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ON A CLASS OF EXPLICIT THREE-STEP RUNGE-KUTTA METHODS WITH EXTENDED REAL STABILITY INTERVALS

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On a class of explicit three-step Runge-Kutta methods with extended real stability intervals*)

by

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ABSTRACT

The paper deals with the numerical integration of semi-discrete parabolic equations, written in the explicit, autonomous form $y' = f(y)$. A class of explicit, 3-step Runge-Kutta methods is considered of which the real boundaries of absolute stability are given by $5.17m^2$ for methods of order 1, and by $2.36m^2$ for methods of order 2. Here m denotes the number of f(y)-evaluations per integration step. This number may be arbitrarily large. The paper also deals with a linearization of the formulas by which m-1 f(y)-evaluations can be replaced by m-1 multiplications of a Jacobian matrix with intermediate vectors. This means that for many problems the linearized schemes will be less expensive. The paper is concluded with a numerical example.

KEY WORDS & PHRASES: *Numerical analysis, Parabolic equations, Method of lines, Stabilized explicit methods*

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*) This report will be submitted for publication elsewhere.

1. INTRODUCTION

This paper deals with the numerical solution of the initial value problem for large systems of ordinary differential equations written in the explicit, autonomous form

$$(1.1) \qquad y' = f(y),$$

and possessing the property that the eigenvalues of the Jacobian matrix $J(y) = \partial f(y)/\partial y$ are situated in a long narrow strip along the negative axis of the complex plane. Such systems frequently arise when discretizing the space variables of initial-boundary value problems for parabolic partial differential equations [7]. We shall focus our attention to these semi-discrete parabolic problems. For our discussion it is not necessary to define a particular class of parabolic problems or to specify the method of semi-discretization. Our only restriction is the location of the eigenvalues of the Jacobian matrix $J(y)$. Further it is always assumed that the problem is sufficiently smooth.

In considering the application of explicit integration methods to semi-discrete parabolic equations one must weigh up an important advantage against an important disadvantage. Their advantage, when compared with implicit or partly implicit methods (see e.g. [7,4]), is that they do not require the solution of large and complicated systems of nonlinear algebraic or transcendental equations (more dimensional problems) and, consequently, that they can be easily applied to large problem classes. Their disadvantage, as is well known, is the conditional stability. Fortunately it is possible to reduce this disadvantage considerably by using so-called stabilized Runge-Kutta methods (cf. [3], section 2.7). Such a method uses a relatively large number of $f(y)$-evaluations per integration step, say m, the majority of which serves to enlarge the real stability boundary. As this boundary increases quadratically with m it certainly pays to employ such a stabilized method instead of a standard explicit one (see [7]). In fact, stabilized Runge-Kutta methods usually become more efficient as the degree m, that is the number of $f(y)$-evaluations per integration step, increases.

In this paper we investigate a class of stabilized, 3-step Runge-Kutta methods containing the 3-step methods earlier reported in [12]. These last methods, however, have two disadvantages. The first is that the integration parameters are not known in closed form. The second, and the most severe one, is that they are internally unstable. That is, within one single integration step they exhibit a severe accumulation of rounding errors, even when satisfying the condition of absolute stability. Because of the fact that this accumulation can easily influence the local accuracy it is desirable to develop internally stable methods. Recently, van der Houwen and Sommeijer [5] reported high degree, one-step Runge-Kutta methods which are indeed internally stable for all values of m. They obtained internal stability after identifying each intermediate stability function with a Chebyshev polynomial via a stable, two-step Chebyshev recursion. Following this idea we develop a class of internally stable, 3-step Runge-Kutta methods. Our absolute stability boundaries are approximately three times larger than the boundaries reported by van der Houwen and Sommeijer [5]. We also discuss a linearization of the new formulas (cf. [10,14]). By linearization we can replace m-1 f(y)-evaluations by m-1 multiplications of a Jacobian matrix with intermediate vectors. This means that for many problems the linearized schemes will be less expensive. The paper is concluded with a numerical example.

2. A CLASS OF THREE-STEP RUNGE-KUTTA FORMULAS OF DEGREE m

Let y_n denote the numerical approximation at $t = t_n$. Let $\tau = t_{n+1} - t_n$ be the (constant) stepsize. Our class of integration formulas then reads

$$y_{n+1}^{(0)} = \theta_0 y_n + \kappa_0 y_{n-1},$$

$$(2.1) \qquad y_{n+1}^{(j)} = \theta_j y_n + \kappa_j y_{n-1} + \tau\Big(\nu_j f(y_n) + \zeta_j f(y_{n-1}) + \sum_{\ell=0}^{j-1} \lambda_{j\ell} f(y_{n+1}^{(\ell)})\Big), \quad j = 1(1)m,$$

$$y_{n+1} = \alpha y_{n+1}^{(m)} + (1-\alpha) y_{n-2}.$$

Formula (2.1) is easily recognized as a 3-step integration formula using m f-evaluations per integration step. Note that $f(y_{n-2})$ does not appear and that y_{n-2} is not used in the intermediate stages. This restriction is made for the sake of the stability analysis. The method of the above type belongs to the wide class of the multistep Runge-Kutta methods (see e.g. [1,3,11,16]). Our purpose is to find, within this class, attractive formulas for semi-discrete parabolic equations. Therefore we shall concentrate on formulas of low order, viz. of order 1 and of order 2, of which the real stability intervals are relatively large. Further we demand internal stability and, as our systems may become very large, limited storage requirements. It should be observed that class (2.1) contains the 3-step formulas from [12]. In the sequel we take $m \geq 2$.

