

**stichting  
mathematisch  
centrum**



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AFDELING NUMERIEKE WISKUNDE  
(DEPARTMENT OF NUMERICAL MATHEMATICS)

NW 72/79

SEPTEMBER

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ON THE INTERNAL STABILITY OF EXPLICIT,  $m$ -STAGE  
RUNGE-KUTTA METHODS FOR LARGE  $m$ -VALUES

Preprint

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**2e boerhaavestraat 49 amsterdam**

BIBLIOTHEEK MATHEMATISCH CENTRUM  
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*Printed at the Mathematical Centre, 49, 2e Boerhaavestraat, Amsterdam.*

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

On the internal stability of explicit, m-stage Runge-Kutta methods for large m-values<sup>\*)</sup>

by

P.J. van der Houwen & B.P. Sommeijer

#### ABSTRACT

Explicit, m-stage Runge-Kutta methods are derived for which the maximal stable integration step per right hand side evaluation is proportional to m when applied to semi-discrete parabolic initial-boundary value problems. The internal stability behaviour of these methods is compared with that of similar Runge-Kutta methods proposed in the literature. Both by analysis and by numerical experiments we show that the value of m in the schemes proposed in this paper is not restricted by internal instabilities.

KEY WORDS & PHRASES: *Numerical analysis, Runge-Kutta methods, internal stability, parabolic equations.*

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<sup>\*)</sup> This report will be submitted for publication elsewhere.



## 1. INTRODUCTION

In various papers stabilized Runge-Kutta methods have been proposed [2, 3, 5] for the time-integration of parabolic differential equations. These methods are characterized by the relatively large number of stages involved. In fact, stabilized Runge-Kutta methods (RK methods) become as a rule more efficient as the number of stages is larger. To be more precise, let the partial differential equation, when space-discretized, be of the form

$$(1.1) \quad \frac{d\vec{y}}{dt} = \vec{f}(t, \vec{y})$$

and let the Jacobian matrix  $J(t, \vec{y}) = \partial \vec{f} / \partial \vec{y}$  have *negative* eigenvalues (*parabolic equations*). Then, the stability condition of an appropriate stabilized RK method is of the form

$$(1.2) \quad \tau \leq \frac{\beta(m)}{\sigma}$$

where  $\tau$  is the integration step  $t_{n+1} - t_n$ ,  $\sigma$  the spectral radius of  $J$  at  $(t_n, \vec{y}_n)$  and  $\beta(m)$  the *stability boundary* of the RK method. Since  $\beta(m)$  increases quadratically with  $m$  it follows that the "stability boundary per function evaluation" increases linearly with  $m$ . Thus, the "integration step per  $\vec{f}$ -evaluation, i.e., the *effective step*, can be made arbitrarily large by choosing  $m$  sufficiently large.

Such schemes would allow unrestricted integration steps as far as stability is concerned by simply adapting the value of  $m$  to the integration step desired. Because  $\sigma$  is usually very large in the case of semidiscrete partial differential equations, realistic  $\tau$ -values will imply large  $m$ -values. Unfortunately, however, most stabilized RK methods proposed in the literature, although satisfying the condition (1.2), become unstable for large  $m$ -values because of *internal instability within the integration steps*. Recently, this phenomenon was discussed in [2] where the authors propose a RK method which is reported to remain stable for extremely high  $m$ -values by a careful ordering of the RK-parameters. It seems, however, that this ordering has to be chosen on the basis of experiments from a one-parameter family of "optimal" orderings. The experiments presented in Section 4 show that this choice is

very critical and depends on the value of  $m$ . This may be inconvenient in actual computation.

In this paper stabilized RK methods are proposed which are uniquely defined and internally stable for arbitrary  $m$ -values. A series of numerical experiments are reported which confirm the theoretical results.

## 2. STABILIZED RUNGE-KUTTA METHODS

Consider Runge-Kutta methods of the form

$$\begin{aligned}
 \vec{y}_{n+1}^{(0)} &= \vec{y}_n, \\
 \vec{y}_{n+1}^{(1)} &= \vec{y}_n + \tilde{\mu}_1 \tau \vec{f}(t_n, \vec{y}_n), \\
 \vec{y}_{n+1}^{(j)} &= \mu_j \vec{y}_{n+1}^{(j-1)} + v_j \vec{y}_{n+1}^{(j-2)} + \tilde{\gamma}_j \tau \vec{f}(t_n, \vec{y}_n) \\
 &\quad + \tilde{\mu}_j \tau \vec{f}(t_n + \theta_{j-1} \tau, \vec{y}_{n+1}^{(j-1)}) + \tilde{v}_j \tau \vec{f}(t_n + \theta_{j-2} \tau, \vec{y}_{n+1}^{(j-2)}), \\
 &\quad j = 2, 3, \dots, m,
 \end{aligned}
 \tag{2.1}$$

