)} - \mu_{m-1}\lambda_0 \Delta\Sigma_n,$$

where

$$(4.5) \qquad \Delta\Sigma_n = \{[E-\rho(E)E^{1-k}] + \tau \frac{\partial f}{\partial y}(y_n)[\sigma(E)E^{1-k}-b_0E]\}\Delta y_n.$$

Here, E denotes the shift operator ($Ey_n = y_{n+1}$) and ρ,σ are the polynomials defined in (3.1).

THEOREM 4.1. *For the model problem* $dy/dt = \delta y$ *the characteristic equation corresponding to (4.4) is given by*

$$(4.6) \qquad Q_m(z)[\rho(\zeta)-z\sigma(\zeta)] + P_m(z)\zeta^{k-1}(1-\zeta) = 0, \qquad z = \tau\delta,$$

where P_m *and* Q_m *are defined in (3.1) and (3.9), respectively.* □

PROOF. It is easily verified (by using lemma 3.1) that (4.4) can be written as

$$(4.4') \qquad \Delta y_{n+1} = P_m(\tau \frac{\partial f}{\partial y}(y_n))\Delta y_n - Q_m(\tau \frac{\partial f}{\partial y}(y_n))\Delta\Sigma_n.$$

From (4.5) the equation (4.6) is now immediate. □

Stability and the stability region can be defined in the usual way. We will use the definitions (cf. [6, p.66]):

DEFINITION 4.1. The scheme (2.2)-(2.3) will be called *stable for given z* if all roots $\zeta_j(z)$ of (4.6) satisfy the inequality

$$(4.7) \qquad |\zeta_j(z)| \le 1, \quad j = 1,2,\ldots,k.$$

This scheme will be called *stable for a given equation* if it is stable for all points in the region $\tau\Delta$; if strict inequality holds in (4.7) we call the scheme *strongly stable*, otherwise *weakly stable*. The scheme will be called *zero-stable* if $|\zeta_j(0)| \le 1$ those on the unit circle being simple roots. □

THEOREM 4.2. *The scheme* (2.2)-(2.3) *is zero-stable if the equation*

$$(4.8)\qquad P_m(0)[\rho(\zeta) - \zeta^k + \zeta^{k-1}] - \rho(\zeta) = 0$$

has its roots on the unit disk those on the unit circle being simple roots.

□

PROOF. The proof is immediate from (4.6) and (3.9).

We remark that $\zeta = 1$ is a root of equation (4.8) for all consistent RKR methods (if $p \geq 1$ then $\phi(0) = \rho(1) = 0$). Hence, zero-stability implies that the derivative of the left hand side of (4.8) at $\zeta = 1$ does not vanish, i.e.

$$(4.9)\qquad P_m(0)[\rho'(1)-1] - \rho'(1) \neq 0.$$

This condition also follows from the convergence condition $F \neq 0$ (cf. (3.21)). A similar situation holds for the linear multistep case (cf. [6, p.33]).

The stability region is most conveniently obtained by applying the boundary locus method (see e.g. [6, p.82]). For that purpose we introduce the trigoniometric polynomials

$$(4.12)\qquad \begin{aligned} C_1(d,\psi) &= \sum_{\ell=0}^{k} a_\ell\, d^{k-\ell}[\sin(\ell-1)\psi - d \sin \ell\, \psi], \\ C_2(d,\psi) &= \sum_{\ell=0}^{k} b_\ell\, d^{k-\ell}[\sin(\ell-1)\psi - d \sin \ell\, \psi], \\ S(d,\psi) &= \sum_{i,\ell=0}^{k} a_i\, b_\ell\, d^{2k-i-\ell} \sin(i-\ell)\psi, \end{aligned}$$

where d is a positive parameter (*damping parameter*).