In the remainder of this section we now shortly discuss some of the basic concepts needed in the next sections. First we give the characteristic equation of (2.1). When applied to the stability test-model

$$y' = \delta y, \quad \delta \in \mathbb{C}, \tag{2.2}$$

(2.1) reduces to the simple scheme

$$y_{n+1}^{(j)} = P_j(z) y_{n-1} + S_j(z) y_n, \qquad j = 0(1)m,$$

(2.3)

$$y_{n+1} = \alpha y_{n+1}^{(m)} + (1-\alpha) y_{n-2},$$

where $z = \tau\delta$ and where P_j and S_j are polynomials of degree j in z. Hence, the characteristic equation is given by

$$\xi^3 - \alpha S_m(z)\xi^2 - \alpha P_m(z)\xi - (1-\alpha) = 0, \tag{2.4}$$

which is of the same form as the characteristic equation of the related methods from [12]. In section 4 it will turn out that the polynomials P_j and S_j belonging to the intermediate stages $y_{n+1}^{(j)}$, play an important role in the internal stability analysis.

Next we give the consistency conditions. We restrict ourselves to order $p = 1$ and order $p = 2$. Let us denote

(2.5) $$S_m(z) = \sum_{i=0}^{m} s_i z^i, \quad P_m(z) = \sum_{i=0}^{m} p_i z^i.$$

Then it is easily shown that method (2.1) is of order p, if and only if (cf.[12]):

(2.6)
$$\begin{array}{c|l} & s_0 = 1 - p_0 \\ p = 1 & s_1 = (3-2\alpha)/\alpha + p_0 - p_1 \\ \hline p = 2 & s_2 = (-1.5 + 2\alpha)/\alpha - \tfrac{1}{2}p_0 + p_1 - p_2 \end{array}$$

Thus, any two polynomials S_m and P_m satisfying conditions (2.6) generate an integration formula of order $p \le 2$. In order to obtain error constants of the same size as in [12], we shall also require $\alpha(s_1+p_1) = 1$, or equivalently ($p \ge 1$),

(2.7) $$\alpha = \frac{2}{2 - p_0} .$$

The effect of this condition is that the error constants, as defined in [2,p.223], cannot become arbitrarily large.

As is the case with linear multistep methods we also have to fulfil the condition of zero-stability in order to obtain convergence [16]. Consequently, at $z = 0$ equation (2.4) has to satisfy the root condition. It turns out that (2.1) is zero stable, if and only if

(2.9) $$p_0 \le \frac{2}{3} .$$

In the following it will always be assumed that conditions (2.7) - (2.8) have been fulfilled.

3. ABSOLUTE STABILITY PROPERTIES

Following Lambert [6], method (2.1) is called absolutely stable for a given $z \in \mathbb{C}$ if, for that z all the roots ξ_i of (2.4) satisfy $|\xi_i| < 1$. Because we did assume that the eigenvalues of $J(y)$ are situated in a long narrow strip along the negative axis we now concentrate on finding polynomials S_m and P_m which lead to such absolute stability regions and which are, in a certain sense, as long as possible. In our analysis z is always assumed to be real and negative.

The starting point is the well-known Routh-Hurwitz criterion which delivers necessary and sufficient conditions for absolute stability [6]. When applied to (2.4) this criterion yields, after a tedious but otherwise elementary calculation, the conditions

$$(3.1)\qquad \begin{aligned} &-1 < A_m(z) < 1, && A_m(z) = \frac{1}{2} + \frac{1}{2}(S_m(z) + P_m(z)),\\ &-1 < B_m(z) < 1, && B_m(z) = \frac{P_0 - 1 + S_m(z) - P_m(z)}{2 - 2p_0},\\ &A_m(z) - B_m(z) > 0. \end{aligned}$$

It is convenient to substitute the consistency relations (2.6) into the first coefficients of A_m and B_m. For order p = 1 this leads to

$$(3.2)\qquad \begin{aligned} A_m(z) &= 1 + (\tfrac{1}{2} - \tfrac{1}{4}p_0)z + \sum_{i=2}^{m} \tfrac{1}{2}a_i z^i, \quad a_i = s_i + p_i,\\ B_m(z) &= \frac{p_0}{2(p_0-1)} + \frac{1 - \tfrac{1}{2}p_0 - 2p_1}{2(1-p_0)} z + \sum_{i=2}^{m} \frac{b_i}{2(1-p_0)} z^i, \quad b_i = s_i - p_i. \end{aligned}$$

For order p = 2 we have the additional relations

$$(3.3)\qquad a_2 = \tfrac{1}{2} + \tfrac{1}{4}p_0 + p_1, \quad b_2 = \tfrac{1}{2} + \tfrac{1}{4}p_0 + p_1 - 2p_2.$$