$$\vec{y}_{n+1} = \vec{y}_{n+1}^{(m)},$$

where the parameters satisfy the relations

$$\begin{aligned}
 \mu_j + v_j &= 1 \\
 \theta_0 &= 0, \theta_1 = \tilde{\mu}_1, \theta_j = \mu_j \theta_{j-1} + v_j \theta_{j-2} + \tilde{\gamma}_j + \tilde{\mu}_j + \tilde{v}_j, \\
 &\quad j = 2, 3, \dots, m.
 \end{aligned}
 \tag{2.2}$$

It is easily verified that  $\vec{y}_{n+1}^{(j)}$  can be written in the form

$$\vec{y}_{n+1}^{(j)} = \vec{y}_n + \tau \sum_{\ell=0}^{j-1} \lambda_{j\ell} \vec{f}(t_n + \theta_\ell \tau, \vec{y}_{n+1}^{(\ell)}), \quad j = 1, 2, \dots, m,
 \tag{2.1'}$$

where the RK parameters  $\lambda_{j\ell}$  are expressions in  $\mu_j$ ,  $\tilde{\mu}_j$ ,  $v_j$ ,  $\tilde{v}_j$  and  $\tilde{\gamma}_j$ , satisfying the condition

$$(2.2') \quad \sum_{\ell=0}^{j-1} \lambda_{j\ell} = \theta_j, \quad j = 1, 2, \dots, m-1.$$

Formula (2.1') is immediately recognized as an explicit m-stage Runge-Kutta formula.

The number of storage arrays needed to implement (2.1) is limited (maximal 6) which is important in view of our aim to apply it to partial differential equations.

## 2.1. Accuracy

We will derive the order equations for first and second order accuracy in terms of the parameters of representation (2.1). Let  $\vec{y}(t)$  denote the exact solution of equation (1.1) through the point  $(t_n, \vec{y}_n)$  and write  $\vec{y}_{n+1}^{(j)}$  in the form

$$(2.3) \quad \vec{y}_{n+1}^{(j)} = \vec{y}_n + c_{1j} \dot{\vec{y}}(t_n) + c_{2j} \ddot{\vec{y}}(t_n) + O(\tau^3).$$

Substitution into (2.1) yields for the coefficients  $c_{1j}$  and  $c_{2j}$  the recurrence relations

$$(2.4) \quad c_{10} = 0, \quad c_{11} = \tilde{\mu}_1, \quad c_{1j} = \mu_j c_{1,j-1} + \nu_j c_{1,j-2} + \tilde{\nu}_j \tilde{\mu}_j + \tilde{\nu}_j, \quad j = 2, 3, \dots, m,$$

$$(2.5) \quad c_{20} = c_{21} = 0, \quad c_{2j} = \mu_j c_{2,j-1} + \nu_j c_{2,j-2} + \tilde{\mu}_j \theta_{j-1} + \tilde{\nu}_j \theta_{j-2}, \quad j = 2, 3, \dots, m.$$

Note that the recurrence relation for  $\theta_j$  is identical to (2.4), hence  $c_{1j} = \theta_j$ . The order equations for p-th order accuracy become

$$(2.6) \quad \begin{aligned} p = 1: & \quad c_{1m} = \theta_m = 1 \\ p = 2: & \quad \theta_m = 1, \quad c_{2m} = \frac{1}{2} \end{aligned}$$

## 2.2. Stability

Let  $\Delta \vec{y}_{n+1}^{(j)}$ ,  $j = 0, 1, \dots, m$ , denote the perturbations of  $\vec{y}_{n+1}^{(j)}$  caused by perturbing  $\vec{y}_n$  by the amount  $\Delta \vec{y}_n$ . When  $\partial \vec{f} / \partial \vec{y}$  is slowly varying with  $t$  and  $\vec{y}$

we find for  $\Delta \vec{y}_{n+1}$  the expression

$$(2.7) \quad \Delta \vec{y}_{n+1}^{(j)} \cong R_j(\tau J_n) \Delta \vec{y}_n,$$

where  $J_n$  is an approximation to  $(\partial \vec{f} / \partial \vec{y})(t_n, \vec{y}_n)$  and  $R_j$  a polynomial of degree  $j$  in  $\tau J_n$  which satisfy the recurrence relation

$$R_0(z) = 1,$$

$$(2.8) \quad R_1(z) = 1 + \tilde{\mu}_1 z,$$

$$R_j(z) = \tilde{\gamma}_j z + (\mu_j + \tilde{\mu}_j z) R_{j-1}(z) + (v_j + \tilde{v}_j z) R_{j-2}(z).$$

