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MC

AFDELING NUMERIEKE WISKUNDE NW 43/77 NOVEMBER
(DEPARTMENT OF NUMERICAL MATHEMATICS)

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EXPERIMENTS WITH STABILIZED RUNGE-KUTTA METHODS FOR SECOND ORDER DIFFERENTIAL EQUATIONS WITHOUT FIRST DERIVATIVES

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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).

AMS(MOS) subject classification scheme (1970): 75L05,M10,M20

Experiments with stabilized Runge-Kutta methods for second order differential equations without first derivatives.

by

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ABSTRACT

In this report, stabilized first, second and third order Runge-Kutta formulas for second order differential equations are tested. These methods are compared with stabilized Runge-Kutta methods for first order differential equations. The tested formulas need low storage, which makes them, together with the large stability interval, suitable for the integration of hyperbolic partial differential equations.

KEYWORDS & PHRASES: *Runge-Kutta formulas, second order differential equations, hyperbolic equations, extended stability region.*

CONTENTS

1. INTRODUCTION.

In order to solve the initial value problem

$$(1.1) \qquad \vec{y}'' = \vec{f}(x,\vec{y}), \quad \vec{y}(x_0) = \vec{y}_0, \quad \vec{y}'(x_0) = \vec{y}'_0$$

one may use a Runge-Kutta method. Through the years a lot of Runge-Kutta formulas have been presented. In this report we concentrate on the stability of such methods. In section 2, first and second order formulas are given with optimal stability intervals. In section 3 we shall derive third order methods (in this connection we observe that the Runge-Kutta scheme by van der Houwen [1975] is only quasi third order, i.e. $\vec{y}$ is third order exact, but $\vec{y}'$ in only a second order approximation).

Finally, the results obtained are listed in section 4. All computations have been carried out on the Control Data CYBER 73-28 of the Stichting Academisch Rekencentrum Amsterdam (SARA).

2. STABILIZED FIRST AND SECOND ORDER RUNGE-KUTTA METHODS.

In this section we briefly give a stability analysis of Runge-Kutta methods for second order differential equations. For further details we refer to van der Houwen [1975,1977].

2.1. An m-point Runge-Kutta formula.

The m-point Runge-Kutta formula for the numerical solution of the initial value problem (1.1) reads as follows

$$(2.1) \qquad \begin{aligned} \vec{y}^{(0)}_{n+1} &= \vec{y}_n, \\ \vec{y}^{(j)}_{n+1} &= \vec{y}_n + \mu_j h_n \vec{y}'_n + \sum_{\ell=0}^{j-1} \lambda_{j\ell}\, h_n^2\, \vec{f}(x_n+\mu_\ell h_n, \vec{y}^{(\ell)}_{n+1}), \qquad j = 1(1)m, \\ \vec{y}'_{n+1} &= \vec{y}'_n + \sum_{\ell=0}^{m-1} \beta_\ell\, h_n\, \vec{f}(x_n+\mu_\ell h_n, \vec{y}^{(\ell)}_{n+1}), \\ \vec{y}_{n+1} &= \vec{y}^{(m)}_{n+1}\,. \end{aligned}$$

In this scheme, $\vec{y}_n$ and $\vec{y}'_n$ are numerical approximations to $\vec{y}(x_n)$ and $\vec{y}'(x_n)$ and $h_n = x_{n+1}-x_n$. In order to be p-th order exact, the Runge-Kutta parameters, i.e. $\mu_{\ell+1},\beta_\ell$, $\ell = 0,\dots,m-1$ and λ_{ij}, $i = 1,\dots,m$, $j = 0,\dots,i-1$, will have to fulfil several consistency conditions. According to Hairer and Wanner [1976], the consistency conditions for scheme (2.1), up to and including order three, are as listed in Table 2.1.

Table 2.1. Consistency conditions for scheme (2.1).

Order	Y	Y'
1	$\mu_m = 1$	$\sum_{i=0}^{m-1} \beta_i = 1$
2	$2\sum_{i=0}^{m-1} \lambda_{mi} = 1$	$2\sum_{i=0}^{m-1} \beta_i\mu_i = 1$
3	$6\sum_{i=0}^{m-1} \lambda_{mi}\mu_i = 1$	$3\sum_{i=0}^{m-1} \beta_i\mu_i^2 = 1$
		$6\sum_{i=0}^{m-1} \beta_i \sum_{j=0}^{i-1} \lambda_{ij} = 1$

It is clear that a third order method not only has to satisfy the p = 3 conditions, but also the conditions for p = 1 and p = 2.

2.2. Stability.

To derive the stability conditions of an m-point formula, we have to apply (2.1) to the test equation

$$\vec{y}'' = J\vec{y}, \quad J \text{ a matrix.}$$

The result, in "matrix-vector" notation is

$$\begin{pmatrix} \vec{y}_{n+1} \\ h\,\vec{y}'_{n+1} \end{pmatrix} = R_m(z) \begin{pmatrix} \vec{y}_n \\ h\,\vec{y}'_n \end{pmatrix}$$

in which $R_m(z)$ denotes the following matrix

$$(2.2)\quad R_m(z) = \begin{pmatrix} 1 + \sum_{\ell=0}^{m-1} \lambda_{m\ell}\, z\, R_{11}^{(\ell)}(z) & 1 + \sum_{\ell=0}^{m-1} \lambda_{m\ell}\, z\, R_{12}^{(\ell)}(z) \\ \sum_{\ell=0}^{m-1} \beta_\ell\, z\, R_{11}^{(\ell)}(z) & 1 + \sum_{\ell=0}^{m-1} \beta_\ell\, z\, R_{12}^{(\ell)}(z) \end{pmatrix},$$

where $R_{11}^{(\ell)}$ and $R_{12}^{(\ell)}$ are defined by

$$R_{11}^{(\ell)} = 1 + \sum_{j=0}^{\ell-1} \lambda_{\ell_j}\, z\, R_{11}^{(j)},$$

$$R_{12}^{(\ell)} = \mu_\ell + \sum_{j=0}^{\ell-1} \lambda_{\ell_j}\, z\, R_{12}^{(j)}, \qquad R_{11}^{(0)} = 1, \quad R_{12}^{(0)} = 0.$$

The matrix R_m is a function of $z = h_n^2\delta$, where h_n equals the stepsize and δ runs through the eigenvalue spectrum of J.

The stability region of formula (2.1) is defined by

$$\{z / |\alpha_j(z)| \le 1,\ j = 1,2\}$$

where $\alpha_j(z)$ are the eigenvalues of $R_m(z)$, $j = 1,2$. The formulas given in this report have optimized negative intervals of strong stability, i.e. $|\alpha_j(z)| < 1$, $j = 1,2$ when z lies in the stability interval.

The formulas discussed in this report turn out to be stable in a part of the complex plane too, as can be seen in the figures (4.1) through (4.5).

