

**stichting
mathematisch
centrum**



AFDELING NUMERIEKE WISKUNDE
(DEPARTMENT OF NUMERICAL MATHEMATICS)

NW 34/76

DECEMBER

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HIGHER ORDER RUNGE-KUTTA METHODS FOR THE NUMERICAL
SOLUTION OF SECOND ORDER DIFFERENTIAL EQUATIONS
WITHOUT FIRST DERIVATIVES

2e boerhaavestraat 49 amsterdam

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).

Higher order Runge-Kutta methods for the numerical solution of second order differential equations without first derivatives

by

P.A. Beentjes & W.J. Gerritsen

ABSTRACT

Runge-Kutta methods are given of order 4 through 8 for the numerical solution of second order differential equations of the type $y'' = f(x,y)$. All schemes presented allow a built-in error estimate that can be used to control the integration step. Special attention is paid to the stability of the methods given.

KEY WORDS & PHRASES: *numerical analysis, second order differential equations, Runge-Kutta methods.*

CONTENTS

1. Introduction	2
2. Notations and outlines of solution techniques	4
3. Fourth order formula using three function evaluations	8
4. Fifth order formula using four function evaluations	9
5. Sixth order formula using six function evaluations	11
6. Seventh order formula using seven function evaluations	14
7. Eighth order formula using nine function evaluations	16
8. Stability analysis	21
9. Subroutines and examples	32
10. Conclusions	43
REFERENCES	44

1. INTRODUCTION

An n-point Runge-Kutta method for the numerical solution of the (vector-) initial value problem

$$(1.1) \quad y'' = f(x, y), \quad y_0 = y(x_0), \quad y'_0 = y'_0(x_0),$$

is given by the following scheme

$$k_i = h_\ell f(x_\ell + M_i h_\ell, y_\ell + h_\ell (M_i y'_\ell + \sum_{j=0}^{i-1} K_{ij} k_j)), \quad i = 0(1)n-1$$

$$(1.2) \quad y_{\ell+1} = y_\ell + h(y'_\ell + \sum_{i=0}^{n-1} A_i k_i),$$

$$y'_{\ell+1} = y'_\ell + \sum_{i=0}^{n-1} a_i k_i, \quad \ell = 0, 1, 2, \dots, L.$$

From now on we assume, like most authors, that $M_0 = 0$. The scheme (1.2) is said to be of order p if the Taylor series of $y_{\ell+1}(y'_{\ell+1})$ and $y(x_{\ell+1}; x_\ell, y_\ell, y'_\ell)$ ($y'(x_{\ell+1}; x_\ell, y_\ell, y'_\ell)$) do agree up to terms h^i , $i = 0(1)p$, where $y(x; x_\ell, y_\ell, y'_\ell)$ stands for the analytical solution of (1.1) proceeding through $(x_\ell, y_\ell, y'_\ell)$. NYSTRÖM [1925], ALBRECHT [1955] and ZONNEVELD [1964] already presented formulas of order p , $p \leq 6$. More recent work in this field was done by FEHLBERG [1972] and HAIRER [1976] who contributed formulas of order p , $p \leq 8$. The formulas of ZONNEVELD and FEHLBERG are of particular interest as they yield some kind of error estimate that can be used to control the integration stepsize. These error estimates are obtained in the following way:

$$(1.3) \quad \rho_y = h \sum_{i=0}^{m-1} C_i k_i, \quad (\text{Zonneveld, Fehlberg}),$$

$$(1.4) \quad \rho'_y = \sum_{i=0}^{m-1} c_i k_i, \quad (\text{Zonneveld}),$$

where C_i and c_i , $i = 0(1)m-1$, are conveniently chosen parameters. Concerning the Zonneveld formulas, ρ_y (ρ'_y) is an approximation of the term of order h^p in the Taylor series for $y_{\ell+1}$ ($y'_{\ell+1}$). A disadvantage, however, lies in the fact that these error estimates are made at the cost of extra function evaluations, i.e. $m > n$. Fehlberg actually obtains ρ_y as the difference between the p -th order approximation $y_{\ell+1}$ and a $(p+1)$ -st order approximation $y_{\ell+1}^*$ as follows

$$\begin{aligned} \rho_y &= y_{\ell+1} - y_{\ell+1}^* = \\ &= y_{\ell} + h(y'_{\ell} + \sum_{i=0}^{n-1} A_i k_i) - y_{\ell} - h(y'_{\ell} + \sum_{i=0}^n B_i k_i) = \\ &= h \sum_{i=0}^n C_i k_i = O(h^{p+1}), \end{aligned}$$

where $k_n = h_{\ell} f(x_{\ell+1}, y_{\ell+1})$, i.e. ρ_y is obtained with the aid of the first function evaluation of the next integration step.

The integration schemes presented in this report have a built-in error estimate of the form (1.3) where $m = n$, and, in some cases, as given in equation (1.4). In fact, these estimates are obtained as

$$(1.5) \quad \rho_y = y_{\ell+1} - y_{\ell+1}^{**},$$

where

$$(1.6) \quad y_{\ell+1}^{**} = y_{\ell} + h(y'_{\ell} + \sum_{i=0}^{n-2} B_i k_i) = y(x_{\ell+1}; x_{\ell}, y_{\ell}, y'_{\ell}) + O(h^p),$$

thus ρ_y is $O(h^p)$. (In the next sections we will refer to $y_{\ell+1}^{**}$ as the *embedded* lower order solution). Although our error estimates are somewhat more conservative than Fehlberg's estimates, we succeeded in constructing p -th order formulas of lower n than those given by Fehlberg. In sections 3-7 we present these formulas of order p , $p = 4(1)8$. In section 8, we shall pay special attention to the stability properties of our schemes. A stability analysis of formulas of type (1.2) is given by van der HOUWEN [1975]. FORTRAN programs for the computation of the Runge-Kutta schemes given in sections 3-8, together with some special examples of these schemes, are given in section 9.

2. NOTATIONS AND OUTLINES OF SOLUTION TECHNIQUES

The procedure of equating Taylor series of $y_{\ell+1}(y'_{\ell+1})$ and $y(x_{\ell+1}; x_{\ell}, y_{\ell}, y'_{\ell})$ ($y'(x_{\ell+1}; x_{\ell}, y_{\ell}, y'_{\ell})$) leads to a number of nonlinear equations in the parameters of (1.2). This number is dependent on the order of accuracy required. Usually, the following assumptions are made to reduce the number of necessary equations

$$(2.1) \quad \sum_{j=0}^{i-1} K_{ij} = M_i^2/2, \quad i = 1(1)n-1.$$

The remaining equations of order p , $p = 1(1)8$, for y' are given in table 2.1.

For reasons of simplicity only the lefthand side of the equations is given in table 2.1; the righthand side equals 1 for all equations.

We have also omitted limits of summation indices; the following conventions are adopted:

An index i is presented to run from N_i up to the value of its preceding index minus 1, where N_i-1 stands for the total number of \sum -signs on the right of the first appearance of index i . Furthermore, the leftmost index has the upper limit $n-1$.