3.1 Upperbounds for real absolute stability boundaries

In section 3.2 we shall, for given order $p \le 2$ and degree $m \ge 2$, construct polynomials A_m and B_m which lead to satisfactory real stability boundaries, say $\beta_p(m)$. First, however, it is of interest to derive upperbounds for $\beta_p(m)$. Consider the inequalities

$$(3.1')\qquad -1 \le A_m(z) \le 1,$$

(3.1") $-1 \le B_m(z) \le 1.$

Let $-\tilde{\beta}_p(m) \le z \le 0$ be the maximal interval where (3.1') - (3.1") can be satisfied. Then, by definition, $\beta_p(m) \le \tilde{\beta}_p(m)$. We need the following result (see e.g. [3]): Let $Q_m(z)$ be a real, m-th degree polynomial with the property $Q_m(0) = Q'_m(0) = 1$. The interval $[-\beta^*(m),0]$ on which the inequality $-1 \le Q_m(z) \le 1$ holds, is maximized by the shifted Chebyshev polynomial

(3.4) $$Q_m(z) = T_m(1 + \frac{z}{m^2}),\ T_m(w) = \cos\,[m \arccos w],\ \beta^*(m) = 2m^2.$$

THEOREM 3.1. *Let the order of consistency* p = 1. *The length of the negative z-interval on which both* (3.1') *and* (3.1") *can be satisfied, is then maximized by* $6m^2$.

PROOF. Consider A_m as defined in (3.2). As a_i, $i \ge 2$, are free parameters, it is obvious to define

(3.5) $$A_m(z) = T_m(1 + (\tfrac{1}{2} - \tfrac{1}{4}p_0)z/m^2).$$

According to (3.4), this polynomial is optimal with respect to (3.1'). The corresponding boundary is $2m^2/(\frac{1}{2}-\frac{1}{4}p_0)$, which is maximized for $p_0 = \frac{2}{3}$. Substituting $p_0 = \frac{2}{3}$, $p_1 = \frac{1}{3}$, and $b_i = 0$ for $i \ge 2$, yields the desired result. □

As a result of this theorem we have that always $\beta_1(m) \le 6m^2$. In fact, the following, somewhat stronger result can be proved: Let A_m and B_m be defined as in the proof of theorem 3.1. Then

(3.6) $$P_m(z) = -\frac{1}{3} + T_m(1 + \frac{z/3}{m^2}),\ S_m(z) = -\frac{1}{3} + P_m(z),$$

and (2.4) can be factorized as $(\xi+1)(2\xi^2-[3P_m(z) + 1]\xi + 1) = 0$. For all $z \in [-6m^2,0]$ the roots of the quadratic equation lie on the unit disk. Hence, we expect that it is possible to construct first order schemes with $\beta_1(m)$-values arbitrarily close to $6m^2$. We return to this point in section 3.2.

THEOREM 3.2. *Let the order of consistency* p = 2. *The length of the negative z-interval on which both* (3.1') *and* (3.2") *can be satisfied cannot exceed* $2.95m^2$.

PROOF. As before, the optimal polynomial A_m is given by (3.5). As p = 2, we have to match quadratic terms. For given p_0, the coefficient p_1 is thus defined by $p_1 = \frac{1}{3}(1-m^{-2})(\frac{1}{2} - \frac{1}{4}p_0)^2 - (\frac{1}{2} + \frac{1}{4}p_0)$. Substitution into $B_m(z)$ yields

$$(3.7) \qquad B_m(z) = \frac{p_0}{2p_0 - 2} + \frac{1 - \frac{1}{12}(1 - \frac{1}{m^2})(1 - \frac{1}{2}p_0)^2}{1 - p_0} z + \sum_{i=2}^{m} \frac{b_i}{2-2p_0} z^i,$$

where p_0 and b_i, $i \geq 2$, are still free (p_2 can be used for the quadratic terms). The optimal polynomial (3.7), with respect to (3.1"), is easily found to be

$$(3.7') \qquad B_m(z) = T_m(1 + \frac{b_1 m^2 T_m'^{-1}(1-z_0/m^2)z - z_0}{m^2}),$$

where b_1 is the second coefficient of (3.7) and where $z_0 > 0$ satisfies $T_m(1-z_0/m^2) = p_0/(2p_0-2)$. Hence

$$(3.8) \qquad z_0 = m^2(1 - \cos[m^{-1} \arccos \frac{p_0}{2(p_0-1)}]).$$

Consequently, the optimal boundary for inequalities (3.1') - (3.1") is

$$(3.9) \qquad \tilde{\beta}_2(m) = \max_{p_0} \min_{p_0} \{(2m^2-z_0)T_m'(1-z_0/m^2)/b_1 m^2, 2m^2/(\tfrac{1}{2}-\tfrac{1}{4}p_0)\}.$$

We computed (3.9) numerically for m = 2(1)100. Within this m-range the $\tilde{\beta}_2(m)/m^2$-values are slightly increasing with m and are converging to a number slightly smaller than 2.95. From this convergence behaviour we are justified to conclude that for all $m \geq 2$, $\tilde{\beta}_2(m)$ is slightly smaller than $2.95m^2$. □

3.2 The construction of nearly optimal polynomials

As noticed before one is not only interested in large boundaries $\beta_p(m)$, but also in absolute stability regions containing a long narrow strip along the negative axis. This can be achieved by requiring damping for negative z-values (except close to z=0). In this section we define polynomials A_m and B_m with appropriate damping properties and which lead to satisfactory $\beta_p(m)$-values.