$R_m(z)$  is called the *stability polynomial* and  $R_j(z)$ ,  $j < m$ , may be considered as an *intermediate stability polynomial*. It can be shown that RK methods of order  $p$  always have a  $p$ -th order consistent stability polynomial, i.e. a polynomial of the form [3]

$$(2.9) \quad R_m(z) = 1 + \beta_1 z + \beta_2 z^2 + \dots + \beta_m z^m, \quad \beta_j = \frac{1}{j!}, \quad j = 1, 2, \dots, p,$$

where the coefficients  $\beta_j$  are certain expressions of the RK parameters. For instance, by writing down the recurrence relations for the coefficient of  $z$  in  $R_j(z)$  we see that relation (2.4) appears, hence  $\beta_1 = c_{1m} = \theta_m$ . Similarly we obtain  $\beta_2 = c_{2m}$ .

Thus, it follows from (2.6) that a *first or second order consistent stability polynomial always implies a first or second order accurate RK method*.

In practice, one often constructs RK methods by identifying its stability polynomial with an appropriate polynomial. From our last remark, first or second order accuracy is then automatically ensured by choosing a first or second order consistent stability polynomial. In this paper we are particularly interested in polynomials with a maximal real interval of stability (we call a polynomial  $P(z)$  stable in a point  $z$  if  $|P(z)| \leq 1$ ). A survey of stability polynomials may be found in [3, p. 86ff]. In our case, where we intend to apply the RK method for very large  $m$ -values, it is convenient to



have an analytical expression at our disposal. Moreover, we shall require that the polynomial is *strongly stable* in the stability interval, that is  $|R_m(z)|$  strictly less than 1 (if  $|R_m(z)| = 1$  at one or more points  $z \in (-\beta, 0)$  we call  $R_m(z)$  *weakly stable*).

In the class of *first order consistent* polynomials we have in the notation of [3]

$$(2.10) \quad \tilde{R}_m^{(1)}(z) = \frac{T_m(w_0 + \frac{w_0+1}{\beta} z)}{T_m(w_0)}, \quad T_m(w) = \cos[m \arccos w], \quad w_0 > 1$$

which is strongly stable in the real interval  $[-\beta, 0]$ ,  $\beta$  being given by

$$(2.11) \quad \beta = \frac{(w_0+1)T'_m(w_0)}{T_m(w_0)} \cong \frac{(w_0+1)[T'_m(1) + (w_0-1)T''_m(1)]}{1 + (w_0-1)T'_m(1)}$$

$$\cong 2m^2 \left[ 1 - \frac{4m^2-1}{6} (w_0-1) \right] \quad \text{as } w_0 \rightarrow 1.$$

The parameter  $w_0$  governs the damping effect of the stability polynomial. It is easily verified that in the stability interval (except for a small neighbourhood of the origin) the polynomial  $\tilde{R}_m^{(1)}(z)$  satisfies the inequality

$$(2.12) \quad |\tilde{R}_m^{(1)}(z)| \leq |T_m^{-1}(w_0)| \cong 1 - (w_0-1)m^2.$$

In the class of *second order consistent* polynomials we find in [3] \*) the weakly stable polynomials

$$(2.13) \quad A_m^{(2)}(z) = 2 \frac{\beta+1}{3\beta+2} + \frac{\beta}{3\beta+2} T_m\left(1 + \frac{2z}{\beta}\right), \quad \beta = \frac{2}{3} (m^2-1)$$

with real stability interval  $[-\beta, 0]$ . We will show that the polynomial  $A_m^{(2)}(z)$  can be modified to obtain a strongly stable, second order consistent polynomial  $\tilde{A}_m^{(2)}(z)$ . The expression (2.13) suggests trying the representation

$$\tilde{A}_m^{(2)}(z) = a + bT_m(w_0 + w_1 z)$$

where  $a$ ,  $b$ ,  $w_0$  and  $w_1$  are determined by the condition  $|\tilde{A}_m^{(2)}(z)| \leq 1 - \varepsilon$ ,  $-\beta \leq z \leq 0$ , i.e.