E.g. (table 2.1, equation 29)

$$1440 \sum a_i M_i \sum K_{ij} M_j \sum K_{jk} M_k$$

stands for

$$1440 \sum_{i=3}^{n-1} a_i M_i \sum_{j=2}^{i-1} K_{ij} M_j \sum_{k=1}^{j-1} K_{jk} M_k = 1.$$

The order equations with respect to y can be easily derived from the equations for y' by the following rule:

Let $f(\vec{a}) = 1$ represent an order- $(p-1)$ equation for y' , then $\text{pf}(\vec{A}) = 1$ represents an order- p equation for y , where $\vec{a} = (a_0, a_1, \dots, a_{n-1})$ and $\vec{A} = (A_0, A_1, \dots, A_{n-1})$.

TABLE 2.1

The order equations for y'

order	equation	no	order	equation	no
1	$\sum a_i$	1	7	$1260 \sum a_i \sum K_{ij} M_j \sum K_{jk} M_k$	20
2	$2 \sum a_i M_i$	2	7	$2520 \sum a_i \sum K_{ij} \sum K_{jk} M_k^2$	21
3	$3 \sum a_i M_i^2$	3	7	$840 \sum a_i M_i \sum K_{ij} \sum K_{jk} M_k$	22
4	$4 \sum a_i M_i^3$	4	8	$8 \sum a_i M_i^7$	23
4	$24 \sum a_i \sum K_{ij} M_j$	5	8	$48 \sum a_i M_i^4 \sum K_{ij} M_j$	24
5	$5 \sum a_i M_i^4$	6	8	$96 \sum a_i M_i^3 \sum K_{ij} M_j^2$	25
5	$60 \sum a_i \sum K_{ij} M_j^2$	7	8	$160 \sum a_i M_i^2 \sum K_{ij} M_j^3$	26
5	$30 \sum a_i M_i \sum K_{ij} M_j$	8	8	$960 \sum a_i M_i^2 \sum K_{ij} \sum K_{jk} M_k$	27
6	$6 \sum a_i M_i^5$	9	8	$240 \sum a_i M_i \sum K_{ij} M_j^4$	28
6	$36 \sum a_i M_i^2 \sum K_{ij} M_j$	10	8	$1440 \sum a_i M_i \sum K_{ij} M_j \sum K_{jk} M_k$	29
6	$72 \sum a_i M_i \sum K_{ij} M_j^2$	11	8	$288 \sum a_i M_i (\sum K_{ij} M_j)^2$	30
6	$120 \sum a_i \sum K_{ij} M_j^3$	12	8	$2880 \sum a_i M_i \sum K_{ij} \sum K_{jk} M_k^2$	31
6	$720 \sum a_i \sum K_{ij} \sum K_{jk} M_k$	13	8	$336 \sum a_i \sum K_{ij} M_j^5$	32
7	$7 \sum a_i M_i^6$	14	8	$2016 \sum a_i \sum K_{ij} M_j^2 \sum K_{jk} M_k$	33
7	$42 \sum a_i M_i^3 \sum K_{ij} M_j$	15	8	$4032 \sum a_i \sum K_{ij} M_j \sum K_{jk} M_k^2$	34
7	$210 \sum a_i \sum K_{ij} M_j^4$	16	8	$6720 \sum a_i \sum K_{ij} \sum K_{jk} M_k^3$	35
7	$140 \sum a_i M_i \sum K_{ij} M_j^3$	17	8	$40320 \sum a_i \sum K_{ij} \sum K_{jk} \sum K_{kl} M_l$	36
7	$84 \sum a_i M_i^2 \sum K_{ij} M_j^2$	18	8	$576 \sum a_i (\sum K_{ij} M_j) (\sum K_{ij} M_j^2)$	37
7	$252 \sum a_i (\sum K_{ij} M_j)^2$	19			

We now present some abbreviations, to be used in the next sections.
We will indicate by (e is a positive integer)

- (ea) : the order equation (e) for $y'_{\ell+1}$ in table 2.1;
 (eA) : the order equation for $y'_{\ell+1}$, resulting from equation (e) of table 2.1 and the rule given above;
 (eB) : the order equation for $y'^{**}_{\ell+1}$ in formula (1.6). This equation is obtained by changing A_i into B_i in order equation (eA) and by lowering the upper limit of the first index to $n-2$;
 (eb) : the order equation for the $n-1$ point $(p-1)$ -st order formula

$$y'^{**}_{\ell+1} = y'_{\ell} + \sum_{i=0}^{n-2} b_i k_i.$$

This equation is obtained by changing a_i into b_i in order equation (ea). Again the upper limit of the first index should be $n-2$;

$$K_i^{(\ell)} : K_i^{(\ell)} = \sum_{j=1}^{i-1} K_{ij} M_j^{\ell};$$

$(n=N, p=P)$ -formula: an N -point P -th order formula of type (2.1);

$(n=N, \tilde{p}=P)$ -formula: an N -point formula of type (2.1), where $y'_{\ell+1}$ is P -th order exact and $y'_{\ell+1}$ is $(P-1)$ -st order exact;

In order to construct an $(n=N, p=P)$ -formula, we transform the original non-linear order equations into sets of linear Van der Monde systems that can be dealt with more or less separately. Concerning the order equations for $y'_{\ell+1}$, the following theorem holds

Theorem 2.1 (HAIRER [1976])

If

$$(2.2) \quad A_i = a_i(1-M_i), \quad i = 0(1)n-1,$$

then the order equations for $y'_{\ell+1}$ are a subset of the order equations for $y'_{\ell+1}$.

In this report we have made the assumption (2.2), thus reducing the order equations to those given in table 2.1, extended with the order equations of the embedded scheme.

For orders p , $p \leq 6$ a solution scheme for the order equations is given by HAIRER [1976].

Given a solution for the equations

$$(2.3) \quad \sum_{i=0}^{n-1} a_i M_i^k = \frac{1}{k+1}, \quad k = 0(1)p-1,$$

this scheme successively determines $K_i^{(\ell)}$, $i = 1(1)n-1$, $\ell = 1(1)i-1$, as functions of a_i and M_i , $i = 0(1)n-1$. This leads to the computation of the parameters K_{ij} , $i = 1(1)n-1$, $j = 1(1)i-1$, from the Van der Monde systems $K_i^{(\ell)}$, $i = 1(1)n-1$, $\ell = 1(1)i-1$.

For higher order methods ($p > 6$), the solution of the order equations proceeds in an analogous way. However, a number of assumptions of the following form has to be made

$$K_i^{(\ell)} = \frac{M_i^{\ell+2}}{(\ell+1)(\ell+2)}, \quad \ell = 1(1)\ell_p,$$

$$a_i = 0, \quad i = 1(1)i_p,$$

and there will be some restrictive conditions with respect to the parameters M_i , $i = 1(1)n-1$.