We shall make use of so-called damped Chebyshev polynomials (see e.g. [3]). This polynomial is defined by

$$(3.10) \qquad R_m(w_0,z) = \frac{T_m(w_0 + (w_0+1)z/\beta)}{T_m(w_0)}, \qquad w_0 > 1,$$

and is, in modulus, strictly less than 1 on the interval $[-\beta(m),0)$, where

$$(3.11) \qquad \beta(m) = \frac{(w_0+1)T'_m(w_0)}{T_m(w_0)} \simeq 2m^2 \left[1 - \frac{4m^2-1}{6}(w_0-1)\right] \quad \text{as} \quad w_0 \to 1.$$

More specific, on the interval $[-\beta(m),(1-w_0)\beta(m)/(1+w_0)]$

$$(3.12) \qquad |R_m(w_0,z)| \le T_m^{-1}(w_0) \simeq 1 - (w_0-1)m^2 \quad \text{as} \quad w_0 \to 1.$$

3.2.1 The first order formulas.

Let the order of consistency p = 1. Let $w_0 > 1$ and $0 < a, b < 1$ be given parameters. Consider the polynomials

$$(3.13) \qquad A_m(z) = 1 - a + a\, R_m(w_0,\, a^{-1}(\tfrac{1}{2} - \tfrac{1}{4}p_0)z),$$

$$(3.14) \qquad B_m(z) = \frac{p_0}{2p_0-2} - b + b\, R_m(w_0, a^{-1}(\tfrac{1}{2} - \tfrac{1}{4}p_0)z).$$

Note that (3.13) is consistent with the polynomial A_m defined by (3.2). Further, the polynomials B_m can always be made consistent by a proper definition of the free parameter p_1 in (3.2). Later we will see that definitions (3.13) - (3.14) are appropriate to establish internal stability (see section 4). Finally, substitution of $p_0 = 2/3$, $w_0 = 1$, $a = 1$ and $b = 0$

yields the polynomials occurring in theorem 3.1.

Let

$$\beta_1(m) = \frac{a(w_0 + 1)\, T'_m(w_0)}{(\tfrac{1}{2} - \tfrac{1}{4}p_0)\, T_m(w_0)} \tag{3.15}$$

and $z \in [-\beta_1(m), (1-w_0)\beta_1(m)/(1+w_0)]$. Then (see (3.1))

$$-1 < 1 - a - a\, T_m^{-1}(w_0) \le A_m(z) \le 1 - a + a\, T_m^{-1}(w_0) < 1, \tag{3.16}$$

$$-1 < \frac{p_0}{2p_0-2} - b - b\, T_m^{-1}(w_0) \le B_m(z) \le \frac{p_0}{2p_0-2} - b + b\, T_m^{-1}(w_0) < 1, \tag{3.17}$$

provided that

$$0 < b < \frac{1 + p_0/(2p_0-2)}{T_m^{-1}(w_0) + 1} . \tag{3.18}$$

As we have much freedom in the choice of b, condition (3.18) is not too restrictive. The last of conditions (3.1) is satisfied if

$$(a-b)\, R_m(w_0, a^{-1}(\tfrac{1}{2} - \tfrac{1}{4}p_0)z) > \frac{p_0}{2p_0 - 2} + a - b - 1. \tag{3.19}$$

The parameters a,b and w_0 should be considered as damping parameters. Because it would require a rather long and tedious calculation to derive an explicit relation between a,b, w_0 and a given parameter $\rho < 1$, such that $|\xi_i| \le \rho$. We prefer to find out whether the polynomials constructed in [12] satisfy inequalities like (3.16) - (3.17). By choosing a,b, p_0 and w_0 accordingly, we then expect similar damping properties as imposed in [12]. As a result of the comparison, we set

$$w_0 = 1 + \frac{1/20}{m^2}, \quad a = 0.975, \; b = 0.2, \; p_0 = \frac{124}{229} . \tag{3.20}$$

Inequalities (3.16), (3.17) and (3.19) then read (approximately)

(3.16') $-1 < -0.90 \le A_m(z) \le 0.95 < 1,$

(3.17') $-1 < -0.98 \le B_m(z) \le -0.60 < 1,$

(3.19') $R_m(w_0, a^{-1}(\frac{1}{2} - \frac{1}{4}p_0)z) > -1.05.$

Consequently, for $z \in [-\beta_1(m), (1-w_0)\beta_1(m)/(1+w_0)]$ inequalities (3.1) have been satisfied. The inspection of the remaining interval $[(1-w_0)\beta_1(m)/(1+w_0), 0]$ is now trivial.

Summarizing, the polynomials (3.13) - (3.14), of which the parameters are listed in (3.20), generate first order integration formulas having stability boundaries

$$(3.15') \qquad \beta_1(m) = \frac{a(w_0+1)\ T_m'(w_0)}{(\frac{1}{2} - \frac{1}{4}p_0)\ T_m(w_0)} \simeq 5.17m^2 \text{ as } m \to \infty.$$

Except close to $z = 0$, the roots ξ_i of (2.4) satisfy $|\xi_i| \le \rho = 0.91$ (we checked ρ for $m = 2(1)25$). This means that the absolute stability regions of the integration formulas are of the same form as the regions plotted in [12], and thus contain a narrow strip along the negative axis.