2.3. The formulas.

To be complete, we give some of the formulas, derived in van der Houwen [1975,77]. In these formulas there is still one free parameter ε left, which has to be chosen in the interval [0,1]. This parameter governs the damping of perturbations of $\vec{y}_n$ and $\vec{y}'_n$ (e.g. caused by rounding errors); for $\varepsilon = 0$ the formulas are weakly stable, which means that the maximum of the absolute values of the eigenvalues of (2.2) equals one.

We mention a first order formula and two second order formulas.

The first order formula is specified by

$$\mu_1 = \frac{1}{2}, \ \mu_2 = 1, \ \beta_1 = 1 \quad \text{and} \quad \lambda_{21} = \frac{4-\varepsilon}{8-6\varepsilon}, \ m = 2. \tag{2.3}$$

The other parameters equal zero. Since $\lambda_{10} = 0$ the first function evaluation is saved. Here the negative stability interval $[-\beta,0]$ is given by

$$[-(4-3\varepsilon),0].$$

The integration formulas in the second order case are defined as follows: Firstly, the two-point formula

$$\begin{aligned} &\mu_1 = \frac{1}{2}\frac{\beta-3\varepsilon}{\beta-\varepsilon}, \quad \mu_2 = \frac{1}{2}, \quad \mu_3 = 1, \\ &\lambda_{21} = \frac{\beta-\varepsilon}{\beta^2}, \quad \lambda_{32} = \frac{1}{2}, \quad \beta_2 = 1. \end{aligned} \tag{2.4}$$

Again the Runge-Kutta parameters not mentioned are equal to zero. In this case the following equation for β holds

$$\beta = 8(1 + \sqrt{1-\varepsilon}).$$

Secondly, the three-point formula

$$\begin{aligned} &\mu_1 = \frac{\sigma_3+\pi_3}{2(\sigma_3-\pi_3)}, \quad \mu_2 = \frac{\sigma_2+\pi_2}{2(\sigma_2-\pi_2)}, \quad \mu_3 = \frac{1}{2}, \quad \mu_4 = 1, \\ &\lambda_{21} = \frac{\sigma_3-\pi_3}{\sigma_2-\pi_2}, \quad \lambda_{32} = \sigma_2-\pi_2, \quad \lambda_{43} = \frac{1}{2}, \quad \beta_3 = 1, \end{aligned} \tag{2.5}$$

where

$$\sigma_2 = -\frac{2}{\gamma^2}\left(6 - \gamma - 3\varepsilon\frac{\gamma^2}{\beta^2}\right), \quad \sigma_3 = -\frac{1}{\gamma^3}\left(8 - \gamma - 4\varepsilon\frac{\gamma^3}{\beta^3}\right),$$

$$\pi_2 = -\frac{3\varepsilon}{\beta^2}, \quad \pi_3 = -\frac{2\varepsilon}{\beta^3}, \quad \gamma = 9 + \frac{9}{32}\varepsilon.$$

For β the approximate expression

$$\beta = 36-9\varepsilon$$

holds.

Note, that in these three cases, β is very close to $4q^2$, where q equals the number of function evaluations per step.

3. STABILIZED THIRD ORDER RUNGE-KUTTA METHODS.

In order to save storage we choose some Runge-Kutta parameters equal to zero

$$
\begin{aligned}
&\lambda_{10} = 0,\\
&\lambda_{j\ell} = 0, \quad j = 2,\ldots,m-1, \quad \ell = 0,\ldots,j-2,\\
(3.1)\qquad &\beta_\ell = \lambda_{m\ell} = 0, \quad \ell \neq 1,\ m-1.
\end{aligned}
$$

Substitution of (3.1) into Table 2.1 yields

$$
\begin{aligned}
&\mu_m = 1,\\
&\beta_1 + \beta_{m-1} = 1,\\
&\lambda_{m1} + \lambda_{mm-1} = \frac{1}{2},\\
(3.2)\qquad &\beta_1\mu_1 + \beta_{m-1}\mu_{m-1} = \frac{1}{2},\\
&\lambda_{m1}\mu_1 + \lambda_{mm-1}\mu_{m-1} = \frac{1}{6},\\
&\beta_1\mu_1^2 + \beta_{m-1}\mu_{m-1}^2 = \frac{1}{3},\\
&\beta_{m-1}\lambda_{m-1m-2} = \frac{1}{6}.
\end{aligned}
$$

From (3.2) it appears that we have seven equations and eight Runge-Kutta parameters. So, we have still one free parameter left and use it to optimize the stability interval. If we express these parameters in terms of μ_1 we find

$$\mu_{m-1} = \frac{3\mu_1-2}{6\mu_1-3},$$

(3.3)
$$\lambda_{m1} = \frac{3\mu_{m-1}-1}{6(\mu_{m-1}-\mu_1)}, \qquad \lambda_{mm-1} = \frac{3\mu_1-1}{6(\mu_1-\mu_{m-1})},$$
$$\beta_1 = \frac{2\mu_{m-1}-1}{2(\mu_{m-1}-\mu_1)}, \qquad \beta_{m-1} = \frac{2\mu_1-1}{2(\mu_1-\mu_{m-1})},$$
$$\lambda_{m-1m-2} = \frac{\mu_1-\mu_{m-1}}{6\mu_1-3}.$$

In order to formulate the stability conditions, we have to calculate the eigenvalues of (2.2). These eigenvalues satisfy the equation

(3.4)
$$\alpha^2 - S(z)\alpha + P(z) = 0,$$

where S(z) equals the trace and P(z) the determinant of (2.2). If we substitute the consistency conditions in (2.2) we find

$$S(z) = 2+z+\sigma_2 z^2+ \ldots + \sigma_{m-1} z^{m-1},$$
$$P)z) = 1+\pi_2 z^2+ \ldots + \pi_{m-1} z^{m-1},$$

where

(3.5)
$$\sigma_2 = \lambda_{mm-1}\lambda_{m-1m-2} + \frac{1}{6}\mu_{m-2},$$
$$\sigma_j = (\lambda_{mm-1}\lambda_{m-1m-2} + \frac{1}{6}\mu_{m-j}) \prod_{\ell=m-j+1}^{m-2} \lambda_{\ell\ell-1}, \qquad j = 3,\ldots,m-1,$$
$$\pi_2 = \sigma_2 - \frac{1}{12},$$
$$\pi_j = \sigma_j - \left\{\frac{1}{6} - \frac{c(\mu_{m-j+1}-\mu_1)\lambda_{m-1m-2}}{\lambda_{m-j+1m-j}}\right\} \prod_{\ell=m-j+1}^{m-2} \lambda_{\ell\ell-1}, \qquad j = 3,\ldots,m-1,$$
$$c = \lambda_{m1}\beta_{m-1} - \lambda_{mm-1}\beta_1 = \frac{1}{12(\mu_{m-1}-\mu_1)}.$$

The Hurwitz criterion tells us, that the roots of (3.4) are within or on the unit circle, when the coefficients of S(z) and P(z) are real and satisfy

(3.6)
$$P(z) \le 1, \quad |S(z)| \le P(z) + 1.$$

From

$$S^2(z) - 4P(z) \le 0$$

it follows that $|S(z)| \le P(z) + 1$.
Thus, by requiring

(3.6') $$P(z) < 1 \quad \text{and} \quad S^2(z) - 4P \le 0$$

we have a more restrictive criterion than (3.6), but (3.6') assures us (since $S^2(z) - 4P(z)$ equals the determinant of (3.4)) that both roots of (3.4) are within the unit circle.