THEOREM 4.3. *Let the RKR method have characteristic roots less than* d *in magnitude in a point* z^* *of the interval* $[z_0, z_1]$. *Then the characteristic roots satisfy* $|\zeta(z)| \leq d$ *for all* $z \in [z_0, z_1]$ *if the curve*

$$(4.13)\qquad \tilde{z} = \frac{P_m(z)}{Q_m(z)}, \qquad z_0 \leq z \leq z_1$$

does not cross the curve

$$(4.14)\qquad z = -\frac{C_1(d,\psi)}{C_2(d,\psi)}, \qquad \tilde{z} = -\frac{S(d,\psi)}{d^{k-1}C_2(d,\psi)},$$

where $0 < \psi < \pi$ *and* $C_2(d,\psi) \neq 0$, *or the straight lines*

$$(4.15)\qquad \tilde{z} = \frac{[\mathrm{Re}\,\sigma(de^{i\psi^*})]z - [\mathrm{Re}\,\rho(de^{i\psi^*})]}{d^{k-1}[\cos(k-1)\psi^* - d\cos k\psi^*]},$$

where ψ^* *is a solution of the three equations*

$$(4.16)\qquad C_1(d,\psi) = 0,\ C_2(d,\psi) = 0,\ S(d,\psi) = 0,\ 0 \le \psi \le \pi. \qquad \square$$

PROOF. Let us write the characteristic equation (4.6) in the form

$$z\sigma(\zeta) - \tilde{z}\,\zeta^{k-1}(1-\zeta) = \rho(\zeta),$$

where $\tilde{z}$ is defined by (4.13).

Considering $\tilde{z}$ temporarily as an independent variable, one may think the $(z,\tilde{z})$-plane as divided into two regions: a region S_+ where $|\zeta| < d$ and a region S_- where $|\zeta| > d$. These regions are separated by the curve (or set of curves) given by (boundary locus method)

$$(4.17)\qquad z\sigma(de^{i\psi}) - \tilde{z}d^{k-1}e^{(k-1)i\psi}(1-de^{i\psi}) = \rho(de^{i\psi}), \quad |\psi| \le \pi.$$

This equation can be represented in the form

$$(4.17')\qquad z\begin{pmatrix}A\\B\end{pmatrix} + \tilde{z}\begin{pmatrix}C\\D\end{pmatrix} = \begin{pmatrix}E\\F\end{pmatrix}$$

with

$$A + iB = \sigma(de^{i\psi}), \qquad E + iF = \rho(de^{i\psi})$$

$$C = d^{k-1}[d\cos k\psi - \cos(k-1)\psi],\ D = d^{k-1}[d\sin k\psi - \sin(k-1)\psi].$$

Let $(z,\tilde{z}) = (Z(\psi), \tilde{Z}(\psi))$ denote the solution of (4.17'). Then this curve separates the stable $(z,\tilde{z})$-points of S_+ and the unstable $(z,\tilde{z})$-points of S_-. Since in our case we are only concerned with points on the curve (4.13), we have stability in the interval $[z_0,z_1]$ if all points on (4.13) are in S_+. Thus, we have to find the location of the curve $(Z(\psi), \tilde{Z}(\psi))$.

Evidently, (4.17') is solved by

$$
\begin{aligned}
&(z,\tilde{z}) = (AD-CB)^{-1}\,(ED-CF, AF-EB) \text{ if } AD-CB \neq 0,\\
&Az + C\tilde{z} = E \text{ if } AD-CB = ED-CF = AF-EB = 0\\
&\qquad\qquad\qquad \wedge\ (A\neq 0 \quad \vee\ C\neq 0),\\
&Bz + D\tilde{z} = F \text{ if } AD - CB = ED - CF = AF - EB = 0\\
&\qquad\qquad\qquad \wedge\ (A=0 \quad \wedge\ C=0).
\end{aligned}
$$

Substitution of the expressions for $A,B,\ldots,F$ reveals that the curve $(Z(\psi),\tilde{Z}(\psi))$ can be presented in the form (4.14) and (4.15). Notice that ψ can be restricted to the interval $[0,\pi]$ because $Z(\psi)$ and $\tilde{Z}(\psi)$ are even functions of ψ.