3.2.2. The second order formulas

As in the preceding subsection we take the polynomials (3.13) and (3.14) as the starting point. Here, however, we have to take account of relations (3.3). Let us consider the polynomials A_m given by (3.2) and (3.13), respectively. Equating these polynomials reveals that p_1 must be used for the quadratic terms. R_m can be written as

$$R_m(w_0,w) = 1 + w + \frac{T_m(w_0)T_m''(w_0)}{2T_m'^2(w_0)} w^2 + \dots \quad ,$$

hence p_1 must satisfy

$$p_1 = \frac{T_m(w_0)\ T_m''(w_0)}{aT_m'^2(w_0)}(\tfrac{1}{2} - \tfrac{1}{4}p_0)^2 - (\tfrac{1}{2} + \tfrac{1}{4}p_0).$$

Substitution of this expression into B_m, given by (3.2), yields

$$(3.2') \qquad B_m(z) = \frac{p_0}{2p_0-2} + \frac{1-a^{-1}T_m(w_0)T_m''(w_0)T_m'^{-2}(w_0)(\tfrac{1}{2}-\tfrac{1}{4}p_0)^2}{1-p_0}z + \sum_{i=2}^{m}\frac{b_i}{2-2p_0}z^i.$$

This polynomial has to be identified with (3.14). Equating linear terms delivers

$$(3.21) \qquad \left(\frac{b}{a} + \frac{T_m(w_0)T_m''(w_0)}{4a\ T_m'^2(w_0)}\right)p_0^2 - \left(\frac{3b}{a} + \frac{T_m(w_0)T_m''(w_0)}{a\ T_m'^2(w_0)}\right)p_0 + \frac{T_m(w_0)T_m''(w_0)}{a\ T_m'^2(w_0)} + \frac{2b}{a} - 4 = 0.$$

Note that in (3.2) the coefficient p_2 can be used to equate quadratic terms.

We now proceed as before. The only extra condition is (3.21). The investigation of the polynomials from [12] decides us to select

$$(3.20') \qquad w_0 = 1 + \frac{1/20}{m^2}, \quad a = 0.81, \quad b = 0.6.$$

Substitution into (3.21) delivers, for large values of m, $p_0 \simeq -0.66$. For these values the inequalities (3.16),(3.17) and (3.19) become (approximately)

$$(3.16'') \qquad -1 < -0.58 \le A_m(z) \le 0.96 < 1,$$

(3.17") $\quad -1 < -0.97 \le B_m(z) \le 0.17 < 1,$

(3.19") $\quad R_m(w_0, a^{-1}(\tfrac{1}{2} - \tfrac{1}{4}p_0)z) > -2.81.$

For low values of m these inequalities have to be checked separately. Fortunately, the parameters p_0 rapidly converge to $p_0(\infty)$. It thus turns out that for all $m \ge 2$ inequalities like (3.16"), (3.17") and (3.19") are satisfied.

Summarizing, the polynomials (3.13) - (3.14), of which the unknown parameters are given by (3.20') and (3.21), generate second order integration formulas with a real absolute stability boundary given by

(3.15") $$\beta_2(m) = \frac{a(w_0+1)\ T_m'(w_0)}{(\tfrac{1}{2} - \tfrac{1}{4}p_0)\ T_m(w_0)} \simeq 2.36m^2 \text{ as } m \to \infty.$$

Except close to $z = 0$, the roots ξ_i of (2.4) satisfy $|\xi_i| \le \rho = 0.95$ (we checked ρ for $m = 2(1)25$). Thus the absolute stability regions of the second order formulas also contain a narrow strip along the negative axis.

4. THREE-STEP RUNGE-KUTTA-CHEBYSHEV FORMULAS

An unpleasant phenomenon in the application of stabilized, explicit methods may be the accumulation of rounding errors within one single integration step. This phenomenon is referred to as internal instability [3,12]. For stabilized methods of a high degree this accumulation may be considerable and can easily influence the local accuracy. It thus is desirable to look for stabilized methods which are internally stable for arbitrary values of m. Recently, van der Houwen and Sommeijer [5] reported a stabilized, one-step Runge-Kutta method which is indeed internally stable for all values of m. They obtained internal stability by making use of a two-step Chebyshev recursion. Following this idea, we now construct internally stable 3-step formulas, of order $p = 1$ and $p = 2$, which possess the absolute stability boundaries derived in the preceding section. Adopting the terminology of

[5] we will call them Runge-Kutta-Chebyshev formulas.

Let us consider the integration scheme

(4.1)
$$
\begin{aligned}
y_{n+1}^{(0)} &= \mu_0 y_n + (1-\mu_0)y_{n-1},\\
y_{n+1}^{(1)} &= \mu_1 y_n + (1-\mu_1)y_{n-1} + \tau(\tilde{\gamma}_1 f(y_n) + \tilde{\delta}_1 f(y_{n-1})),\\
y_{n+1}^{(j)} &= \mu_j y_{n+1}^{(j-1)} + (1-\mu_j)y_{n+1}^{(j-2)} + \tau\tilde{\mu}_j f(y_{n+1}^{(j-1)}), j = 2(1)m,\\
y_{n+1} &= \alpha(\alpha_0 y_{n+1}^{(m)} + \alpha_1 y_n + \alpha_2 y_{n-1}) + (1-\alpha)y_{n-2}, \ m \geq 2.
\end{aligned}
$$

In (4.1) the formula for the intermediate results $y_{n+1}^{(j)}$ may be interpreted as a particular two-step formula using the previous results $y_{n+1}^{(j-1)}$ and $y_{n+1}^{(j-2)}$. Internal stability is a stability property of this two-step formula. When applied to test-model (2.2) $y_{n+1}^{(j)}$ satisfies the recurrence relation

(4.2)
$$y_{n+1}^{(j)} = (\mu_j + \tilde{\mu}_j z)y_{n+1}^{(j-1)} + (1-\mu_j)y_{n+1}^{(j-2)}.$$

If this homogeneous recursion is stable for all z from the absolute stability interval $[-\beta_p(m),0)$, we may expect internal stability.