This guarantee is also given by the criterion used by van der Houwen, i.e.

(3.7) $$P(z) < 1, \; z < 0, \; \frac{1}{2}\,|S(z)| \le P(z).$$

From (3.6') and (3.7) we obtain an interval of negative z-values for which the Runge-Kutta formula is strongly stable. When P(z) is close to unity this interval is only slightly smaller than the weak stability interval. If all coefficients $\sigma_2,\ldots,\sigma_{m-1}$, $\pi_3,\ldots,\pi_{m-1}$ are determined, we have to express the Runge-Kutta parameters in terms of these coefficients. For that purpose we rewrite (3.5) in the form

(3.8)
$$\sigma_2 = \lambda_{mm-1}\lambda_{m-1m-2} + \frac{1}{6}\,\mu_{m-2},$$

$$\sigma_{m-k+1} = (\lambda_{mm-1}\lambda_{m-1m-2} + \frac{1}{6}\,\mu_{k-1})Q_k, \qquad k = 2,\ldots,m-2,$$

$$\pi_2 = \sigma_2 - \frac{1}{12},$$

$$\pi_3 = \sigma_3 - \left\{\frac{1}{6}\,\lambda_{m-2m-3} - c(\mu_{m-2}-\mu_1)\lambda_{m-1m-2}\right\},$$

$$\pi_{m-k+2} = \sigma_{m-k+2} - \left\{\frac{1}{6}\,Q_{k-1} - c(\mu_{k-1}-\mu_1)\lambda_{m-1m-2}\,Q_k\right\}, \quad k = 3,\ldots,m-2,$$

$$c = \frac{1}{12(\mu_{m-1}-\mu_1)},$$

where $$Q_k = \prod_{j=k}^{m-2} \lambda_{jj-1}.$$

Since λ_{mm-1} and λ_{m-1m-2} are already known as functions of μ_1 (see (3.3)), we may calculate μ_{m-2} as function of μ_1 from the first equation of (3.8). If we substitute the expression of μ_{m-2} in the fourth equation of (3.8), we find λ_{m-2m-3} in terms of μ_1. Note, that $Q_{m-2} = \lambda_{m-2m-3}$.

In general, we see from the second equation of (3.8) that

$$\mu_{k-1} = 6\,\frac{\sigma_{m-k+1} - \lambda_{mm-1}\lambda_{m-1m-2}Q_k}{Q_k} \tag{3.9}$$

and from the fifth equation of (3.8) that

$$Q_{k-1} = 6\left\{\sigma_{m-k+2} - \pi_{m-k+2} + c(\mu_{k-1}-\mu_1)\,\lambda_{m-1m-2}Q_k\right\}. \tag{3.10}$$

Substitution of (3.9) into (3.10) yields

$$Q_{k-1} = 6\left[\sigma_{m-k+2} - \pi_{m-k+2} + c\left\{6(\sigma_{m-k+1} - \lambda_{mm-1}\lambda_{m-1m-2}Q_k) - \mu_1 Q_k\right\}\lambda_{m-1m-2}\right]. \tag{3.11}$$

Since Q_{m-2} is known in terms of μ_1 we find from (3.11) $Q_{m-3},\ldots,Q_2$ as functions of μ_1. At last μ_1 is calculated by means of (3.9)

$$\mu_1 = 6\left(\frac{\sigma_{m-1}}{Q_2} - \lambda_{mm-1}\lambda_{m-1m-2}\right). \tag{3.12}$$

Equation (3.12) is a polynomial in μ_1, of which the coefficients are functions of σ_2, σ_j and π_j, $j = 3,\ldots,m-1$. It is clear that calculating μ_1 means calculating the zeroes of a polynomial. An additional problem is that μ_1 has to be real. If μ_1 is determined we are able to calculate all Runge-Kutta parameters by (3.3) and by considering that

$$\lambda_{kk-1} = \frac{Q_k}{Q_{k+1}}, \qquad k = 2,\ldots,m-2.$$

3.1. A two point Runge-Kutta formula

For m = 3 we have, according to (3.5),

$$S(z) = 2 + z + \sigma_2 z^2,$$

$$P(z) = 1 + (\sigma_2 - \frac{1}{12})\,z^2,$$

where $$\sigma_2 = \lambda_{32}\lambda_{21} + \frac{1}{6}\mu_1 .$$

From the last equation follows

$$(3.12') \qquad \mu_1^2 - 6\sigma_2\mu_1 + 3\sigma_2 - \frac{1}{6} = 0.$$

Since we have the extra condition that μ_1 has to be real, we may immediately conclude that

$$(3.13) \qquad \sigma_2 \leq \frac{3-\sqrt{3}}{18} \quad \text{or} \quad \sigma_2 \geq \frac{3+\sqrt{3}}{18} .$$

In this case we apply (3.6'). From the first equation of (3.6'), it immediately follows that

$$\sigma_2 < \frac{1}{12} ,$$

and this results, together with (3.13) in

$$(3.14) \qquad \sigma_2 \leq \frac{3-\sqrt{3}}{18} .$$

The second equation of (3.6') leads to

$$4 + \frac{4}{3} z + 2\sigma_2 z^2 + \sigma_2^2 z^3 \geq 0.$$

Consider

$$F(z) = z^3 + \frac{2}{\sigma_2} z^2 + \frac{4}{3\sigma_2^2} z + \frac{4}{\sigma_2^2} .$$

From Abramowitz and Stegun [1964] we learn that this polynomial has one real root z_0 and two complex conjugate roots. A calculation yields

$$(3.15) \qquad z_0 = \frac{2}{3\sigma_2} \left(\sqrt[3]{1 - \frac{27}{2}\sigma_2} - 1 \right) .$$