The a priori solution for a_i , $i = 0(1)n-1$ of equation (2.3) can be given in terms of M_i , $i = 1(1)n-1$, as (2.3) is a Van der Monde system for the a_i , $i = 0(1)n-1$. If n_r is the number of non-zero a_i 's and $p > n_r + 1$, then there are $(p - n_r - 1)$ restrictive conditions for M_i , $i = i_1(1)i_{n_r}$ (cf. HILDEBRAND [1956], p 351-357). As for our higher order formulas ($p > 5$) some of the lower indexed a_i 's have to be equal to zero (in order to facilitate the solvability of the remaining order equations), we have identified the non-zero a_i 's and corresponding M_i 's to the weight factors and abscissas of the Gauss-Radau quadrature formula

$$(2.4) \quad \int_0^1 f(x) dx \simeq w_1 f(0) + \sum_{i=2}^{n_r} w_i f(x_i).$$

It is well known that (2.4) is exact for polynomials up to a degree of $2n_r - 2$. Thus, an application of (2.4) to the set $\{x_i\}_{i=0}^{2n_r-2}$ leads to

$$\sum_{i=1}^{n_r} w_i x_i^k = \frac{1}{k+1}, \quad x_1 = 0, \quad k = 0(1)2n_r - 2,$$

which, in connection with (2.3), justifies the identification of the quadrature coefficients to the Runge-Kutta parameters a_i and M_i , $i = 1(1)n_r$. The expressions for w_i and x_i , $i = 1(1)n_r$ are given in ABRAMOWITZ and STEGUN [1964], p 888.

On page 921 of this handbook numerical values are given for w_i/x_i and x_i , $i = 2(1)n_r$, $n_r = 2(1)9$. For our purposes we only need the $n_r = 4$ and $n_r = 5$ quadrature coefficients. These coefficients are given in section 9 to 27 decimal places.

In the next sections we will often omit the expressions for a_0 , B_0 , A_i , $K_{i+1,0}$, $i = 0(1)n-1$. These parameters are easily obtained from the equations (1a), (1B), (1A), (2.1) and (2.2).

3. FOURTH ORDER FORMULA USING THREE FUNCTION EVALUATIONS

The $(n=3, p=4)$ scheme with an embedded $(n=2, \tilde{p}=3)$ scheme is easily found from equations (1a) through (5a).

The resulting formula, which has one free parameter (e.g. M_1), is given by

$$(3.1) \quad M_1 M_2 / 2 - (M_1 + M_2) / 3 + 1/4 = 0,$$

$$(3.2) \quad a_1 = \frac{M_2/2 - 1/3}{M_1(M_2 - M_1)}, \quad a_2 = \frac{M_1/2 - 1/3}{M_2(M_1 - M_2)}, \quad B_1 = \frac{1}{6M_1},$$

$$K_{21} = \frac{1}{24a_2 M_1}.$$

Substituting $M_1 = \frac{1}{2}$, we arrive at Nyström's formula of order four (see NYSTRÖM [1925], p 24). In section 8 we will give a value for M_1 which leads to optimal stability properties of our $(n=3, p=4)$ scheme.

4. FIFTH ORDER FORMULA USING FOUR FUNCTION EVALUATIONS

In this section we will derive $(n=4, p=5)$ schemes with an embedded $(n=3, p=4)$ scheme.

The general formula turns out to have two free parameters, e.g. M_2 and M_3 . The solution of equations (1a) through (8a) proceeds as follows. Equations (2a) through (4a) and equation (6a) are linear in a_i , $i = 1, 2, 3$. The solution is

$$a_1 = \frac{M_2 M_3 / 2 - (M_2 + M_3) / 3 + 1/4}{M_1 (M_2 - M_1) (M_3 - M_1)},$$

and similar expressions for a_2 and a_3 , together with the condition

$$(4.1) \quad M_1 M_2 M_3 / 2 - (M_1 M_2 + M_1 M_3 + M_2 M_3) / 3 + (M_1 + M_2 + M_3) / 4 - 1/5 = 0.$$

From equations (5a) and (8a) it follows that

$$(4.2) \quad K_{21} = \frac{M_3 / 24 - 1/30}{a_2 M_1 (M_3 - M_2)},$$

$$K_3^{(1)} = \frac{M_2 / 24 - 1/30}{a_3 (M_2 - M_3)}.$$

The latter equation yields, together with equation (7a)

$$(4.3) \quad K_{31} = \frac{(M_3 / 24 - 1/30) / (M_3 - M_2) + M_2 / 24 - 1/60}{a_3 M_1 (M_2 - M_1)},$$

$$(4.4) \quad K_{32} = \frac{M_1 / 24 - 1/60}{a_3 M_2 (M_1 - M_2)}.$$

The parameters B_i , $i = 1, 2$, are easily derived from equation (2B) and (3B), e.g.

$$B_1 = \frac{M_2 / 6 - 1/12}{M_1 (M_2 - M_1)}.$$

There are some limitations with respect to the values of the (free) parameters. As can easily be checked, we have

$$M_1 \neq 0, M_2 \neq 0, M_1 \neq M_2, M_2 \neq M_3, a_2 \neq 0, a_3 \neq 0.$$

We shall now briefly present some extra schemes, which are specific examples of the solution given above.

- (i) The particular choice $M_{2,3} = \frac{6 \pm \sqrt{6}}{10}$ leaves M_1 as a free parameter, because (4.1) is fulfilled independent on the value of M_1 .

$$\text{The scheme is given by } a_0 = \frac{1}{9}, a_1 = 0, a_2 = \frac{16+p}{36}, a_3 = \frac{16-p}{36}, \\ M_2 = \frac{6-p}{10}, M_3 = \frac{6+p}{10}, p = \pm \sqrt{6}.$$

K_{21} , K_{31} and K_{32} are obtained from (4.2), (4.3) and (4.4).

- (ii) If we choose $M_1 = M_3$ in case (i), a_3 becomes a free parameter and the

$$\text{solution is } a_0 = \frac{1}{9}, a_2 = \frac{16+p}{36}, \tilde{a}_3 = \frac{16-p}{36}, a_1 = \tilde{a}_3 - a_3,$$

$$M_1 = M_3 = \frac{6+p}{10}, M_2 = \frac{6-p}{10}, p = \pm \sqrt{6}.$$

- (iii) The particular choice $M_3 = 0$, implying that a_3 can again be chosen arbitrarily, leads to $M_{1,2} = \frac{6 \pm \sqrt{6}}{10}$.

$$\text{The resulting scheme is given by } a_0 = \frac{1}{9} - a_3, a_1 = \frac{16-p}{36},$$

$$a_2 = \frac{16+p}{36}, M_1 = \frac{6+p}{10}, M_2 = \frac{6-p}{10}, M_3 = 0, p = \pm \sqrt{6}.$$

Equations (4.2) through (4.4) determine K_{21} , K_{31} and K_{32} .