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\*) see also: M. BAKKER, MC report TN 62/71, Mathematisch Centrum, Amsterdam, 1971, (Dutch).

$$(2.14) \quad a+b = 1-\varepsilon, \quad a > 0, \quad w_0 - w_1\beta = -1,$$

and the consistency conditions

$$(2.15) \quad \begin{aligned} \tilde{A}_m^{(2)}(0) &= a + bT_m(w_0) = 1, \\ (\tilde{A}_m^{(2)})'(0) &= bw_1T_m'(w_0) = 1, \\ (\tilde{A}_m^{(2)})''(0) &= bw_1^2T_m''(w_0) = 1. \end{aligned}$$

Here,  $\varepsilon > 0$  and serves to make the polynomial strongly stable. Solving (2.14)-(2.15) leads to the strongly stable, second order consistent polynomial

$$(2.16) \quad \begin{aligned} \tilde{A}_m^{(2)}(z) &= a + bT_m(w_0 + \frac{w_0+1}{\beta}z), \quad a = \frac{T_m(w_0)-1-\varepsilon T_m(w_0)}{T_m(w_0)-1}, \\ b &= \frac{\varepsilon}{T_m(w_0)-1}, \quad \varepsilon = \frac{T_m''(w_0)[T_m(w_0)-1]}{[T_m'(w_0)]^2}, \end{aligned}$$

where

$$(2.17) \quad \beta = \frac{(w_0+1)T_m''(w_0)}{T_m'(w_0)} \cong \frac{2}{3} (m^2-1) \left[1 - \frac{2}{5}\varepsilon \frac{m^2-1/4}{m^2-1}\right] \quad \text{as } \varepsilon \rightarrow 0.$$

This polynomial assumes extrema  $1 - \varepsilon$  in the real stability interval  $[-\beta, 0)$ . In order to know what value for  $w_0$  should be chosen to get a prescribed  $\varepsilon$ , one may use the formula  $w_0 \cong 1 + 3\varepsilon/(m^2-1)$  provided that  $\varepsilon$  is sufficiently small. It should be remarked that polynomials  $\tilde{R}_m^{(2)}(z)$  exist [3] with a real stability interval approximately given by  $[-.80m^2, 0)$ . These polynomials, however, are not available in closed form and therefore not suitable to our purposes unless relatively small values for  $m$  are used ( $m \leq 12$ ). The polynomials  $\tilde{A}_m^{(2)}(z)$  used here, although not optimal, cover roughly 80% of the stability interval of the optimal polynomials  $\tilde{R}_m^{(2)}(z)$ .

### 2.3. Internal stability

It is well-known that RK methods with many stages may exhibit an unstable behaviour in spite of a strongly stable stability polynomial  $R_m(z)$ .

The reason is the development of instabilities within a single integration step (cf. [3, 5]). Fortunately, the identification of  $R_m(z)$  with a prescribed polynomial does not uniquely define the parameters in the scheme (2.1) and we may try to exploit this freedom by improving the internal stability of the method.

Let us consider the points  $t_n + \theta_j \tau$  in the scheme (2.1) as step points, then one integration step with scheme (2.1) may be considered as the performance of one Euler step and  $m-1$  steps with a multistep formula. From the point of view of stability these steps may be considered three-term relations involving  $\vec{y}_{n+1}^{(j)}$ ,  $\vec{y}_{n+1}^{(j-1)}$  and  $\vec{y}_{n+1}^{(j-2)}$ . By requiring that all these relations are stable we are led to the condition that the roots of the equations

$$(2.18) \quad \begin{aligned} \xi - (1 + \tilde{\mu}_1 z) &= 0, \\ \xi^2 - (\mu_j + \tilde{\mu}_j z)\xi - (v_j + \tilde{v}_j z) &= 0, \quad j = 2, 3, \dots, m \end{aligned}$$

are on the unit disk, those on the unit circle having multiplicity 1 if  $z = 0$ . Here,  $z$  runs through the eigenvalues of  $\tau J_n$ . Assuming that the stability condition (1.2) is satisfied we have  $-\beta \leq z \leq 0$  and are led to the *internal stability conditions* [4]

$$(2.19) \quad \begin{aligned} 0 \leq \tilde{\mu}_1 \leq \frac{2}{\beta}, \quad |\mu_j| \leq 1 - v_j, \quad |\mu_j - \tilde{\mu}_j \beta| \leq 1 - v_j + \tilde{v}_j \beta, \\ v_j > -1, \quad v_j \geq \beta \tilde{v}_j - 1, \quad j = 2, 3, \dots, m. \end{aligned}$$

We remark that an alternative condition for internal stability reads

$$(2.19') \quad |R_j(z)| \leq 1, \quad -\beta \leq z \leq 0, \quad j = 1, 2, \dots, m.$$

These conditions are sometimes easier to verify.