Firstly, however, we have to take care of absolute stability. Application of (4.1) to (2.2) yields a scheme of type (2.3), where

(4.3)
$$
\begin{aligned}
&P_0(z) = 1-\mu_0, \ S_0(z) = \mu_0, \ P_1(z) = 1-\mu_1 + \tilde{\delta}_1 z, \ S_1(z) = \mu_1+\tilde{\gamma}_1 z,\\
&P_j(z) = (\mu_j+\tilde{\mu}_j z)P_{j-1}(z) + (1-\mu_j)P_{j-2}(z), \ j = 2(1)m-1,\\
&S_j(z) = (\mu_j+\tilde{\mu}_j z)S_{j-1}(z) + (1-\mu_j)S_{j-2}(z), \ j = 2(1)m-1,\\
&P_m(z) = \alpha_2 + \alpha_0[(\mu_m+\tilde{\mu}_m z)P_{m-1}(z) + (1-\mu_m)P_{m-2}(z)],\\
&S_m(z) = \alpha_1 + \alpha_0[(\mu_m+\tilde{\mu}_m z)S_{m-1}(z) + (1-\mu_m)S_{m-2}(z)].
\end{aligned}
$$

The polynomials S_m and P_m are fixed by our absolute stability requirements. An easy calculation (see (3.1) and (3.13)-(3.14)) shows that

$$S_m(z) = a' + \frac{a''}{T_m(w_0)} T_m(w_0+w_1 z), \quad P_m(z) = b' + \frac{b''}{T_m(w_0)} T_m(w_0+w_1 z), \tag{4.4}$$

where

$$\begin{aligned} &a' = (1-b)(1-p_0)-a, \quad a'' = a+b(1-p_0), \quad w_1 = \frac{(\tfrac{1}{2}-\tfrac{1}{4}p_0)T_m(w_0)}{a\, T_m'(w_0)}, \\ &b' = p_0 - a + b(1-p_0), \quad b'' = a - b(1-p_0), \end{aligned} \tag{4.5}$$

a,b,p_0 and w_0 being the parameters of (3.13)-(3.14). Thus, if (4.3) leads to polynomials (4.4) the absolute stability properties of our special scheme (4.1) are determined by the polynomials A_m and B_m from (3.13)-(3.14). The particular choice of p_0, a and b determines the order of consistency.

Next we shall define the polynomials S_j and P_j for $j < m$. These polynomials govern the internal stability. Let, for $0 \le j \le m-1$,

$$S_j(z) = \frac{a''}{(a''+b'')T_j(w_0)} T_j(w_0+w_1 z), \quad P_j(z) = \frac{b''}{(a''+b'')T_j(w_0)} T_j(w_0+w_1 z). \tag{4.6}$$

Substitution into (4.3) yields

$$\begin{aligned} &\mu_0 = \mu_1 = a''/(a''+b''), \quad \tilde{\gamma}_1 = w_1 a''/(w_0(a''+b'')), \quad \tilde{\delta}_1 = w_1 b''/(w_0(a''+b'')), \\ &\mu_j = 2w_0 T_{j-1}(w_0)/T_j(w_0), \quad \tilde{\mu}_j = 2w_1 T_{j-1}(w_0)/T_j(w_0), \quad j = 2(1)m-1, \end{aligned} \tag{4.7}$$

and (4.4) is obtained if

$$\alpha_0 = a'' + b'', \quad \alpha_1 = a', \quad \alpha_2 = b'. \tag{4.8}$$

Recursion (4.2) is now immediately recognized as a standard 2-step Chebyshev recursion which is stable for all z from the stability interval $[-w_1^{-1}(1+w_0),0)$. Note that all integration parameters of (4.1) have been defined by relations (4.7)-(4.8). Also note that with respect to internal stability the definition of S_j and P_j in (4.6) is not unique.

To save space we omit a discussion of the local truncation error of (4.1). We confine ourselves with the remark that the accuracy of the method is almost independent of m and that the error constants are approximately equal to the error constants of the related three-step formulas from [12]. A complete discussion can be found in the appendix given in [15]. A nice property of (4.1) is that each intermediate formula defining $y_{n+1}^{(j)}$, $j = 2(1)m$, may be interpreted as a first order consistent 2-step formula. This property can be shown by a straightforward Taylor expansion at the point $y_{n+1}^{(j-1)}$. Consequently, apart from the first and the last stage, each application of (4.1) may be interpreted as an integration with m-1 different, and stable 2-step formulas. The stepsizes for these formulas are much smaller than τ. It is expected that this property advantages the accuracy of (4.1), in particular the accuracy of the first order formulas.

5. LINEARIZED RUNGE-KUTTA-CHEBYSHEV FORMULAS

Suppose we are given a semi-discrete parabolic equation (1.1) for which it is not too cumbersome to write down the Jacobian $J(y)$, and for which an $f(y)$-evaluation requires significantly more computational work than a multiplication of $J(y)$ with some vector. For such problems the costs of one integration step with (4.1), performed with a large value of m, can be reduced considerably by replacing $f(y_{n+1}^{(j-1)})$ by the linearization (see also [10,14])

$$(5.1) \qquad f(y_n) + J(y_{n+\eta})(y_{n+1}^{(j-1)} - y_n).$$

Substitution of this expression into (4.1), yields an integration formula using one $f(y)$-evaluation and m-1 matrix-vector multiplications per integration step. In (5.1) the vector $y_{n+\eta}$ is assumed to be a first order approximation at some point $t = t_n + \eta\tau$. Because our formulas (4.1) are of order $p \leq 2$, substitution of (5.1) does not influence the order.