Nyström's ($n=4, p=5$) formula with $M_2 = \frac{2}{3}$ and $M_3 = 1$ fits equations (4.1) through (4.4), but because $M_3 = 1$ the embedded ($n=3, \tilde{p}=4$) formula is in fact ($n=3, \tilde{p}=5$). The latter implies that no truncation error can be calculated in the sense of (1.5).

In section 9, a program for the two-parameter scheme is given by the subroutine RKP45.

5. SIXTH ORDER FORMULA USING SIX FUNCTION EVALUATIONS

The equations to be solved are given by (1a) through (13a). To start off, we will indicate how a family of ($n=5, p=6$) formulas can be obtained. Equations (2a) - (4a), (6a) and (9a) give the condition

$$M_1 M_2 M_3 M_4 / 2 - (M_1 M_2 M_3 + M_1 M_2 M_4 + M_1 M_3 M_4 + M_2 M_3 M_4) / 3 + \\ + (M_1 M_2 + M_1 M_3 + M_1 M_4 + M_2 M_3 + M_2 M_4 + M_3 M_4) / 4 - (M_1 + M_2 + M_3 + M_4) / 5 + 1/6 = 0.$$

The solution for the a_i , $i = 1(1)4$, is given by

$$a_1 = \frac{M_2 M_3 M_4 / 2 - (M_2 M_3 + M_2 M_4 + M_3 M_4) / 3 + (M_2 + M_3 + M_4) / 4 - 1/5}{M_1 (M_2 - M_1) (M_3 - M_1) (M_4 - M_1)},$$

and, by permuting indices in the last formula, similar expressions hold for a_2 through a_4 .

From (5a), (8a) and (10a) follows

$$K_2^{(1)} = \frac{M_3 M_4 / 24 - (M_3 + M_4) / 30 + 1/36}{a_2 (M_3 - M_2) (M_4 - M_2)}$$

(similar expressions hold for $K_3^{(1)}$ and $K_4^{(1)}$).

Equations (7a) and (11a) yield

$$K_3^{(2)} = \frac{(1/60 - a_2 K_2^{(2)}) M_4 - (1/72 - a_2 K_2^{(2)}) M_2}{a_3 (M_4 - M_3)}$$

(similar expression for $K_4^{(2)}$). Thus, with $K_4^{(3)}$ resulting from (12a), we can express all K_{ij} , $i = 2(1)4$, $j = 1(1)i-1$, in terms of a_i and M_i , $i = 1(1)4$.

There is still one equation, (13a), to be satisfied. By substituting all the expressions found in this equation, a quite laborious computation leads to the simple condition

$$(5.1) \quad M_4 = 1.$$

Thus, we have found a two-parameter family (e. g. M_2 and M_3) of $(n=5, p=6)$ formulas. A member of this family ($M_2 = \frac{1}{2}, M_3 = \frac{3}{4}$) is given by ALBRECHT [1955]. However, since we did not succeed in finding an embedded $(n=3, \tilde{p}=5)$ formula of the family above (because of (5.1) the integration formula for y is already of type $(n=4, \tilde{p}=5)$), we will now proceed to derive an $(n=6, p=6)$ formula with an embedded $(n=5, \tilde{p}=5)$ formula.

By substituting

$$(5.2) \quad a_1 = 0,$$

$$(5.3) \quad K_i^{(j)} = \frac{M_i^{j+2}}{(j+1)(j+2)}, \quad i = 2(1)5, \quad j = 1, 2,$$

the equations (2a) through (13a) are reduced to

$$(5.4) \quad \sum_{i=2}^5 a_i \sum_{j=1}^{i-1} K_{ij} M_j^3 = \frac{1}{120},$$

$$(5.5) \quad \sum_{i=2}^5 a_i K_{i1} = 0,$$

$$(5.6) \quad \sum_{i=2}^5 a_i M_i^k = \frac{1}{k+1}, \quad k = 1(1)5.$$

It is easily verified that, if

$$(5.7) \quad \sum_{i=2}^5 a_i M_i \sum_{j=1}^{i-1} K_{ij} M_j^3 = \frac{1}{140},$$

$$(5.8) \quad \sum_{i=3}^5 a_i M_i \sum_{j=1}^{i-1} K_{ij} \sum_{\ell=1}^{j-1} K_{j\ell} M_\ell = \frac{1}{840},$$

and

$$(5.9) \quad \sum_{i=2}^5 a_i M_i^6 = \frac{1}{7},$$

the resulting scheme becomes of type $(n=6, \tilde{p}=7)$.

To solve (5.6) and (5.9), we put $a_2 = 0$ and respectively identify a_i , $i = 0, 3, 4, 5$ with the weight factors, and M_i , $i = 0, 3, 4, 5$ ($M_0 \equiv 0$), with the abscissas of the 4-point Radau quadrature formula. Note there are 6 possible identifications. From (5.3) easily results $M_1 = M_2/2$.

The solution of (5.4) through (5.7) proceeds as follows. Equations (5.4) and (5.7) are solved for $K_4^{(3)}$ and $K_5^{(3)}$. As K_{51} is given by (5.5) we are able to determine all parameters K_{ij} , $i = 2(1)5$, $j = 1(1)i-1$, by solving linear Van der Monde systems. Using all the expressions found above, equation (5.8) leads to the condition

$$(5.10) \quad M_2 = \frac{(M_5/5-1/6)M_3/12-(M_5/6-1/7)/20}{(M_5/4-1/5)M_3/6-(M_5/5-1/6)/12}.$$

A similar formula for M_3 is obtained if we take $a_3 = 0$ instead of $a_2 = 0$, bringing the total number of possible solutions, as indicated above, to 12.

The equations (1B) through (5B) for the embedded $(n=5, \tilde{p}=5)$ scheme reduce, with the aid of the assumptions (5.3), to the Van der Monde system

$$\sum_{i=2}^4 B_i M_i^k = \frac{1}{(k+1)(k+2)}, \quad k = 1, 2, 3.$$

Finally, we remark that it is possible to obtain an embedded $(n=5, \tilde{p}=6)$ scheme for the formula given above by taking $M_2 = M_5$ instead of the value of M_2 determined by (5.9).

It is easily verified that, in that case, the weights b_i , $i = 1(1)4$, are given by

$$b_2 = a_5,$$

$$b_3 = a_3,$$

$$b_4 = a_4.$$

The consequence, however, for taking $M_2 = M_5$ is that the scheme is no longer of type $(n=6, \tilde{p}=7)$, because equation (5.8) does not hold. On the other hand, it is useful to have an embedded $(n=5, \tilde{p}=6)$ scheme,

thus being able to control errors in y' as well as in y .

In section 9, a program for the solution above (with $a_3 = 0$) is given by the subroutine RKPAP 66.

6. SEVENTH ORDER FORMULA USING SEVEN FUNCTION EVALUATIONS

In this section an $(n=7, p=7)$ formula with an embedded $(n=6, \tilde{p}=6)$ formula is derived.