### 3. SPECIFICATION OF RK FORMULAS

The RK method (2.1) can be uniquely defined by prescribing the stability polynomial  $R_m(z)$  to obtain the parameters  $\tilde{\mu}_j$  (say) and specifying the

parameters  $\mu_j$ ,  $\nu_j$ ,  $\tilde{\nu}_j$  and  $\tilde{\gamma}_j$  or, alternatively, by prescribing all intermediate stability polynomials  $R_j(z)$ ,  $j = 1, 2, \dots, m$  occurring in (2.8). We shall consider the methods listed in table 3.1. All methods are strongly

Table 3.1. Specification of RK methods

Method	m	$R_m(z)$	$\beta$	$\mu_j$	$\nu_j$	$\tilde{\nu}_j$	$\tilde{\gamma}_j$	$R_j(z)$
Diagonal schemes	$m \leq 12$	$\tilde{R}_m^{(1)}(z)$	$1.93m^2$					
		$\tilde{R}_m^{(2)}(z)$	$0.80m^2$			$1 \ 0 \ -\tilde{\mu}_{j-1} \ 0$		
Factorized schemes	depends on the ordering of $\mu_j$	$\tilde{R}_m^{(1)}(z)$	$1.93m^2$	1	0	0	0	
Runge-Kutta-Chebyshev schemes	unlimited	$\tilde{R}_m^{(1)}(z)$	$1.93m^2$			(3.8)		(3.6)
		$\tilde{A}_m^{(2)}(z)$	$.65m^2$			(3.11)		(3.9)

stable with  $|R_m(z)| \leq .95$  in the stability interval (excluding the direct neighbourhood of the origin). The order of accuracy equals the order of consistency of  $R_m(z)$  and appears as the upper index of the stability polynomials.

The diagonal and factorized schemes were proposed in [3] and [2], respectively. The Runge-Kutta-Chebyshev schemes are derived in Sections 3.3 and 3.4.

### 3.1. The diagonal schemes

The reason to call the first two methods in Table 3.1 *diagonal schemes* is the diagonal form of the matrix  $(\lambda_{j\ell})$  when it is represented in the form (2.1'). In fact, we have  $\lambda_{j\ell} = \tilde{\mu}_j \delta_{j,\ell+1}$ ,  $\delta_{j\ell}$  denoting the Kronecker symbol.

The values of the parameters  $\tilde{\mu}_j$  follow from the coefficients of the stability polynomial  $\tilde{R}_m^{(p)}(z)$ . Since  $R_m(z)$  is easily varied to assume the form

$$R_m(z) = 1 + z + \tilde{\mu}_m \tilde{\mu}_{m-1} z^2 + \tilde{\mu}_m \tilde{\mu}_{m-1} \tilde{\mu}_{m-2} z^3 + \dots + \prod_{j=1}^m \tilde{\mu}_j z^m,$$

the identification with  $\tilde{R}_m^{(p)}(z)$  yields

$$(3.1) \quad \tilde{\mu}_m = 1, \quad \tilde{\mu}_{m-1} = \tilde{\beta}_2, \quad \tilde{\mu}_{m-j} = \frac{\tilde{\beta}_{j+1}}{\tilde{\beta}_j}, \quad j = 2, 3, \dots, m-1,$$

where the  $\tilde{\beta}_j$  denote the coefficients of  $\tilde{R}_m^{(p)}(z)$ . In Table 3.2 the values of the parameters  $\tilde{\mu}_j$  are given for  $p = 1, 2$  and  $m = 12$ . Higher  $m$ -values are not recommended because of internal instabilities. Only those stages which satisfy the conditions (2.19), i.e.

$$(3.2) \quad \tilde{\mu}_1 \leq \frac{2}{\beta}, \quad \tilde{\mu}_j \geq \tilde{\mu}_{j-1} \geq 0, \quad \tilde{\mu}_j + \tilde{\mu}_{j-1} \leq \frac{2}{\beta}$$

are stable. For  $m = 12$  this is only the case in the first four stages.