Since we assumed stability in at least one point $z^* \in [z_0,z_1]$, the point $(z^*, P_m(z^*)/Q_m(z^*))$ lies in the region S_+: we may conclude that we have stability if the curve (4.13) does not cross the curves (4.14) and (4.15). □

We observe that in the special case where

$$\sigma(\zeta) = b_0\zeta^k + b_1\zeta^{k-1}$$

the equations (4.16) only possess the common roots $\psi^* = 0$ and $\psi^* = \pi$ so that the lines (4.15) are given by

$$(4.15') \qquad \tilde{z} = \frac{\sigma(d)z - \rho(d)}{d^{k-1}[1-d]}\ , \quad \tilde{z} = \frac{\sigma(-d)z - \rho(-d)}{(-d)^{k-1}[1+d]}\ .$$

In figure 4.1 we have illustrated a typical example of the location of the curve $z = Z(\psi)$, $\tilde{z} = \tilde{Z}(\psi)$ (for $d = 1$) and the curve (4.13).

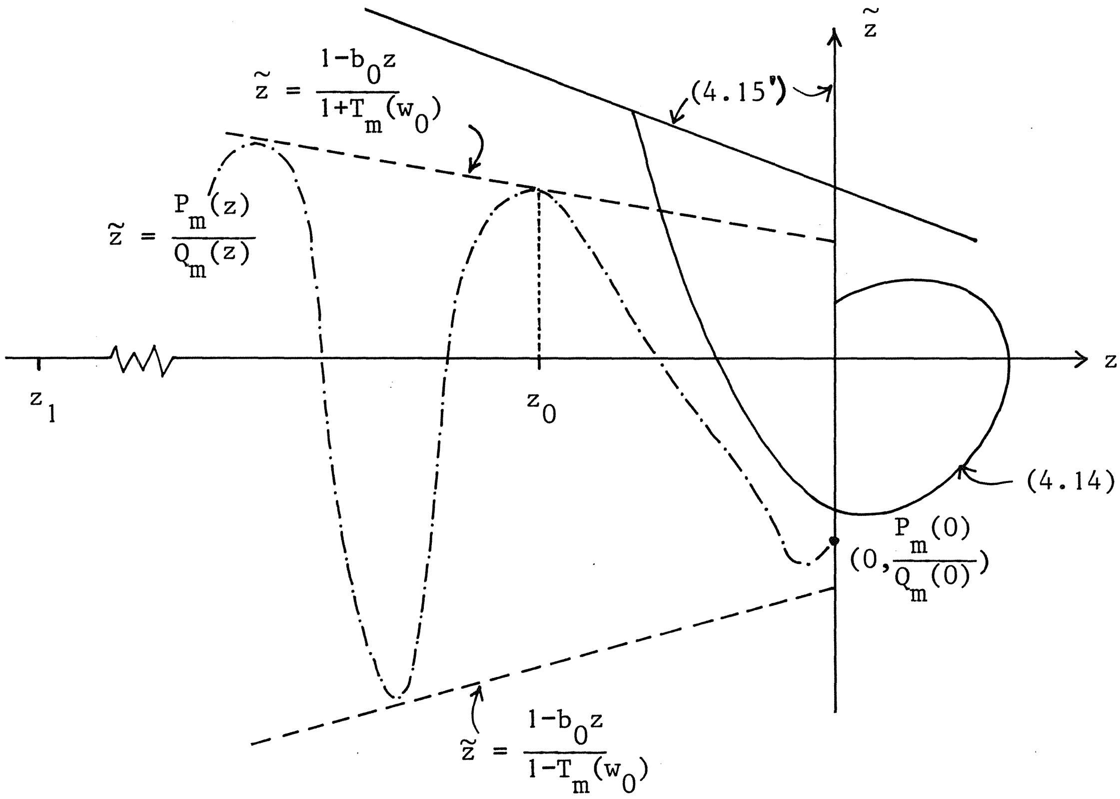

Figure 4.1. The curves $z = Z(\psi)$, $\tilde{z} = \tilde{Z}(\psi)$ ————

and $\tilde{z} = P_m(z)/Q_m(z)$ —— • —— • —— , for d = 1

This figure suggests to force the curve $\tilde{z} = P_m(z)/Q_m(z)$ "below" the curve $z = Z(\psi)$, $\tilde{z} = \tilde{Z}(\psi)$. The following Corollary of theorem 4.3 reflects such a situation.