The equations to be solved are given by equations (1a) through (22a). First we put

$$K_i^{(j)} = \frac{M_i^{j+2}}{(j+1)(j+2)}, \quad i = 2(1)6, \quad j = 1, 2,$$

$$a_1 = 0.$$

Under these assumptions, the equations (1a) through (22a) reduce to

$$(6.1) \quad \sum_{i=2}^6 a_i M_i^k = \frac{1}{k+1}, \quad k = 1(1)6,$$

$$(6.2) \quad \sum_{i=2}^6 a_i \sum_{j=1}^{i-1} K_{ij} M_j^3 = \frac{1}{120},$$

$$(6.3) \quad \sum_{i=2}^6 a_i K_{i1} = 0,$$

$$(6.4) \quad \sum_{i=2}^6 a_i \sum_{j=1}^{i-1} K_{ij} M_j^4 = \frac{1}{210},$$

$$(6.5) \quad \sum_{i=2}^6 a_i M_i \sum_{j=1}^{i-1} K_{ij} M_j^3 = \frac{1}{140},$$

$$(6.6) \quad \sum_{i=2}^6 a_i M_i K_{i1} = 0.$$

If we solve the additional equations

$$(6.7) \quad \sum_{i=2}^6 a_i M_i^7 = \frac{1}{8},$$

$$(6.8) \quad \sum_{i=2}^6 a_i M_i \sum_{j=1}^{i-1} K_{ij} M_j^4 = \frac{1}{240},$$

$$(6.9) \quad \sum_{i=2}^6 a_i M_i^2 \sum_{j=1}^{i-1} K_{ij} M_j^3 = \frac{1}{160},$$

$$(6.10) \quad \sum_{i=2}^6 a_i M_i^2 K_{i1} = 0.$$

we have an $(n=7, \tilde{p}=8)$ formula.

However, we only succeed to solve (6.1) through (6.9). The solution of these equations proceeds as follows.

First we put $a_2 = 0$ and we take for a_i and M_i , $i = 0, 3, 4, 5, 6$, the values of the weight factors and abscissas of the 5-point Radau quadrature formula, thus satisfying equations (6.1) and (6.7). The expressions for $K_i^{(3)}$, $i = 4, 5, 6$, follow from (6.2), (6.5) and (6.9). Equations (6.4) and (6.8) are solved for $K_j^{(4)}$, $i = 5, 6$. K_{61} follows from (6.3) and, by substituting all the expressions found into the equation (6.6), we obtain the following relation

$$M_2 = \frac{M_3 M_4 (M_6/5 - 1/6)/12 - (M_3 + M_4)(M_6/6 - 1/7)/20 + (M_6/7 - 1/8)/30}{M_3 M_4 (M_6/4 - 1/5)/6 - (M_3 + M_4)(M_6/5 - 1/6)/12 + (M_6/6 - 1/7)/20}.$$

The equations (2B) through (8B) reduce, under the assumptions made above, to the Van der Monde system

$$\sum_{i=2}^5 B_i M_i^k = \frac{1}{(k+1)(k+2)}, \quad k = 1(1)4.$$

It is possible to interchange the values of M_2 and M_3 in the solutions given above (making $a_3 = 0$).

Thus, the total number of indicated solutions is 48.

In section 9 we present a subroutine, RKPAP 77, for the computation of the parameters of the solutions corresponding to the case $a_3 = 0$.

7. EIGHTH ORDER FORMULA USING NINE FUNCTION EVALUATIONS

In this section we give solutions for an $(n=9, p=8)$ formula with an embedded $(n=8, \tilde{p}=7)$ formula.

The equations to be solved are given by the equations (1a) through (37a). By the assumptions

$$a_1 = a_2 = a_3 = 0,$$

$$K_i^{(j)} = \frac{M_i^{j+2}}{(j+1)(j+2)}, \quad i = 2(1)8, \quad j = 1, 2,$$

$$K_i^{(3)} = M_i^5/20, \quad i = 4(1)8,$$

these equations reduce to

$$(7.1) \quad \sum_{i=4}^8 a_i M_i^k K_{i1} = 0, \quad k = 0, 1, 2,$$

$$(7.2) \quad \sum_{i=4}^8 a_i M_i^k \sum_{j=1}^{i-1} K_{ij} M_j^4 = \frac{1}{30(k+7)}, \quad k = 0, 1,$$

$$(7.3) \quad \sum_{i=4}^8 a_i \sum_{j=1}^{i-1} K_{ij} M_j^5 = \frac{1}{336},$$

$$(7.4) \quad \sum_{i=4}^8 a_i \sum_{j=2}^{i-1} K_{ij} \sum_{\ell=1}^{j-1} K_{j\ell} M_\ell^3 = \frac{1}{6720},$$

$$(7.5) \quad \sum_{i=4}^8 a_i \sum_{j=3}^{i-1} K_{ij} \sum_{\ell=2}^{j-1} K_{j\ell} \sum_{m=1}^{\ell-1} K_{\ell m} M_m = \frac{1}{40320},$$

$$(7.6) \quad \sum_{i=4}^8 a_i M_i^k = \frac{1}{k+1}, \quad k = 1(1)7.$$

There are several ways for solving equations (7.1) through (7.6). We will only deal with the following two cases, both having

$$K_{i1} = 0, \quad i = 4(1)8.$$

By this assumption equation (7.1) is satisfied.

CASE 1 $a_5 = 0.$

Equation (7.2) is fulfilled by taking

$$K_i^{(4)} = M_i^6/30, \quad i = 4,6,7,8.$$

From the assumptions made so far, $K_{41} = 0$ and $K_4^{(4)} = M_4^6/30$ lead to the condition

$$M_{2,3} = M_4 \frac{5 \pm \sqrt{5}}{10}.$$

We now concentrate first on the solution of (7.6) and the equations of the embedded ($n=8, \tilde{p}=7$) scheme, (1B)-(13B). Under the assumptions made, together with $B_1 = B_2 = B_3 = 0$, these latter equations reduce to

$$(7.7) \quad \sum_{i=4}^7 B_i M_i^k = \frac{1}{(k+1)(k+2)}, \quad k = 1(1)5.$$

Equations (7.6) and (7.7) are simply solved by substituting for a_i and M_i , $i = 0,4,6,7,8$, the values of the weight factors and abscissas of the 5-point Radau quadrature formula (2.4) and, moreover, by substituting

$$M_5 = M_8,$$

$$B_i = A_i, \quad i = 0,4,6,7,$$

$$B_5 = A_8.$$

In a simple way, equations (7.4) and (7.5) can be reduced to

$$(7.7) \quad \sum_{i=4}^8 a_i \sum_{j=2}^3 K_{ij} K_{j1} = 0,$$

and

$$(7.8) \quad \sum_{i=4}^8 a_i (K_{i3} K_{32} M_2^3 - \frac{1}{20} \sum_{j=2}^3 K_{ij} M_j^5) = 0.$$