A simple investigation delivers that z_0 is minimized, on condition (3.14), by

$$(3.14') \qquad \sigma_2 = \frac{3-\sqrt{3}}{18} ,$$

which gives rise to

$$z_0 \simeq -6.$$

The Runge-Kutta formula is defined by

$$\mu_1 = \frac{3-\sqrt{3}}{6}, \quad \mu_2 = \frac{3+\sqrt{3}}{6}, \quad \mu_3 = 1,$$

$$(3.16) \qquad \lambda_{21} = \frac{1}{3}, \quad \lambda_{31} = \frac{3+\sqrt{3}}{12}, \quad \lambda_{32} = \frac{3-\sqrt{3}}{12},$$

$$\beta_1 = \beta_2 = \frac{1}{2}.$$

The stability interval $[-\beta,0]$ is given by

$$[-6,0].$$

Finally, the parameter ε is determined by the relation

$$P(-\beta) = 1-\varepsilon,$$

which yields

$$\varepsilon \simeq .4641.$$

3.2. A three-point Runge-Kutta formula

In this case, the following equations for $S(z)$ and $P(z)$ hold

$$S(z) = 2 + z + \sigma_2 z^2 + \sigma_3 z^3,$$

$$P(z) = 1 + (\sigma_2 - \frac{1}{12})z^2 + \pi_3 z^3,$$

where, according to (3.5),

$$\sigma_2 = \lambda_{43}\lambda_{32} + \frac{1}{6}\mu_2,$$

$$\sigma_3 = (\lambda_{43}\lambda_{32} + \frac{1}{6}\mu_1)\lambda_{21},$$

$$\pi_3 = \sigma_3 - \frac{1}{6}\lambda_{21} + \frac{(\mu_2-\mu_1)\lambda_{32}}{12(\mu_3-\mu_1)} .$$

For the polynomial P(z) we choose

(3.17) $$P(z) = 1 - \frac{3\varepsilon}{\beta^2} z^2 - \frac{2\varepsilon}{\beta^3} z^3, \qquad 0 \le \varepsilon \le 1.$$

This leads immediately to

(3.18) $$\sigma_2 = \frac{-3\varepsilon}{\beta^2} + \frac{1}{12} .$$

From (3.17) it follows that

$$P(-\beta) = 1-\varepsilon.$$

Applying (3.7) leads to

(3.19) $$-P(z) \le S_1(z) + S_2(z) \le P(z),$$

where

$$S_1(z) = \frac{1}{2} S(z) - \frac{1}{2}\sigma_3 z^3,$$

$$S_2(z) = \frac{1}{2}\sigma_3 z^3.$$

Since z runs through the negative axis, (3.19) delivers

(3.20) $$z^{-3}(P(z)-S_1(z)) \le \frac{1}{2}\sigma_3 \le -z^{-3}(P(z)+S_1(z)).$$

Let $\ell(z)$ and r(z) denote the left and right hand side of (3.20). An investigation reveals that the behaviour of $\ell(z)$ and r(z) is for $\varepsilon \neq 0$, as illustrated in figure 3.1.

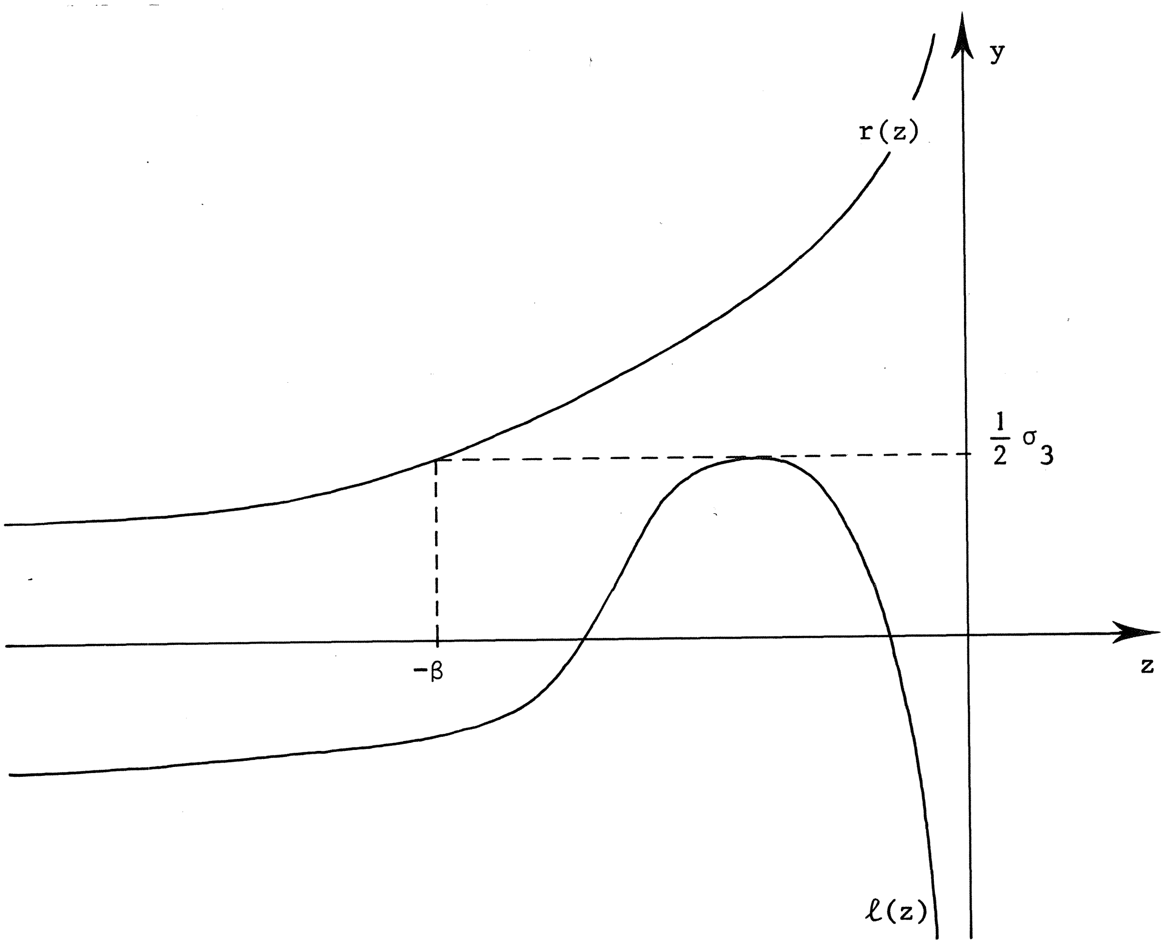

fig. 3.1 The behaviour of $\ell(z)$ and $r(z)$ for $\varepsilon \neq 0$.

For $\varepsilon = 0$ holds

$$\lim_{z\to-\infty} \ell(z) = \lim_{z\to-\infty} r(z) = 0.$$

In van der Houwen [1970] it is proved, that the best choice for $y = \frac{1}{2}\sigma_3$ is the line which touches $y = \ell(z)$. Thus, if we calculate the maximum of $\ell(z)$, we find the optimal value for σ_3.