Table 3.2. Parameters  $\tilde{\mu}_j$  defined by (3.1) for  $p = 1, 2$ .

j	p = 1	p = 2
1	.59855019853748 10 <sup>-3</sup>	.14655103357686 10 <sup>-2</sup>
2	.13680675530244 10 <sup>-2</sup>	.33579537473672 10 <sup>-2</sup>
3	.23814095294512 10 <sup>-2</sup>	.58641787543279 10 <sup>-2</sup>
4	.37550786293928 10 <sup>-2</sup>	.92868907459439 10 <sup>-2</sup>
5	.56849352386342 10 <sup>-2</sup>	.14143642717242 10 <sup>-1</sup>
6	.85214009286744 10 <sup>-2</sup>	.21381220113453 10 <sup>-1</sup>
7	.12943371721975 10 <sup>-1</sup>	.32889580915313 10 <sup>-1</sup>
8	.20412750851429 10 <sup>-1</sup>	.52908291207994 10 <sup>-1</sup>
9	.34579560109742 10 <sup>-1</sup>	.92622927228129 10 <sup>-1</sup>
10	.66851127311726 10 <sup>-1</sup>	.18919569639556
11	.17003903575641	.5
12	1	1

### 3.2. Factorized schemes

The stability polynomial of the factorized schemes is given by

$$R_m(z) = \prod_{j=1}^m (1 + \tilde{\mu}_j z) = 1 + z + \sum_{j=2}^m \tilde{\mu}_j \sum_{\ell=1}^{j-1} \tilde{\mu}_\ell z^2 + \dots$$

Let us write the polynomial  $\tilde{R}_m^{(1)}(z)$  in the form

$$(3.3) \quad \prod_{j=1}^m \left(1 - \frac{z}{\omega_j}\right),$$

where  $\omega_j$  represent the zeros of  $\tilde{R}_m^{(1)}(z)$ . Then, identification with  $R_m(z)$  yields

$$(3.4) \quad \tilde{\mu}_j = -\frac{1}{\omega_j}, \quad \theta_j = \sum_{\ell=1}^j \frac{-1}{\omega_\ell}, \quad j = 1, 2, \dots, m.$$

The stages of this method may be considered as a sequence of Euler steps with stepsizes  $|\tau/\omega_j|$ . This factorization into Euler steps explains the characterization *factorized schemes*.

From (2.10) the zeros of  $\tilde{R}_m^{(1)}(z)$  can be derived, so that by (3.4) the values of the parameters  $\tilde{\mu}_j$  are given by

$$(3.4') \quad \frac{\sqrt{w_0^2 - 1}}{m \tanh[m \ln(w_0 + \sqrt{w_0^2 - 1})]} \cdot \frac{1}{\cos\left[\frac{(\ell - 1/2)\pi}{m}\right] - w_0}, \quad \ell = 1, \dots, m.$$

The ordering of the Euler steps is free but extremely important in view of internal instabilities. Checking the conditions (2.19) reveals that half of the stages are unstable. In [2], however, special orderings are proposed which are claimed to give an overall stable behaviour. These orderings belong to the class

$$(3.5) \quad j = \ell \equiv i\chi \pmod{m}, \quad i = 1, 2, \dots, m; \ell, \chi \in [1, m].$$

In Section 4, a number of  $\chi$ -values will be tested and indeed we verified that once a suitable  $\chi$ -value is found, relatively large  $m$ -values are possible. However, the optimal  $\chi$ -value depends on  $m$  and it is not clear how to

predict a priori its value. This makes the factorization method less attractive from a computational point of view.

Finally, we remark that factorization methods of second or higher order are difficult to construct because of the requirement that the parameters  $\tilde{\mu}_j$  should be highly accurate. This implies that we should have a polynomial  $R_m(z)$  with  $m$  real roots which can be analytically expressed in terms of its coefficients. Such a requirement excludes the application of factorized schemes with  $\tilde{R}_m^{(2)}(z)$  or  $\tilde{A}_m^{(2)}(z)$  as its stability polynomial (note that  $\tilde{A}_m^{(2)}(z)$  only has complex roots).

### 3.3. First order Runge-Kutta-Chebyshev scheme

Let  $\beta$  be given by (2.11) and consider the polynomials

$$(3.6) \quad P_j(z) = T_j^{-1}(w_0) T_j\left(w_0 + \frac{w_0+1}{\beta} z\right), \quad j \geq 0.$$