The parameter η has been introduced in order to indicate that we have some freedom in the choice of the evaluation point of J (see also [8,9]). In particular, it shows that when the Jacobian matrix is kept fixed during some finite number of integration steps the order of consistency remains unchanged. The practical relevance of this aspect has still to be investigated. In the next section the linearized method is applied to a non-linear problem where $y_{n+\eta} = y_n$. The results of this experiment are encouraging.

For a derivation of the local truncation error of the linearized method the reader is referred to the appendix given in [15]. It appears that if $\eta = 0$ the linearization hardly changes the error constants of (4.1).

6. A NUMERICAL EXAMPLE

The application of the Runge-Kutta-Chebyshev method (4.1) and its linearization will be illustrated by integrating the rather non-linear partial differential equation (Richtmyer & Morton [7], p. 201)

$$(6.1) \qquad u_t = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right)(u^5),$$

where $u(t,x_1,x_2) = [\frac{4}{5}v(2vt+x_1+x_2)]^{1/4}$ and $v = 1$. We assume Dirichlet boundary conditions on the unit square and $0 \le t \le 1$.

By imposing a uniform grid on $\{(x_1,x_2)\,|\,0 \le x_1,x_2 \le 1\}$, having $(N-1)^2$ interior gridpoints, and by replacing the Laplacian by the standard 5-point difference operator, the initial-boundary value problem is converted into a nonlinear semi-discrete system (1.1) having $(N-1)^2+1$ components (autonomous form). We take N fixed and equal to 20.

For a given stepsize τ the condition of absolute stability is, at each step, $\tau\sigma(J(y)) \le \beta_p(m)$ where σ denotes the spectral radius. In our case $\sigma(J(y(t_n))) \simeq 64(1+t_n)/N^2 = 25600(1+t_n)$. We always integrated with the minimal value of m still satisfying the absolute stability condition, i.e.

$$(6.2) \qquad m_n = \begin{cases} 1 + \text{entier}\,[(25600\,\tau(1+t_n)/5.17)^{1/2}], & p = 1, \\ 1 + \text{entier}\,[(25600\,\tau(1+t_n)/2.36)^{1/2}], & p = 2. \end{cases}$$

Hence m varies with n. For convenience we used $\beta_2(m) = 2.36m^2$. For low values of m the actual $\beta_2(m)$-values are slightly smaller. In practical situations it is of course desirable to have an automatic check on stability (see e.g. [13]).

Altogether 20 integrations have been carried out. For τ = 1/5, 1/10, 1/20, 1/40/, 1/80 and p = 1,2 we applied method (4.1) and its linearization where η = 0. The additional starting vectors y_0, y_1 and y_2 were determined using the exact solution of (6.1). For method (4.1) we tabulated $sd = -{}^{10}\log(\text{max. abs. errors at } t=1)$, m_{max} = the maximal value of m being used, and fev = the total number of f(y)-evaluations. For the linearized method we tabulated sd, m_{max}, ev = the total number of f(y)-evaluations + J(y)-evaluations, and mv = the total number of matrix-vector multiplications.

τ	p = 1			p = 2		
	sd	m_{max}	fev	sd	m_{max}	fev
1/5	1.40	43	121	1.72	63	178
1/10	1.48	31	226	2.11	46	331
1/20	2.72	22	356	3.52	33	525
1/40	3.78	16	537	3.98	24	785
1/80	4.41	12	789	4.66	17	1150

Table 6.1 Results of method (4.1)

	p = 1				p = 2			
	sd	m_{max}	ev	mv	sd	m_{max}	ev	mv
1/5	1.36	43	6	118	1.85	63	6	175
1/10	1.80	31	16	218	2.65	46	16	323
1/20	2.85	22	36	338	3.79	33	36	507
1/40	3.85	16	76	499	4.04	24	76	747
1/80	4.48	12	156	711	4.80	17	156	1072

Table 6.2 Results of the linearized method

From tables 6.1 and 6.2 we can conclude that all integrations have been performed successfully, that is, without numerical instabilities. Further we see that the results of the linearized method are even slightly more accurate than those of method (4.1). It should also be noted that if the results are plotted in an accuracy-efficiency diagram we can conclude that the first order results are somewhat better than the second order ones. This may be due to the property mentioned at the end of section 4. To be able to give a more general, and more reliable indication on the accuracy-efficiency performance of the various schemes it is necessary to perform an extensive numerical comparison. In the near future we intend to carry out such a comparison for our schemes and for the related one-step schemes reported in [5].