A calculation reveals that for

$$z = \frac{-24\beta^2}{36\varepsilon+\beta^2}$$

the function $\ell(z)$ assumes its maximal value ℓ_{max}, for which holds

(3.21) $$\ell_{max} = \frac{1}{2}\sigma_3 = \frac{1}{2}\left(\frac{36\varepsilon+\beta^2}{24\beta^2}\right)^2 - \frac{2\varepsilon}{\beta^3} .$$

From $r(-\beta) = \ell_{max}$ it follows that

(3.22) $$\beta^4 - 48\beta^3 + (72\varepsilon+576)\beta^2 + (576\varepsilon-2304)\beta + 1296\varepsilon^2 = 0,$$

which, for $\varepsilon = 0$, reduces to

(3.22') $$\beta^3 - 48\beta^2 + 576\beta - 2304 = 0.$$

The real zero β_o of (3.22') is given by

$$\beta_o = 4(\sqrt[3]{4} + 2\sqrt[3]{2}) + 16 \approx 32{,}428972607031.$$

Neglecting all terms of order ε^2 and substituting $\beta = \beta_o - c\varepsilon$, into (3.22), we find

$$c = \frac{24(\beta_o+8)}{(\beta_o-8)(\beta_o-24)} \cong 4.7122041975066.$$

Summarizing, for small ε holds

(3.22") $$\beta \cong \beta_o - 4.71\varepsilon.$$

Substituting the preset values of σ_2 and π_3 and the expression for σ_3 (i.e. (3.21)) in (3.11), the polynomial in μ_1 which is obtained by (3.12), is

(3.23) $$\{2592(\pi_3-\sigma_3)-36\}\mu_1^4+\{2592(2\sigma_3-\pi_3)+216\sigma_2\}\mu_1^3+\{216(\pi_3-19\sigma_3)-108\sigma_2+12\}\mu_1^2$$
$$+\{432(\pi_3+3\tfrac{1}{2}\sigma_3)-36\sigma_2\}\mu_1-108(\pi_3+2\sigma_3)+18\sigma_2-1 = 0 .$$

For $\varepsilon = 0$, (3.23) reduces to

$$(3.23') \qquad 324\mu_1^4 - 216\mu_1^3 + 33\mu_1^2 + 3\mu_1 - 1 = 0\,.$$

Of the two real roots of (3.23'), we have chosen

$$(3.24) \qquad \mu_1^* = .40543044569291\,.$$

If we rewrite (3.23) to

$$(3.23'') \qquad F(\mu_1;\varepsilon) \equiv \sum_{i=0}^{4} a_i(\varepsilon)\mu_1^i = 0$$

and substitute $a_i(\varepsilon)$ by its Taylorseries

$$a_i(0) + \varepsilon.\ a_i'(0), \qquad i = 0,\ldots,4,$$

we may replace (3.23') by

$$\sum_{i=0}^{4} a_i(0)\mu_1^i + \varepsilon \sum_{i=0}^{4} a_i'(0)\mu_1^i = 0$$

or

$$F(\mu_1;0) + \varepsilon\, G(\mu_1;0) = 0$$

According to Stoer [1972] the root $\mu_1(\varepsilon)$ of the last equation, is a perturbation of (3.24)

$$(3.24') \qquad \mu_1(\varepsilon) = \mu_1^* - \varepsilon \frac{G(\mu_1^*;0)}{F'(\mu_1^*;0)}\,.$$

A tedious calculation reveals that for small ε

$$(3.25) \qquad \mu_1(\varepsilon) = \mu_1^* - 1.12_{10}{-4}\varepsilon.$$

is a root of (3.23).

Using for μ_1 formula (3.25), we may calculate all the other Runge-Kutta parameters as indicated before and obtain thereby a three-point third order method.

4. NUMERICAL EXPERIMENTS.

To start off, we investigate the stability regions of the five methods. By discretiscing the second quadrant of the complex plane, we obtain a set of complex numbers and for each of these numbers, the functions S(z) and P(z) are evaluated. Finally we calculate the roots of (3.4) and make a distinction between three cases. If the maximum of the absolute values of the roots

a) is bigger than one, we print a space on the spot of z in the complex plane,
b) equals one, we print a W (weakly stable),
c) is smaller than one, we print an S (strongly stable).

The stability regions presented in figures 4.1 through 4.5 have been calculated for $\varepsilon = .1$, except in the two point third order case because in that case ε has a preset value. From figure 4.4 it appears that (3.16) is also stable for z-values smaller than -6. This is explained by observing that (3.6') is a sufficient condition but not a necessary one to obtain strong stability.

The testing of the integration schemes is done by solving four dependent problems and by comparing the results of the procedure STARK in which the five schemes discussed in this report are united, with the results of the procedure ARK (see BEENTJES [1972]), which contains stabilized Runge-Kutta formulas for first order differential equations upto and including order three. In order to test STARK we put $\varepsilon = .1$.

The right hand side of the problems contains differential operators with respect to the space variable x. If we semi-discretise with respect to x, we obtain a system of ordinary differential equations. In the four problems we replace the x-interval by 25 grid points. By doing this, the differential operators with respect to the space variable reduce to central differences defined at these grid poitns. By means of a higher order Runge-Kutta method we computed a reference solution.

The spectral radius of the Jacobian matrix is calculated by Gerschgorin's theorem in the linear cases and in the non-linear cases we use a safe upperbound. For each problem we calculate the total number of function evaluations needed to reach the endpoint of the integration interval and the number of correct digits of the least accurate component of the solution at the endpoint.

Problem 1.

Initial boundary value problem (see ANDRADE & McKEE [1977]).

$$\frac{\partial^2 u}{\partial x^2} = -\left(\frac{1}{x} + \frac{1}{120} x^4\right) \frac{\partial^4 u}{\partial x^4}, \quad \frac{1}{2} \le x \le 1, \quad t \ge 0. \tag{4.1}$$

The initial conditions are

$$u(x,0) = 0 \quad \text{and} \quad \frac{\partial u}{\partial t}(x,0) = 1 + \frac{1}{120} x^5.$$

The boundary conditions

$$u(\tfrac{1}{2}, t) = (1 + \frac{1}{120} . 2^{-5}) \sin t, \quad u(1,t) = (1 + \frac{1}{120}) \sin t,$$

$$\frac{\partial^2 u}{\partial x^2}(\tfrac{1}{2}, t) = \frac{1}{48} \sin t \quad \text{and} \quad \frac{\partial^2 u}{\partial x^2}(1,t) = \frac{1}{6} \sin t.$$

The theoretical solution of (4.1) is

$$u(x.t) = (1 + \frac{1}{120} x^5) \sin t$$

The endpoint of integrating is te = 0.01.

Problem 2.