From (2.10) it follows that  $P_m(z) \equiv \tilde{R}_m^{(1)}(z)$ . Furthermore, the polynomials  $P_j(z)$  are stable in the sense of (2.19') and satisfy the condition  $P_j(0) = 1$ . They are therefore suitable as intermediate stability polynomials. Hence, by putting  $P_j(z) = R_j(z)$ ,  $R_j(z)$  being defined by (2.8) for  $j = 0, 1, \dots, m$ , we generate a method with  $\tilde{R}_m^{(1)}(z)$  as its stability polynomial. By observing that  $P_j(z)$  satisfies the recurrence relation (cf. the construction of the second order Richardson method for the iterative solution of elliptic difference equations [1])

$$(3.7) \quad \begin{aligned} P_0(z) &= 1, \\ P_1(z) &= 1 + \frac{w_0+1}{\beta w_0} z, \\ P_j(z) &= 2\left(w_0 + \frac{w_0+1}{\beta} z\right) \frac{T_{j-1}(w_0)}{T_j(w_0)} P_{j-1}(z) - \frac{T_{j-2}(w_0)}{T_j(w_0)} P_{j-2}(z) \end{aligned}$$

the identification with (2.8) yields

$$\begin{aligned}
(3.8) \quad \tilde{\mu}_1 &= \frac{w_0+1}{\beta w_0}, \\
\tilde{\gamma}_j &= \tilde{v}_j = 0, \quad \mu_j = 2w_0 \frac{T_{j-1}(w_0)}{T_j(w_0)}, \\
\tilde{\mu}_j &= 2 \frac{w_0+1}{\beta} \frac{T_{j-1}(w_0)}{T_j(w_0)}, \quad v_j = 1 - \mu_j, \quad j = 2, 3, \dots, m.
\end{aligned}$$

It is easily verified that the internal stability conditions (2.19) are satisfied by these parameters.

Since the stability polynomials  $R_j(z)$  of the successive stages are all shifted Chebyshev polynomials we will call the method defined by (3.8) a *Runge-Kutta-Chebyshev scheme*.

#### 3.4. Second order Runge-Kutta-Chebyshev scheme

Consider the polynomials

$$\begin{aligned}
(3.9) \quad P_0(z) &= 1, \\
P_j(z) &= a + b \frac{T_m(w_0)}{T_j(w_0)} T_j\left(w_0 + \frac{w_0+1}{\beta} z\right), \quad j \geq 1,
\end{aligned}$$

$a$ ,  $b$  and  $\beta$  being given by (2.16) and (2.17). Then  $P_m(z) \equiv \tilde{A}_m^{(2)}(z)$ ,  $P_j(0) = 1$  and (2.19') is satisfied. These polynomials satisfy the recurrence relation

$$\begin{aligned}
(3.10) \quad P_0(z) &= 1, \\
P_1(z) &= 1 + \frac{b(w_0+1)T_m(w_0)}{\beta w_0} z, \\
P_j(z) &= -\frac{2a(w_0+1)T_{j-1}(w_0)}{\beta T_j(w_0)} z + 2\left(w_0 + \frac{w_0+1}{\beta} z\right) \frac{T_{j-1}(w_0)}{T_j(w_0)} P_{j-1}(z) \\
&\quad - \frac{T_{j-2}(w_0)}{T_j(w_0)} P_{j-2}(z).
\end{aligned}$$

Identification of (2.8) and (3.10) yields



$$\begin{aligned}
(3.11) \quad \tilde{\mu}_1 &= \frac{b(w_0+1)T_m(w_0)}{\beta w_0}, \\
\tilde{\gamma}_j &= -\frac{2a(w_0+1)T_{j-1}(w_0)}{\beta T_j(w_0)}, \quad \mu_j = 2w_0 \frac{T_{j-1}(w_0)}{T_j(w_0)}, \quad \tilde{\mu}_j = 2 \frac{(w_0+1)T_{j-1}(w_0)}{\beta T_j(w_0)}, \\
v_j &= -\frac{T_{j-2}(w_0)}{T_j(w_0)}, \quad \tilde{v}_j = 0, \quad j = 2, 3, \dots, m.
\end{aligned}$$

These parameters satisfy the internal stability conditions (2.19).

As in the preceding section the internal stability polynomials  $R_j(z)$  are related to Chebyshev polynomials. Therefore, the method defined by (3.11) will also be called a Runge-Kutta-Chebyshev scheme.