COROLLARY 4.1. *Let the RKR method have characteristic roots satisfying* $|\zeta(-cm^2)| < d \leq 1$. *Let the equations (4.16) have no solutions except for* $\psi^* = 0$ *and* $\psi^* = \pi$, *and let the following conditions be satisfied*

$$\text{(4.18a)}\quad b_0 \le \frac{-\sigma(\mp d)[1+T_m(w_0)]}{(\mp d)^{k-1}[1\pm d]},$$

$$(1\pm d)d^{k-1}(1-b_0z_0) \le (\mp 1)^{k-1}[1+T_m(w_0)][\sigma(\mp d)z_0-\rho(\mp d)] ;$$

$$\text{(4.18b)}\quad \frac{P_m(z)}{Q_m(z)} \le \frac{1}{2}(-1)^{k-1}[\sigma(-1)z-\rho(-1)] \text{ for } z_0 \le z \le 0;$$

$$\text{(4.18c)}\quad \frac{1 + b_0C_1(d,\psi)C_2^{-1}(d,\psi)}{1 + T_m(w_0)} \le -\frac{S(d,\psi)}{d^{k-1}C_2(d,\psi)}$$

$$\text{for } -cm^2 \le -\frac{C_1(d,\psi)}{C_2(d,\psi)} \le z_0 \text{ and } 0 < \psi < \pi;$$

$$\text{(4.18d)}\quad \frac{P_m(-C_1(1,\psi)C_2^{-1}(1,\psi))}{Q_m(-C_1(1,\psi)C_2^{-1}(1,\psi))} \le -\frac{S(1,\psi)}{C_2(1,\psi)}$$

$$\text{for } z_0 \le -\frac{C_1(1,\psi)}{C_2(1,\psi)} \le 0 \text{ and } 0 < \psi < \pi,$$

where z_0 is some point in the interval $[-cm^2,0]$. Then the method is stable for all $z \in [-cm^2,0]$ and the characteristic roots are bounded by d in the interval $[-cm^2,z_0]$. □

PROOF. The interval $[-cm^2,0]$ is divided into two parts $[-cm^2,z_0]$ and $[z_0,0]$. In the interval $[-cm^2,z_0]$ we have used the inequality

$$\frac{P_m(z)}{Q_m(z)} \le \frac{1-b_0z}{1+T_m(w_0)},$$

and in the interval $[z_0,0]$ we required that

$$\frac{P_m(z)}{Q_m(z)} \le \tilde{Z}(\psi).$$

Application of theorem 4.3 yields the inequalities (4.18). □

It should be remarked that the conditions (4.18) simplify if we choose $z_0 = 0$, $d = 1$. Then (4.18a) reduces to a simple condition on the coefficients a_ℓ and b_ℓ

$$(4.18a') \qquad \sum_{\ell \le k/2} a_{2\ell} \le \frac{-1}{T_m(w_0)+1}, \qquad b_0 \ge \frac{1+T_m(w_0)}{1-T_m(w_0)} \cdot \sum_{\ell=1}^{k} (-1)^\ell b_\ell,$$

where we have used the relation $\rho(1) = 0$; the conditions (4.18b) and (4.18d) are automatically satisfied. However, the condition (4.18c) becomes rather restrictive and we are in danger of throwing away some interesting formulas. On the other end of the scale one has $z_0 = -cm^2$ which takes all stable formulas into account. On the basis of figure 4.1 it seems that the point where $P_m(z)$ assumes its first extreme value (when starting in z=0) is a reasonable choice, i.e.

$$(4.19) \qquad z_0 = \frac{\cos\frac{\theta}{m} - \cos\frac{\pi}{m}}{b_0(\cos\frac{\theta}{m} - w_0)}, \qquad 0 \le \theta \le \pi .$$

The reason for introducing the parameter z_0 in corollary 4.1 is the reduction of the computational labour in checking the stability conditions in theorem 4.3 numerically.