Initial boundary value problem (see VAN DER HOUWEN [1977]).

$$\frac{\partial^2 u}{\partial t^2} = g\, h(x) \frac{\partial^2 u}{\partial x^2} + \frac{1}{4} \lambda u + \exp(\tfrac{1}{2} \lambda t)\, \omega(x), \quad 0 \le x \le 10^5, \quad t \ge 0.$$

The initial conditions are

$$u(x,0) = \frac{\partial u}{\partial t}(x,0) = 0.$$

The boundary conditions

$$\frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(10^5,x) = 0.$$

The constants used in this problem are

$$g = 9.81, \qquad \lambda = 25_{10}{-6}.$$

The functions h(x) and w(x) represent

$$h(x) = 10\{2+\cos(2_{10}{-5}\ \pi x) \quad \text{and} \quad w(x) = {}_{10}{-3}\ \sin({}_{10}{-5}\ \pi x).$$

The endpoint of the integrating is te = 3600.

Problem 3.

Initial boundary value problem

$$\frac{\partial^2 u}{\partial t^2} = u^2\left(\frac{\partial^2 u}{\partial x^2} + t^2 \ \sin(xt)\right) - x^2 \ \sin(xt), \qquad 0 \le x \le 1, \quad t \ge 0.$$

The initial conditions are

$$u(x,0) = x(1-x) \quad \text{and} \quad \frac{\partial u}{\partial t}(x,0) = x.$$

The boundary conditions

$$u(0,t) = 0 \quad \text{and} \quad u(1,t) = \sin t.$$

The endpoint of integrating is te = 1.

Problem 4.

Initial boundary value problem

$$(4.2) \qquad \rho_h \frac{\partial^2 u}{\partial t^2} + c\,\frac{\partial u}{\partial t} = -E\,\frac{\partial^4 u}{\partial x^4} + T\,\frac{\partial^2 u}{\partial x^2} + f(u), \qquad 0 \le x \le 200, \quad t \ge 0.$$

The initial conditions for (5.2) with c = 0, are calculated by solving (5.2) with c = 2.7 and $a_1 = 0$ until $\frac{\partial u}{\partial t} = 0$.

The boundary conditions

$$u(0,t) = 0, \qquad u(200,t) = a_0 + a_1 \sin(\omega t),$$

$$\frac{\partial^2 u}{\partial x^2}(0,t) = 0 \quad \text{and} \quad \frac{\partial^2 u}{\partial x^2}(200,t) = 0,$$

where

$$a_0 = 15, \qquad a_1 = 1 \quad \text{and} \quad \omega = \frac{\pi}{6} .$$

The constants and functions which appear in (4.2) are

$$\rho_h = 50, \qquad E = 1.39\;10^{6}, \qquad T = 10^{5},$$

$$f(u) = \begin{cases} -50\,u & , \quad \text{if } u < 0 \\ 375\,u^2 - 750\,u & , \quad \text{if } 0 \le u \le 1 \\ -375 & , \quad \text{else} \end{cases}$$

The endpoint of integrating is te = 12.

In the following tables fe denotes the number of function evaluations and sd represents the number of correct digits of the least accurate component.

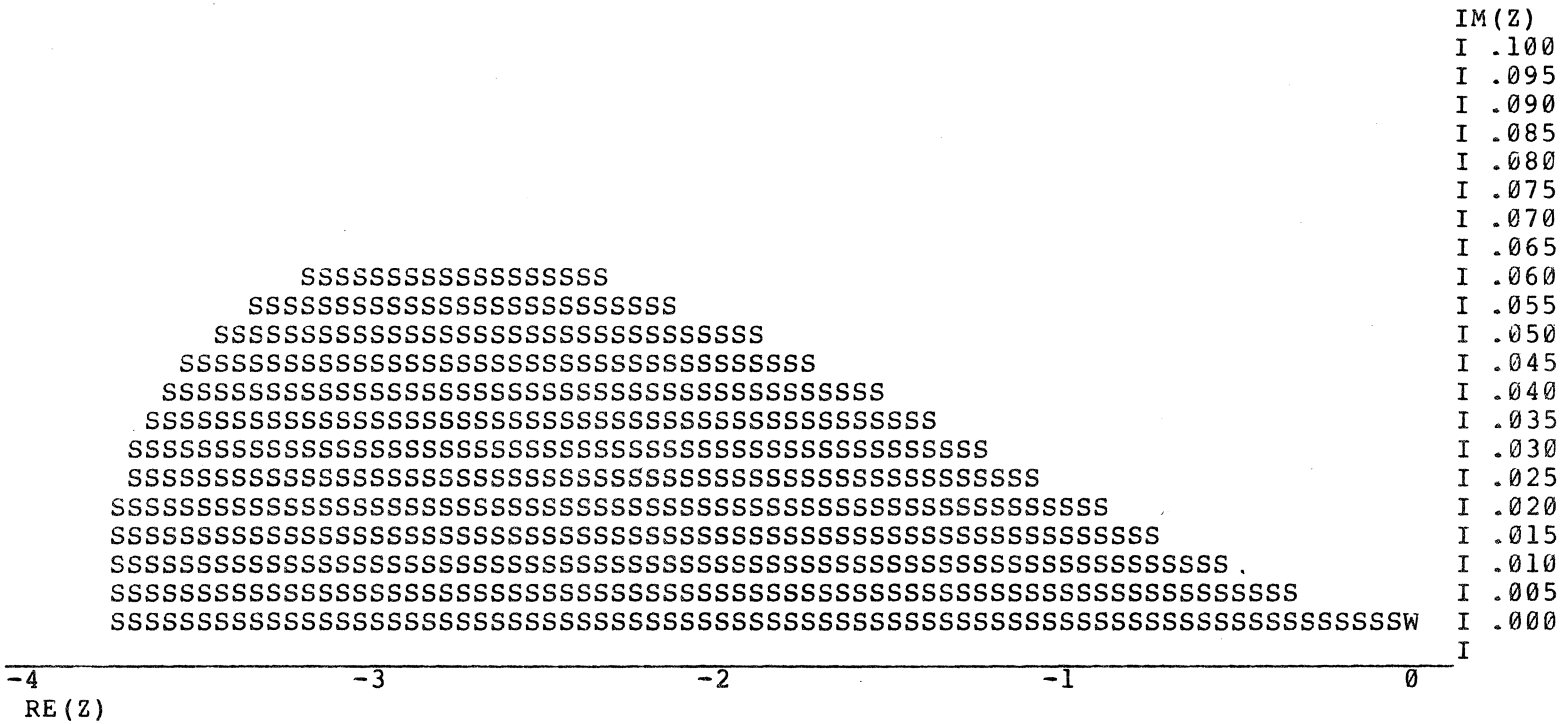

FIG. 4.1. THE STABILITY-REGION OF SCHEME (2.3) .

```
                                                                                    IM(Z)
                                                                                    I .500
                                                                                    I .475
                                         S                                          I .450
                                         S                                          I .425
                                         S                                          I .400
                                         S                                          I .375
                                         S                                          I .350
                                         S                                          I .325
                                         S                                          I .300
                                         S                                          I .275
                                         S                                          I .250
                                         S                                          I .225
                                         SS                                         I .200
                                         SS                                         I .175
                                         SS                                         I .150
                                        SSS                                         I .125
           SSSSSSSSSSSS                SSSS                                         I .100
      SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                                        I .075
    SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                                      I .050
   SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                              I .025
   SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSW  I .000
                                                                                    I
------------------------------------------------------------------------------------
-16                 -12                 -8                  -4                   0
 RE(Z)
```