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APPENDIX

THE LOCAL TRUNCATION-ERROR OF METHOD (4.1) AND OF THE LINEARIZED METHOD

Associate (4.1) and its linearized version with the operator equations $y_{n+1} = E_n[\tau, y_n, y_{n-1}, y_{n-2}]$ and $y_{n+1} = L_n[\tau, y_n, y_{n-1}, y_{n-2}]$, respectively. Let $E_n^{(j)}$ and $L_n^{(j)}$ denote the operators for the intermediate stages. Let y denote an exact solution vector of (1.1). Using tensor notation, we then find the expansions, for j = 0(1)m,

(a1)
$$E_n^{(j)}[\tau, y(t_n), y(t_{n-1}), y(t_{n-2})] =$$
$$y(t_n) + c_{1j}\tau f + c_{2j}\tau^2 f_j f^j + c_{3j}\tau^3 f_j f_k^j f^k + c_{4j}\tau^3 f_{jk} f^j f^k + O(\tau^4),$$

(a2)
$$L_n^{(j)}[\tau, y(t_n), y(t_{n-1}), y(t_{n-2})] =$$
$$y(t_n) + c_{1j}\tau f + c_{2j}\tau^2 f_j f^j + c_{3j}\tau^3 f_j f_k^j f^k + \bar{c}_{4j}\tau^3 f_{jk} f^j f^k + O(\tau^4),$$

where

(a3)
$$c_{10} = \mu_0 - 1,\ c_{20} = \tfrac{1}{2}(1-\mu_0),\ c_{30} = \bar{c}_{40} = \frac{1}{6}(\mu_0 - 1),$$
$$c_{11} = \tilde{\gamma}_1 + \tilde{\delta}_1 + \mu_1 - 1,\ c_{21} = \tfrac{1}{2}(1-\mu_1) - \tilde{\delta}_1,\ c_{31} = c_{41} = \bar{c}_{41} = \tfrac{1}{2}\tilde{\delta}_1 + \frac{1}{6}(\mu_1 - 1),$$

and where c_{1j}, c_{2j}, c_{3j}, c_{4j} and $\bar{c}_{4j}$ for j ≥ 2 are given by the (weakly stable) recurrence relations

(a4)
$$\begin{aligned}
c_{1j} &= \mu_j c_{1j-1} + (1-\mu_j) c_{1j-2} + \tilde{\mu}_j, \\
c_{2j} &= \mu_j c_{2j-1} + (1-\mu_j) c_{2j-2} + \tilde{\mu}_j c_{1j-1}, \\
c_{3j} &= \mu_j c_{3j-1} + (1-\mu_j) c_{3j-2} + \tilde{\mu}_j c_{2j-1}, \\
c_{4j} &= \mu_j c_{4j-1} + (1-\mu_j) c_{4j-2} + \tfrac{1}{2}\tilde{\mu}_j c_{1j-1}^2, \\
\bar{c}_{4j} &= \mu_j \bar{c}_{4j-1} + (1-\mu_j) \bar{c}_{4j-2} + \eta\tilde{\mu}_j c_{1j-1}.
\end{aligned}$$

It should be observed that the constants c_{1j}, c_{2j} and c_{3j} can be obtained in closed form by expanding the particular formulas (2.3). Because the resulting expressions will be rather lengthy we prefer to use (a3)-(a4). The local truncation errors of E_n and L_n are given by

(a5) $$y(t_{n+1}) - E_n[\tau, y(t_n), y(t_{n-1}), y(t_{n-2})] =$$
$$C_2\tau^2 f_j f^j + C_3\tau^3 f_j f_k^j f^k + C_4\tau^3 f_{jk} f^j f^k + O(\tau^4),$$

(a6) $$y(t_{n+1}) - L_n[\tau, y(t_n), y(t_{n-1}), y(t_{n-2})] =$$
$$C_2\tau^2 f_j f^j + C_3\tau^3 f_j f_k^j f^k + \bar{C}_4\tau^3 f_{jk} f^j f^k + O(\tau^4),$$

where

(a7) $$\begin{aligned} C_2 &= -\frac{3}{2} - \alpha(\alpha_0 c_{2m} + \frac{1}{2}\alpha_2 - 2), \\ C_3 &= \frac{3}{2} - \alpha(\alpha_0 c_{3m} - \frac{1}{6}\alpha_2 + \frac{8}{6}), \\ C_4 &= \frac{3}{2} - \alpha(\alpha_0 c_{4m} - \frac{1}{6}\alpha_2 + \frac{8}{6}), \\ \bar{C}_4 &= \frac{3}{2} - \alpha(\alpha_0 \bar{c}_{4m} - \frac{1}{6}\alpha_2 + \frac{8}{6}). \end{aligned}$$

Note that $\bar{C}_4$ depends on η. It appears that the error constants occurring in (a5)-(a6) are almost independent of m. Consequently, we may expect that the accuracy behaviour of the methods is also almost independent of m. This has been corroborated by numerical experiments. Approximations to the error constants are given below for $\eta = 0$.

	C_2	C_3	C_4	$\bar{C}_4$
p=1	1.26	-0.41	-0.29	-0.21
p=2	0	0.45	0.37	0.41

Observe that these constants are approximately equal to the corresponding ones of the related three-step formulas from [12]. It should also be observed that for $\eta = 0$ the constant $\bar{C}_4$ is close to C_4. The parameter η can be chosen in such a way that even $C_4 = \bar{C}_4$, i.e., that the difference of the errors (a5) and (a6) is $O(\tau^4)$. If η decreases with increasing n, i.e. if

$y_{n+\eta}$ is kept fixed during some finite number of integration steps, then $|\bar{C}_4|$ will grow with n. Thus in this situation, unless J(y) is nearly constant, we have to reckon with a decreasing accuracy.