Finally, we remark that the condition on the characteristic roots at $z = -cm^2$ implies the necessary condition $\sigma(1) > 0$. This immediately follows from (4.6) if $z = -cm^2$ is substituted, i.e.

$$\rho(\zeta) + cm^2\sigma(\zeta) + \frac{1+b_0m^2c}{1-(-1)^m T_m(w_0)} \zeta^{k-1}(1-\zeta) = 0.$$

For large positive values of ζ the left hand side is positive, hence if $\zeta = 1$ the left hand side, i.e. $cm^2\sigma(1)$, should also be positive otherwise at least one characteristic zero > 1 exists.

4.3. Derivation of stability intervals for second order formulas

In this section we consider the stability interval for a few methods discussed in section 3.

k = 1

Application of corollary 4.1 with $z_0 = 0$ and $d = 1$ yields

$$(4.19) \qquad b_1 \leq \frac{T_m(w_0)-1}{T_m(w_0)+1} b_0, \qquad b_0 + b_1 > 0 .$$

From (3.13a) and (3.13b) it follows that for a given pair (θ,ε) the second order RKR method is uniquely defined by

$$(4.20) \qquad a_1 = 1, \; b_0 = \frac{Q_m(0)}{2\tilde{Q}_m'(0)}, \quad b_1 = -\frac{Q_m(0)}{2\tilde{Q}_m'(0)} - \frac{1}{Q_m(0)} .$$

Substitution into (4.19) results in the condition

$$(4.19') \qquad b_0 = \frac{Q_m(0)}{2\tilde{Q}_m'(0)} \geq \frac{T_m(w_0)+1}{2(T_m(w_0)-\cos\theta)} .$$

Since we want a stability boundary β as large as possible we should identify b_0 with the lower bound in (4.19') (cf. (3.16a)). Solving the resulting relations leads to

$$(4.21) \qquad \theta = \pi, \; b_0 = \tfrac{1}{2}, \; b_1 = \tfrac{1}{2}\,\frac{T_m(w_0)-1}{T_m(w_0)+1}, \quad a_1 = 1, \; \beta = \frac{8m^2}{\pi^2+\varepsilon^2} ,$$

where ε is still free and m should be sufficiently large in order to satisfy (3.16b).

The error constants in the local error follow from (3.12) and are given by

$$(4.22)\qquad C_{31} = -\frac{1}{6}\,,\qquad C_{32} \cong \frac{1}{4} - \frac{\pi^2}{32(1+T_m(w_0))}\qquad \text{as } m \gg 1.$$

It is interesting to observe that the method (4.21) almost possesses the maximal real stability boundary attainable within the class of all second order, m-stage Runge-Kutta methods. In [3] it was calculated that the maximal stability constant c is a slowly increasing function as m increases with limiting value .82 ..., whereas in (4.21) we find $c \cong .81$ for small values of ε.

In the preceding analysis we chose $z_0 = 0$ (and therefore $d = 1$) in order to derive the optimal formula by analytical means. In practice, one wishes of course some damping of the higher harmonics and should choose $d < 1$ and consequently $z_0 < 0$. The optimal formula is then to be obtained by checking numerically the conditions of corollary 4.1 over a range of values for θ and selecting that formula which gives rise to a maximal stability boundary β.