FIG. 4.2. THE STABILITY-REGION OF SCHEME (2.4) .

```
                                                                          IM(Z)
                                                                          I .600
                                                                          I .575
                                                                          I .550
                 SSS                                                      I .525
               SSSSSSSS                                                   I .500
              SSSSSSSSSSS                                                 I .475
             SSSSSSSSSSSSS                                                I .450
            SSSSSSSSSSSSSSSS                                              I .425
            SSSSSSSSSSSSSSSSS                                             I .400
           SSSSSSSSSSSSSSSSSSSS                                           I .375
           SSSSSSSSSSSSSSSSSSSSS                                          I .350
           SSSSSSSSSSSSSSSSSSSSSS                                         I .325
          SSSSSSSSSSSSSSSSSSSSSSSSS                                       I .300
          SSSSSSSSSSSSSSSSSSSSSSSSSS                                      I .275
          SSSSSSSSSSSSSSSSSSSSSSSSSSSS                                    I .250
          SSSSSSSSSSSSSSSSSSSSSSSSSSSSS                                   I .225
          SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                                 I .200
          SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                               I .175
         SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                              I .150
         SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                            I .125
         SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                         I .100
         SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                       I .075
         SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                    I .050
         SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS                I .025
         SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSW  I .000
                                                                          I
--------------------------------------------------------------------------
-7        -6        -5        -4        -3        -2        -1         0
 RE(Z)
```

FIG. 4.4. THE STABILITY-REGION OF SCHEME (3.16) .

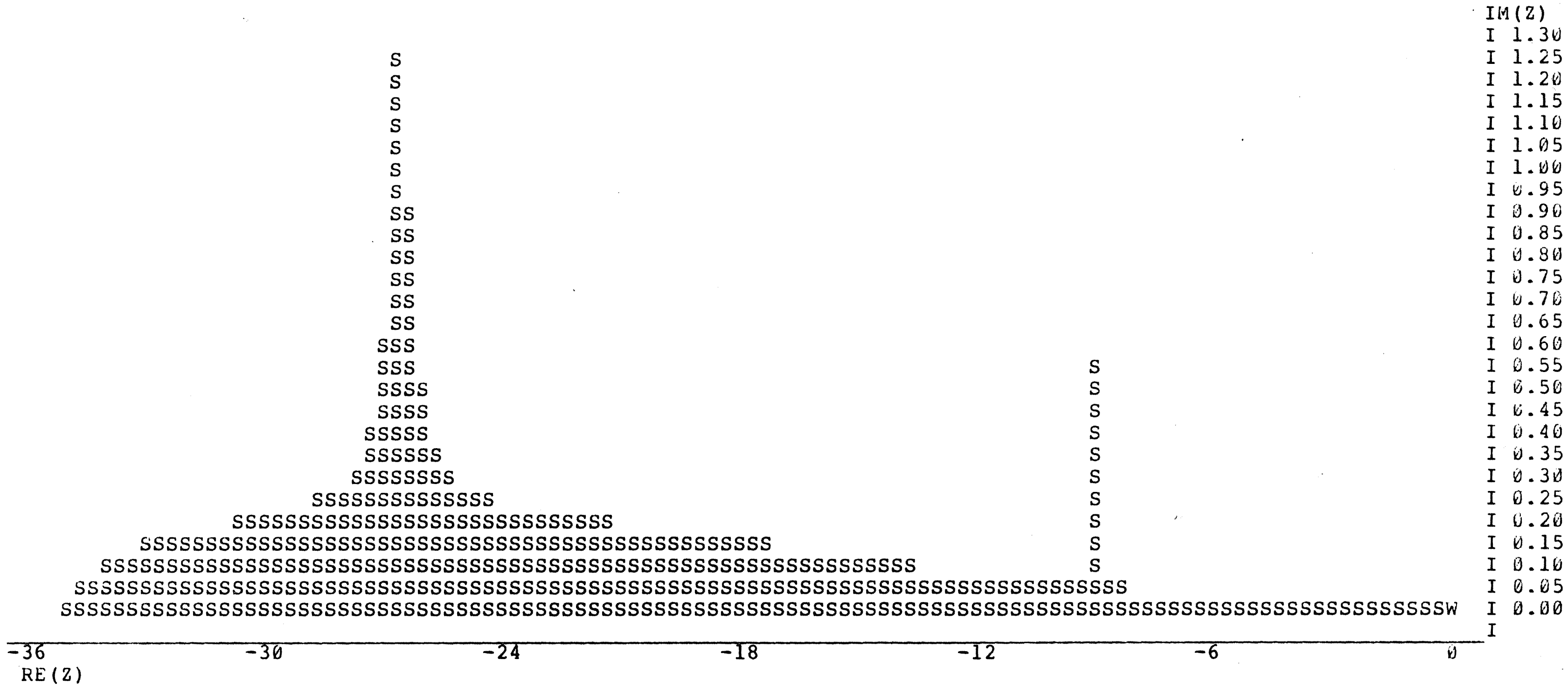

FIG. 4.3. THE STABILITY-REGION OF SCHEME (2.5) .