We may rewrite these equations as

$$(7.9) \quad c_2 (-\frac{1}{20} M_2^5) + c_3 (K_{32} M_2^3 - \frac{1}{20} M_3^5) = 0,$$

$$(7.10) \quad c_2 K_{21} + c_3 K_{31} = 0,$$

where
$$c_j = \sum_{i=4}^8 a_i K_{ij}, \quad j = 2, 3.$$

The only possible solution of (7.9) and (7.10) is given by

$$(7.11) \quad c_2 = c_3 = 0,$$

as can be shown by using the expressions for K_{21} , K_{31} and K_{32} , together with $M_1 = M_2/2$ and $M_{2,3} = \frac{5+\sqrt{5}}{10} M_4$. More generally, by taking

$$(7.12) \quad c_j = \sum_{i=2}^8 a_i K_{ij}, \quad j = 1(1)7,$$

we obtain the equations

$$(7.13) \quad \sum_{i=1}^7 c_i M_i^k = \frac{1}{(k+1)(k+2)(k+3)}, \quad k = 1(1)5.$$

We observe that (7.13) represents five order equations; e.g., the $k = 5$ - equation corresponds to (7.3), being the last equation from the system (7.1)-(7.6) not yet taken into account.

Since $c_i = 0$, $i = 1, 2, 3$, the existence of a solution of (7.13) for c_i , $i = 4(1)7$, is guaranteed if the following condition holds

$$(7.14) \quad \sum_{i=1}^5 (-1)^i x_i / (i+1) / (i+2) / (i+3) = 0,$$

where

$$x_1 = M_4 M_5 M_6 M_7,$$

$$x_2 = M_4 M_5 M_6 + M_4 M_5 M_7 + M_4 M_6 M_7 + M_5 M_6 M_7,$$

$$(7.15) \quad x_3 = M_4 M_5 + M_4 M_6 + M_4 M_7 + M_5 M_6 + M_5 M_7 + M_6 M_7,$$

$$x_4 = M_4 + M_5 + M_6 + M_7,$$

$$x_5 = 1.$$

We will show that (7.14) does indeed hold.

PROPERTY 7.1 If

$$\sum_{\substack{i=4 \\ i \neq 5}}^8 a_i M_i^k = \frac{1}{k+1}, \quad k = 1(1)7, \quad \text{and} \quad M_5 = M_8 \quad \text{then}$$

$$\sum_{i=1}^5 (-1)^i x_i / (i+1) / (i+2) / (i+3) = 0,$$

where x_i , $i = 1(1)5$ is defined by (7.15).

PROOF. From the Van der Monde system

$$\sum_{\substack{i=4 \\ i \neq 5}}^8 a_i M_i^k = \frac{1}{k+1}, \quad k = 1(1)4,$$

we can obtain the quantities a_i in terms of M_i , $i = 4, 6, 7, 8$.

The remaining equations

$$\sum_{\substack{i=4 \\ i \neq 5}}^8 a_i M_i^k = \frac{1}{k+1}, \quad k = 5, 6, 7,$$

lead to the conditions

$$(7.16) \quad \begin{pmatrix} 1/2 & -1/3 & 1/4 & -1/5 \\ 1/3 & -1/4 & 1/5 & -1/6 \\ 1/4 & -1/5 & 1/6 & -1/7 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} -1/6 \\ -1/7 \\ -1/8 \end{pmatrix},$$

where, as $M_8 = M_5$, x_i , $i = 1(1)4$, is given by (7.15). Denoting the i -th equation of (7.16) by r_i , $i = 1, 2, 3$, we obtain (7.14) by taking $(r_1 - 2r_2 + r_3)/2$. \square

To complete the solution of our eighth order formula, we proceed as follows. First, the parameter K_{87} is obtained as

$$K_{87} = c_7/a_8.$$

We are then left with 8 linear equations $K_i^{(j)}$, $i = 7, 8$, $j = 1(1)4$, and 10 unknowns, K_{ij} , $i = 7, 8$, $j = 2(1)6$. However, instead of two, we have only one free parameter, since a preset value of K_{72} (say) immediately leads to

$$K_{82} = c_2 - \sum_{i=2}^7 a_i K_{i2}.$$

CASE 2 $a_4 = 0$.

In this case the solution is found in a quite similar way. In particular we have

$$\begin{aligned} M_4 &= M_8, \\ B_i &= A_i, \quad i = 0, 5, 6, 7, \\ B_4 &= A_8. \end{aligned}$$

Again, M_i and a_i , $i = 5(1)8$ are related to Radau quadrature coefficients. The assumptions $K_{41} = K_{51} = 0$ and $K_5^{(4)} = M_5^6/30$ lead to the following conditions for M_2 and M_3

$$\begin{aligned} -5M_4(M_2 + M_3) + 10M_2M_3 &= -3M_4^2, \\ (5M_4 - 3M_5)M_5(M_2 + M_3) + (5M_5 - 10M_4)M_2M_3 &= (3M_4 - 2M_5)M_5^2, \end{aligned}$$

of which the solution is

$$M_2 = M_5 \frac{6p^3 - 3p^2 - 6p + 4 \pm \sqrt{36p^6 - 156p^5 + 309p^4 - 356p^3 + 1236p^2 - 596p + 16}}{2(10p^2 - 15p + 6)},$$

(7.9)

$$M_3 = \frac{M_4(5M_2 - 3M_4)}{10M_2 - 5M_4}, \quad p = M_4/M_5.$$

An investigation of the zeroes (all complex) of the square root argument appearing in the expression for M_2 , shows that M_2 is real-valued for arbitrary M_4 and M_5 .

In section 9 a FORTRAN routine of case 2 is given by subroutine RKPARG. For reasons of simplicity we only consider those schemes of the two cases treated above for which $K_{72} = 0$. Note that this choice leads to 48 possible solutions for each case.

8. STABILITY ANALYSIS

In this section we will investigate the stability properties of the schemes developed.

In Van der HOUWEN [1975] the following amplification matrix for an n -point Runge-Kutta formula is presented:

$$R^{(n)}(z) = \begin{pmatrix} 1 + \sum_{\ell=0}^{n-1} A_{\ell} \cdot z \cdot R_{11}^{(\ell)}(z) & \sum_{\ell=0}^{n-1} A_{\ell} \cdot z \cdot R_{12}^{(\ell)}(z) \\ \sum_{\ell=0}^{n-1} a_{\ell} \cdot z \cdot R_{11}^{(\ell)}(z) & 1 + \sum_{\ell=0}^{n-1} a_{\ell} \cdot z \cdot R_{12}^{(\ell)}(z) \end{pmatrix},$$

with

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

$$R_{12}^{(j)} = M_j + \sum_{\ell=0}^{j-1} K_{j\ell} \cdot z \cdot R_{12}^{(\ell)}, \quad j = 1(1)n-1,$$

$$R_{11}^{(0)} = R_{12}^{(0)} + 1 = 1,$$

$z = h^2 \delta$, $\delta \in \Delta$, Δ denotes the eigenvalue spectrum of the Jacobian matrix of the right-hand side of (1.1); h represents the stepsize. A Runge-Kutta scheme is said to be *stable* when $|\alpha_{1,2}| < 1$ and *weakly stable* if $|\alpha_{1,2}| \leq 1$, where $\alpha_{1,2}$ are the eigenvalues of $R^{(n)}(z)$.