#### 4. NUMERICAL RESULTS

In the preceding section, three types of methods are presented: the *diagonal schemes* extremely simple in structure but possessing unfavourable internal stability properties for larger  $m$ -values, the *factorized schemes* similarly simple in structure but very sensitive to the optimal ordering of the RK parameters and finally the *Runge-Kutta-Chebyshev schemes* satisfying the internal stability conditions for arbitrary  $m$ -values at the cost of a more complicated form of the formulas and a few additional storage arrays. It is the aim of this section to test numerically the internal stability behaviour of the various schemes. In order to isolate this aspect from other sources of inaccuracy, such as the discretization error and the stability at the step points, we have chosen a problem which would be exactly solved by the numerical schemes if no round-off errors enter in the computation (provided that the parameters of the schemes are exactly given). The initial-boundary value problem is given by

$$(4.1) \quad u_t = u_{xx} + u_{yy},$$

defined on  $\{(t,x,y) \mid t \geq 0, 0 \leq x, y \leq 1\}$ . The Dirichlet boundary conditions as well as the initial condition are set to 1. After semi-discretization using central differences on a uniform grid with gridsize equal to  $1/20$ ,

the resulting system was integrated by just one integration step with the maximal stable steplength  $\tau = \beta(m)/\sigma$ . Here  $\sigma$  is equal to 3200. The exact solution of this system equals 1 for all components and for all values of  $t$ .

By perturbing the initial vector and comparing the numerical result after one integration step with the exact solution, we get insight into the damping effect of the numerical scheme on the initial perturbation. We chose the components of the initial vector equal to  $1 + r \cdot 10^{-14}$ , where  $r$  denotes a random number  $\in (-1, 1)$  being different for each component. The factor  $10^{-14}$  has been chosen because the experiments were carried out on a CDC Cyber 73-28 computer using an accuracy of about 14 digits. In Table 4.1 we have listed for the various schemes the amplification factors

$$(4.2) \quad \alpha = 10^{14} \max_P |y_1^{(P)} - 1|,$$

where  $y_1^{(P)}$  denotes the numerical solution at the grid point  $P$  for  $t = \tau$ .

Table 4.1. Amplification factors in the various schemes

Diagonal scheme				Factorized scheme			Runge-Kutta-Chebyshev scheme			
p = 1 $\tau = 1.93m^2/\sigma$		p = 2 $\tau = 0.8m^2/\sigma$		p = 1 $\tau = 1.93m^2/\sigma$			p = 1 $\tau = 1.93m^2/\sigma$		p = 2 $\tau = 0.65m^2/\sigma$	
m	$\alpha$	m	$\alpha$	m	$\chi$	$\alpha$	m	$\alpha$	m	$\alpha$
12	.23 <sub>10</sub> <sup>8</sup>	12	.17 <sub>10</sub> <sup>8</sup>	41	1	.20 <sub>10</sub> <sup>5</sup>	41	.65 <sub>10</sub> <sup>1</sup>	36	.56 <sub>10</sub> <sup>2</sup>
				41	21	.16 <sub>10</sub> <sup>2</sup>	82	.85 <sub>10</sub> <sup>1</sup>	71	.76 <sub>10</sub> <sup>2</sup>
				41	31	.25 <sub>10</sub> <sup>2</sup>	164	.18 <sub>10</sub> <sup>2</sup>	142	.93 <sub>10</sub> <sup>2</sup>
				41	40	.12 <sub>10</sub> <sup>16</sup>			284	.76 <sub>10</sub> <sup>2</sup>
				82	1	.69 <sub>10</sub> <sup>25</sup>				
				82	61	.19 <sub>10</sub> <sup>6</sup>				
				82	71	.51 <sub>10</sub> <sup>5</sup>				
				82	81	.14 <sub>10</sub> <sup>34</sup>				

This table shows that the amplification of rounding errors in the diagonal scheme is already considerable for  $m = 12$  and therefore  $m$  should not be increased. With the factorized scheme it is possible to use high  $m$ -values provided an appropriate value of  $\chi$  is chosen. Since it is not clear how to choose such a  $\chi$ -value for a given value of  $m$ , this scheme needs careful handling.

For the Runge-Kutta-Chebyshev scheme we may conclude that the propagation of rounding errors is neglectable and almost independent of  $m$ .

#### REFERENCES

- [1] FRANK, W., *Solution of linear systems by Richardson's method*, J. Assoc. Comp. Mach. 7, 274-286 (1960).
- [2] GENTSCH, W. & A. SCHLÜTER, *Über ein Einschrittverfahren mit zyklischer Schrottweitenänderung zur lösung parabolische Differentialgleichungen*, ZAMM 58, 415-416 (1978).
- [3] HOUWEN, P.J. van der, *Construction of integration formulas for initial value problems*, North-Holland Publ. Comp., Amsterdam (1977).
- [4] LAMBERT, J.D., *Computational methods in ordinary differential equations*, John Wiley & Sons, London (1973).
- [5] VERWER, J.G., *A class of stabilized three-step Runge-Kutta methods for the numerical integration of parabolic equations*, J. Comp. Appl. Math. 3, 155-166 (1977).

ONTVANGEN: 17 OKT. 1979