$\underline{k = 2}$

Again we apply corollary 4.1 with $z_0 = 0$ and $d = 1$. Condition (4.18) reduces to

$$(4.24)\qquad a_1 \geq \frac{1}{1+T_m(w_0)}\,,\qquad b_0 \geq (b_2-b_1)\,\frac{1+T_m(w_0)}{1-T_m(w_0)}\,.$$

Defining a_1 and b_1 by (3.13a) and a_2 by (3.13'b) we obtain a family of second order formulas in which the coefficients b_0 and b_2 are free for any given (θ,ε). Choosing b_0 as small as possible, i.e. b_0 satisfies

$$(4.25)\qquad b_0 = (b_2-b_1)\,\frac{1+T_m(w_0)}{1-T_m(w_0)}\,,$$

we find for β an expression in terms of ε and θ. For large values of m this expression reduces to

(4.26) $$\beta \cong \left[\frac{4[1+2T_m(w_0) - \cos\theta]}{(1+T_m(w_0))(\theta^2+\varepsilon^2)} - \frac{2\sin\theta}{\theta(T_m(w_0) - \cos\theta)} \right] m^2 .$$

The remaining stability conditions of the corollary were checked numerically over a range of (θ,ε,b_2) values. In the table 4.1 we have listed a few triples (θ,ε,b_2) and corresponding values of c,F,C_{31} and C_{32} which generate a stable formula for $m >> 1$. These figures show that the stability constant and the normalizing factor, respectively, slowly increase and decrease if θ and ε decrease (with the limiting value $c = 4/3$ as θ and $\varepsilon \to 0$). However, the coefficient b_0 becomes rather large for small values of θ and ε (for

Table 4.1 Stability constants, error constants and normalizing factors for the RKR method (3.27), (4.23) if $m >> 1$

ε	θ	b_2	c	F	C_{31}	C_{32}
.2	$\pi/2$	0	1.153	1.398	-.233	.096
.2	$\pi/3$	-.2	1.245	1.252	-.260	.092
.2	$\pi/4$	-.6	1.280	1.106	-.277	.090
.2	$\pi/5$	-1.0	1.296	1.069	-.282	.089
.1	$\pi/5$	-1.0	1.301	1.095	-.280	.089
.05	$\pi/5$	-1.1	1.303	1.062	-.283	.089
0	0	-	4/3			

$\theta = \pi/5$ and $\varepsilon = .05$ we found $b_0 \cong 7.7$), so that it is recommended to choose for example $\varepsilon = .2$, $\theta = \pi/3$ and $b_2 = -.2$ which results in $b_0 \cong 2.8$, $b_1 \cong -.17$ and $a_1 \cong a_2 \cong .5$.

<u>$k \geq 3$</u>

For k = 3 and k = 4 we checked the conditions of corollary 4.1 by numerical means. In table 4.2 the values of those coefficients a_ℓ and b_ℓ are given which were used as optimization parameters in our numerical program. The remaining coefficients immediately follow from the order equations (3.13a) and (3.13b). In all cases listed in this table, a zero-value for the parameter θ turned out to generate the largest c-values for a prescribed value of the normalizing factor F and the parameter ε. It is clear from the values found for c and F that large stability constants are to be paid for by small normalizing factors and consequently reduced accuracy.

Finally, we consider the case of vanishing error constants. From (3.13c') and (3.16a) it follows that

$$c = 2\,\frac{\eta[(\theta^2+\varepsilon^2)\cos\theta + (3\theta^2-\varepsilon^2)\,\frac{\sin\theta}{\theta}\,] - 4\sin^2\theta}{\theta^2(\theta^2+\varepsilon^2)\eta[\frac{\sin\theta}{\theta} - \eta]} \quad \text{as } m \to \infty.$$

It can be verified that $c = c(\theta)$ increases from $c(0) = 4/10$ to $c(\pi) = 1/2$. In table 4.3 a few cases are listed which satisfy the conditions of corollary 4.1.