An investigation how perturbations are analytically propagated for equations of type $y'' = Jy$, reveals that the "analytic" amplification matrix is of the following form

$$A = \begin{pmatrix} \cosh(Dh) & (Dh)^{-1} \sinh(Dh) \\ Dh \sinh(Dh) & \cosh(Dh) \end{pmatrix},$$

where $D^2 = J$. The matrix A is the analytic analogue of the matrix $R^{(n)}(z)$. The eigenvalues of A satisfy:

$$\alpha^2 - 2 \cosh \sqrt{z} \alpha + 1 = 0, \quad z = h^2 \delta, \quad \delta \in \Delta.$$

From this it follows that $\alpha_{\pm} = \exp(\pm \sqrt{z})$. This means that there is weak stability at points on the negative z -axis and no stability for other z -values. For this reason, we concentrate on those schemes which have the longest negative stability interval, i.e. the interval $[\beta, 0]$ of negative z -values for which $|\alpha_{1,2}| \leq 1$. We define β to be the *stability bound* of the method.

Evidently, an n -point Runge-Kutta formula, with a stability bound β is stable, if $|h| \leq |h_{\max}| = \sqrt{\frac{-\beta}{1 \delta 1_{\max}}}$. Concerning the eigenvalues of $R^{(n)}(z)$, the following equation holds

$$(8.1) \quad \alpha^2 - S\alpha + P = 0,$$

where S equals the sum of the diagonal elements of $R^{(n)}(z)$ and P denotes the determinant of $R^{(n)}(z)$. Applying the Hurwitz-criterion to (8.1) leads to $|\alpha_{1,2}| \leq 1$ if

$$(8.2) \quad P_1(z) = P - 1 \leq 0,$$

$$(8.3) \quad P_2(z) = S - P - 1 \leq 0,$$

$$(8.4) \quad P_3(z) = -S - P - 1 \leq 0.$$

For each polynomial $P_i(z)$ there is a maximal interval $[\beta_i, 0]$, $i = 1, 2, 3$, for which the relevant equation of (8.2) through (8.4) holds.

It is clear that the stability bound β is found by

$$[\beta, 0] = \bigcap_{i=1,2,3} [\beta_i, 0].$$

By calculating the zeroes of $P_i(z)$, β_i ($i=1,2,3$) is easily derived.

EXAMPLE :

In the ($n=3, p=4$) case we have one free parameter left and this will be used to optimize the stability bound.

Using (3.1) and (3.2) it is easily verified that

$$R^{(3)}(z) = \begin{pmatrix} 1 + \frac{1}{2}z + \frac{1}{24}z^2 + \frac{(1-M_2)M_1}{48}z^3 & 1 + \frac{1}{6}z + \frac{1}{24}(1-M_2)z^2 \\ z + \frac{1}{6}z^2 + \frac{1}{48}M_1z^3 & 1 + \frac{1}{2}z + \frac{1}{24}z^2 \end{pmatrix}.$$

Thus, we have

$$P_1(z) = \frac{1}{144} \left\{ M_2(6-3M_1) - 4 \right\} z^3,$$

$$P_2(z) = z \left\{ 1 + \frac{1}{12}z + \frac{1}{144}(3M_1 - 6M_2 + 4)z^2 \right\},$$

$$P_3(z) = -4 - z - \frac{1}{12}z^2 - \frac{1}{144} \left\{ 3M_1 - 6M_1M_2 + 6M_2 - 4 \right\} z^3.$$

We now solve (8.2) through (8.4) using these $P_i(z)$, $i = 1, 2, 3$. Equation (8.2) yields

$$\frac{1}{144} \left\{ M_2(6-3M_1) - 4 \right\} z^3 \leq 0.$$

Considering only negative z -values we may write

$$-3M_1M_2 + 6M_2 - 4 \geq 0.$$

Applying (3.1) yields

$$(8.5) \quad M_1 < \frac{2}{3}.$$

Equation (8.3) leads to

$$z \left\{ 1 + \frac{1}{12} z + \frac{1}{144}(3M_1 - 6M_2 + 4)z^2 \right\} \leq 0.$$

Since, again, z runs through the negative-axis, we obtain

$$(8.6) \quad 1 + \frac{1}{12} z + \frac{1}{144}(3M_1 - 6M_2 + 4)z^2 \geq 0.$$

There are two possibilities.

CASE 1 Suppose $3M_1 - 6M_2 + 4 \geq 0$.

A calculation, using (3.1), yields : $M_1 = \frac{1}{3}$ ($M_1 \geq \frac{2}{3}$ is contradicted by (8.5)).

Substituting $M_1 = \frac{1}{3}$ in (3.1) and (8.6) respectively, we find $M_2 = \frac{5}{6}$ and $z \geq -12$.

Using the values $M_1 = \frac{1}{3}$ and $M_2 = \frac{5}{6}$, it follows that (8.4) is fulfilled if $z \geq -12$.

Thus we find $\beta \leq -12$.

CASE 2 Suppose

$$(8.7) \quad 3M_1 - 6M_2 + 4 < 0.$$

Furthermore suppose case 2 leads to $\beta \leq -12$.

Substituting $z = -12$ in (8.6), results in $3M_1 - 6M_2 + 4 \geq 0$. But this contradicts (8.7).

The conclusion is that for $M_1 = \frac{1}{3}$ we find the optimal stability bound

$$\beta = -12.$$

The resulting scheme is given in table 8.1.

TABLE 8.1 The (n=3,p=4) scheme with optimal stability bound $\beta = -12$.

$$\begin{aligned}
M_0 &= 0 & M_1 &= \frac{1}{3} & M_2 &= \frac{5}{6} \\
K_{10} &= \frac{1}{18} \\
K_{20} &= \frac{5}{144} & K_{21} &= \frac{5}{16} \\
A_0 &= \frac{1}{10} & A_1 &= \frac{1}{3} & A_2 &= \frac{1}{15} \\
a_0 &= \frac{1}{10} & a_1 &= \frac{1}{2} & a_2 &= \frac{2}{5} \\
B_0 &= \frac{1}{6} & B_1 &= \frac{1}{3}
\end{aligned}$$

In the (n=4,p=5) case, two free parameters are left (M_1 and M_3).

We did not succeed in calculating by analytical means a scheme with an optimal stability bound.

The best combination of M_1 and M_3 we have found numerically, is given by

$$M_1 = .2776745182, \quad M_3 = .7366565518,$$

yielding a stability bound

$$\beta = -8.4622662640723.$$

The resulting scheme will be presented in section 9.