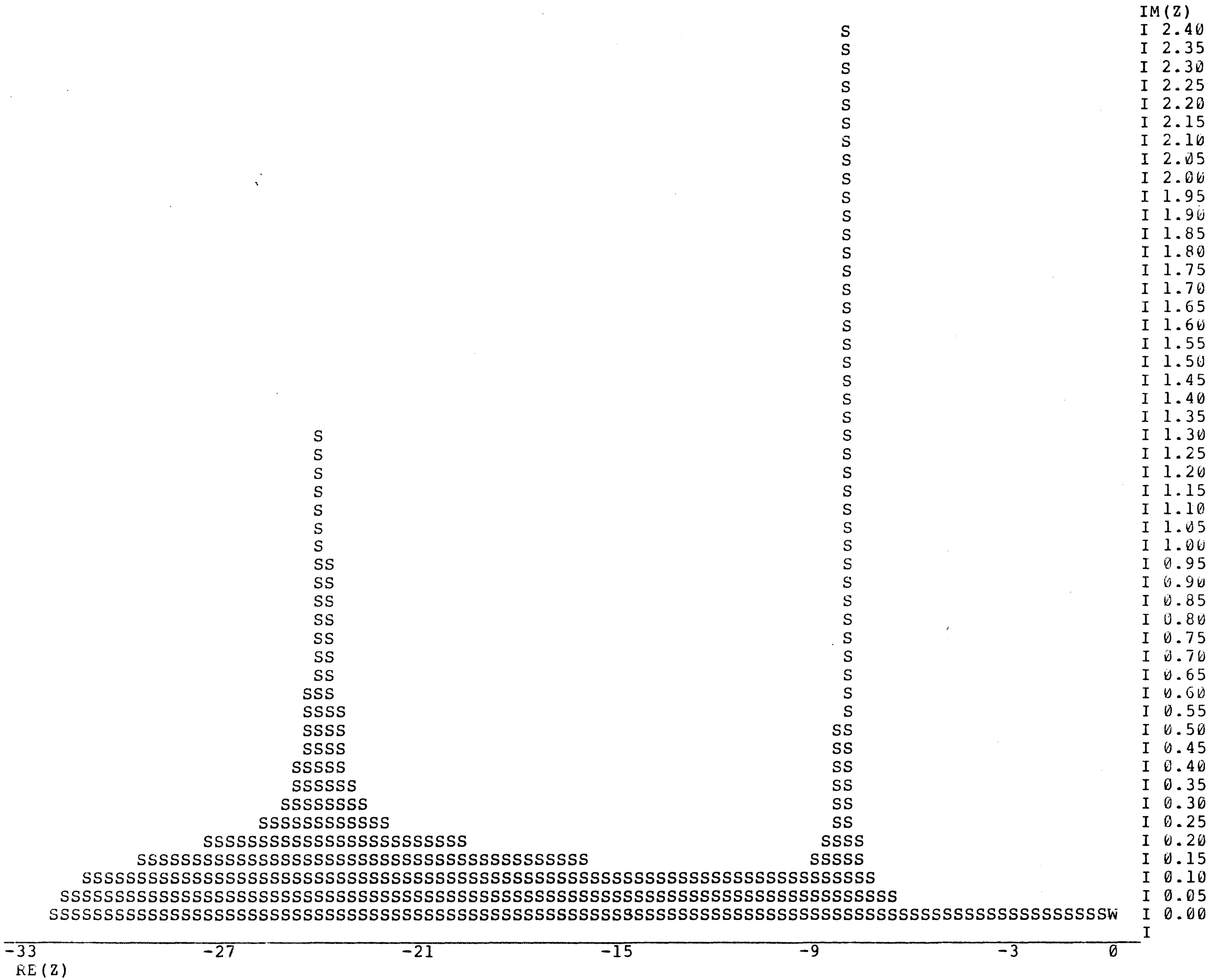

FIG. 4.5. THE STABILITY-REGION OF THE M=4,P=3 SCHEME .

Table 4.1.1. First order tests.

ARK	m = 2	STARK	m = 2
FE	SD	FE	SD
307	6.42	80	7.68
385	6.52	100	7.78
511	6.64	133	7.91
767	6.82	199	8.09
1531	7.12	398	8.40

Table 4.1.2. Second order tests.

ARK	m = 3	m = 3	STARK		m = 4
FE	SD	FE	SD	FE	SD
232	8.62	78	8.23	78	7.79
289	8.82	98	8.42	99	8.05
385	9.07	130	8.67	132	8.30
577	9.42	194	9.02	195	8.65
1150	10.02	388	9.62	390	9.26

Table 4.1.3. Third order tests

ARK	m = 4	m = 3	STARK		m = 4
FE	SD	FE	SD	FE	SD
221	9.72	126	10.21	84	5.70
273	9.83	158	11.15	102	6.51
365	10.45	210	11.59	138	8.92
545	11.14	314	12.20	204	9.93
10.85	12.25	626	12.76	408	10.79

The numerical results of problem 1.

Table 4.2.1. First order tests.

ARK m = 2		STARK m = 2	
FE	SD	FE	SD
61	1.16	16	2.23
77	1.25	20	2.32
101	1.38	26	2.44
151	1.55	39	2.61
299	1.85	78	2.91

Table 4.2.2. Second order tests.

ARK m = 3		STARK m = 3		STARK m = 4	
FE	SD	FE	SD	FE	SD
46	3.00	16	3.16	18	3.22
58	3.21	20	3.41	21	3.11
76	3.48	26	3.68	27	3.34
115	3.85	38	4.08	39	3.88
226	4.49	76	4.71	78	4.63

Table 4.2.3. Third order tests.

ARK m = 4		STARK m = 3		STARK m = 4	
FE	SD	FE	SD	FE	SD
45	3.79	26	4.12	18	1.70
57	4.13	32	4.25	21	1.89
73	4.44	42	4.52	27	2.99
109	5.10	62	5.01	42	4.04
213	6.34	122	5.91	81	4.93

The numerical results of problem 2.

Table 4.3.1. First order tests.

ARK	m = 2	STARK	m = 2
FE	SD	FE	SD
129	2.36	34	3.45
161	2.46	42	3.58
215	2.58	56	3.73
321	2.75	83	3.94
639	3.05	166	4.27

Table 4.3.2. Second order tests.

ARK	m = 3	STARK m = 3		STARK m = 4	
FE	SD	FE	SD	FE	SD
97	3.76	34	3.67	33	3.39
121	3.96	42	3.87	42	3.57
163	4.22	54	4.12	54	3.86
241	4.58	82	4.47	81	4.21
481	5.16	162	5.08	162	4.81

Table 4.3.3. Third order tests.

ARK	m = 4	STARK m = 3		STARK m = 4	
FE	SD	FE	SD	FE	SD
93	4.80	52	5.24	36	3.29
117	5.24	66	5.53	45	3.78
153	5.67	88	5.89	57	4.44
229	6.40	132	6.40	87	4.78
453	7.60	260	7.29	171	6.15

The numerical results of problem 3.

Table 4.4.1. First order tests.

ARK m = 2		STARK m = 2	
FE	SD	FE	SD
391	1.50	102	1.54
489	1.49	127	1.68
651	1.50	169	1.80
975	1.51	254	2.09
1949	1.59	507	2.46

Table 4.4.2. Second order tests.

ARK m = 3		STARK m = 3		STARK m = 4	
FE	SD	FE	SD	FE	SD
295	1.71	100	-.03	99	-.40
367	1.83	124	1.74	126	1.71
490	1.87	166	1.91	165	1.93
733	1.94	248	2.09	249	2.16
1462	2.25	494	2.65	495	2.63

Table 4.4.3. Third order tests.

ARK m = 3		STARK m = 3		STARK m = 4	
FE	SD	FE	SD	FE	SD
277	1.92	160	2.04	105	-1.71
349	2.01	200	2.27	132	- .06
461	2.24	266	2.57	174	1.41
693	2.70	398	2.97	261	2.49
1381	3.73	796	3.75	519	3.69

The numerical results of problem 4.

ACKNOWLEDGEMENTS

The author wishes to thank Prof.dr. P.J. van der Houwen for his improving remarks. He is also grateful to drs. P.A. Beentjes for the nice cooperation during his stay at the Mathematical Centre.

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