<u>Table 4.2</u>. Stability constants, error constants and normalizing factors for three- and four-step RKR methods with $\theta = 0$, $\varepsilon = \frac{1}{2}$ and d = 0.9

	b_0	b_1	b_2	b_3	b_4	a_4	c	F	c^*	C_{31}	C_{32}	m_1
I	$\frac{36}{5}$	.8354	$\frac{4}{5}$	0	0	0	2.22	1.0	2.22	-.56	.06	7
II	$\frac{55}{10}$	-.2823	$-\frac{2}{5}$	$-\frac{2}{5}$	0	0	2.91	.5	2.06	-.70	.05	6
III	$\frac{35}{10}$	-.6165	$-\frac{6}{5}$	$-\frac{4}{5}$	0	0	4.57	.1	1.45	-.83	.03	4
IV	1	-.9116	$-\frac{1}{5}$	$\frac{1}{5}$	0	0	16.00	.01	1.60	-.96	.01	5
V	$\frac{18}{5}$	.8177	$\frac{1}{2}$	$-\frac{1}{2}$	0	4	4.44	.5	3.14	-1.24	.03	4

Table 4.3. Stability constants and normalizing factors for three-step RKR methods with vanishing error constant and d = 0.9

	ε	θ	b_0	b_1	b_2	b_3	C	F	c^*	m_1
VI	1	0	10.752	-8.763	1.053	$-\frac{1}{5}$	.37	1	.372	2
VII	1	0	10.752	-7.466	4.838	$\frac{2}{5}$	.37	3	.537	2
VIII	$\frac{1}{2}$	π	.821	- .366	.340	0	.48	1.5	.551	9

5. NUMERICAL EXPERIMENTS

We will demonstrate that the RKR methods derived in this paper can be used for the integration of nonlinear parabolic initial-boundary value problems. In particular, we will show that the extremely large integration step allowed by the linear stability theory can actually be used in (highly) nonlinear problems.

As test problem we chose [8]

$$(5.1)\qquad \frac{\partial u}{\partial t} = \Delta u^5, \qquad 0 \le t \le 1$$

with initial and boundary conditions on the unit square such that the exact solution is given by

$$(5.2)\qquad u(t,x_1,x_2) = [\tfrac{4}{5}(2t+x_1+x_2)]^{1/4}.$$

This problem was semi-discretized on a uniform grid in the (x_1,x_2) domain with square meshes of width h = 1/20 using the usual five-point difference formulas.

The resulting system of ODE's was integrated by the RKR methods listed in the tables 4.2 and 4.3. The starting values $y_0,y_1,\ldots,y_{k-1}$ for these methods were derived from the exact solution (5.2). This of course implies that the accuracy at the end point for large τ may be considerably higher than the accuracy obtained if the starting values are computed numerically. The numbers of significant digits defined by the expression

$$(5.3) \qquad sd = -\log_{10}\|\text{exact solution of (1.1)} - \text{numerical solution}\|_\infty$$

obtained in t = 1 are given in table 5.1 for a few values of the integration step τ. In addition, the total number of right hand side evaluations is given. This number is related to τ by the formula

$$(5.4) \qquad N = \sum_{n=1}^{1/\tau} m_n,$$

where

$$m_n = \sqrt{\frac{\text{spectral radius}\cdot\tau}{c}} \cong \sqrt{\frac{\tau}{c}\frac{64}{h^2}(1+t_n+\tau)} \ .$$

Table 5.1. (sd/N)-values for the methods I,II,...,VIII listed in the tables 4.2 and 4.3 obtained for problem (5.1).

	τ=1/5	τ=1/10	τ=1/20	τ=1/40	τ=1/80	τ=1/160
I	3.89/305	3.03/425	4.32/599	4.81/849	5.35/1212	5.91/1730
II	3.18/267	3.24/372	4.08/524	4.18/797	5.07/1064	5.62/1529
III	2.53/213	3.18/295	3.35/422	3.99/598	4.50/856	5.11/1240
IV	1.91/115	2.53/160	2.09/229	1.14/327	unstable ($m<m_1$)	
V	2.69/217	3.58/304	3.97/428	4.66/607	5.18/867	5.83/1259
VI	3.64/741	3.87/1034	4.22/1451	4.31/2050	4.58/2906	5.45/4129
VII	4.11/741	4.48/1034	4.64/1451	4.96/2050	5.05/2906	5.94/4129
VIII	3.41/652	4.22/917	4.75/1279	4.46/1805	4.28/2558	5.30/3638

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