For the higher order formulas of section 5 through 7, only a finite number of schemes is derived.

We determined β by using a numerical procedure to calculate the zeroes of the polynomials $P_i(z)$, $i = 1, 2, 3$, for each of those schemes. The schemes with the longest stability intervals are listed in section 9.

In table 8.2 we give the results we have found, not only for the schemes we developed, but also for the schemes presented by Fehlberg and other authors.

If no non-zero stability interval is found, this is denoted by $\beta = 0$.

At last, the stability-regions of the schemes presented in the tables 8.1 and 9.1 - 9.4, are given in the figures 8.1 - 8.5.

An s is printed at each investigated point z of the complex plane where the formula is weakly stable.

TABLE 8.2 The stability bound of some Runge-Kutta formulas.

Runge-Kutta formula	Characteristics	β
TABLE 8.1	(n=3,p=4)	-12
NYSTRÖM [1925]	(n=3,p=4)	$4(-2-\sqrt[3]{2+\sqrt[3]{4}}) \approx -6.6900799917069$
FEHLBERG [1972]	(n=4,p=4)	$-\frac{72}{17} \approx -4.2352941176476$
TABLE 9.1	(n=4,p=5)	-8.4622662640723
NYSTRÖM [1925]	(n=4,p=5)	0
ZONNEVELD [1970]	(n=4,p=5)	0
FEHLBERG [1972]	(n=6,p=5)	0
TABLE 9.2	(n=6,p=6)	-10.396968386386
ALBRECHT [1955]	(n=5,p=6)	-9.2426036128093
FEHLBERG [1972]	(n=7,p=6)	0
FEHLBERG [1972]	(n=9,p=7)	-9.8569225631423
TABLE 9.3	(n=7,p=7)	-9.784342857982
HAIRER [1976]	(n=7,p=7)	-5.7532375998338
TABLE 9.4	(n=9,p=8)	-26.617539426346
FEHLBERG [1972]	(n=11,p=8)	0

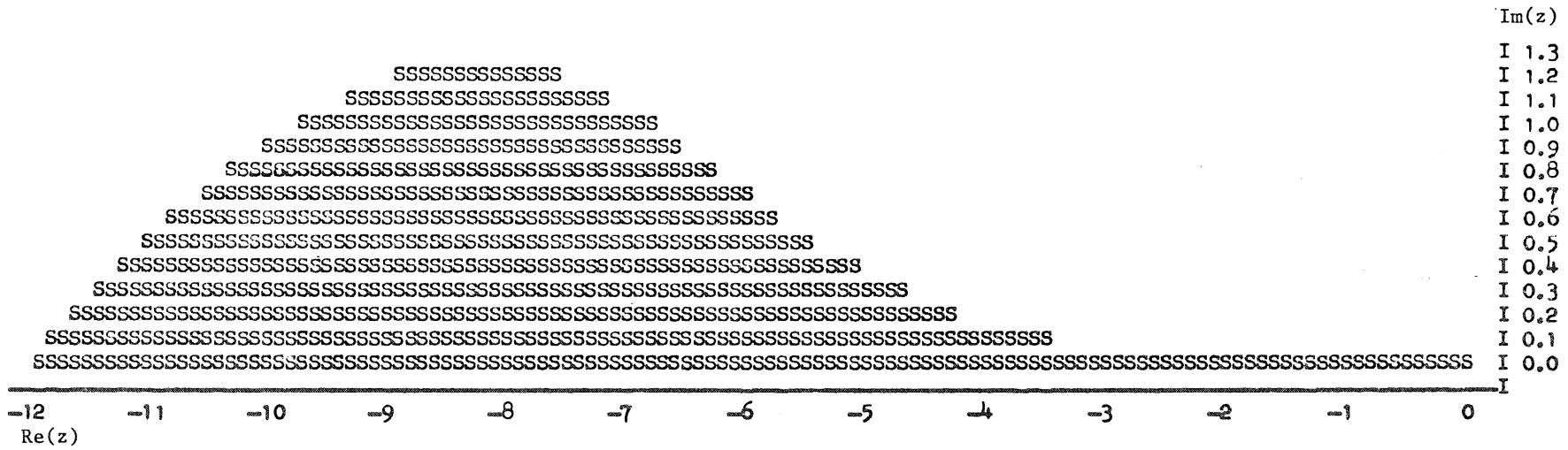


Fig. 8.1. THE STABILITY - REGION OF THE SCHEME GIVEN BY TABLE 8.1

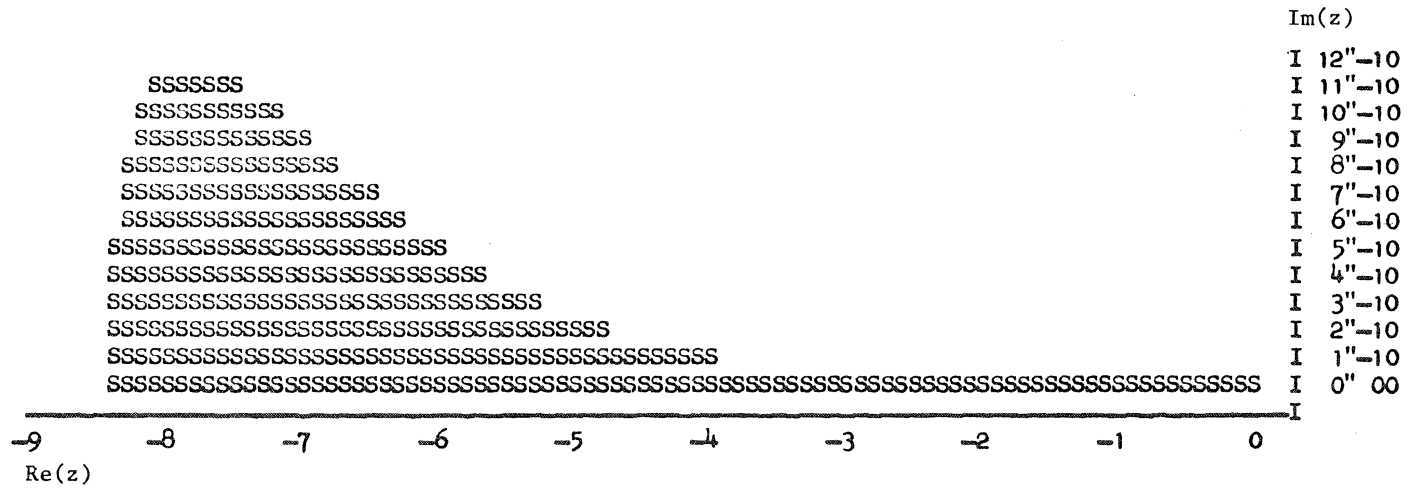


Fig. 8.2. THE STABILITY - REGION OF THE SCHEME GIVEN BY TABLE 9.1

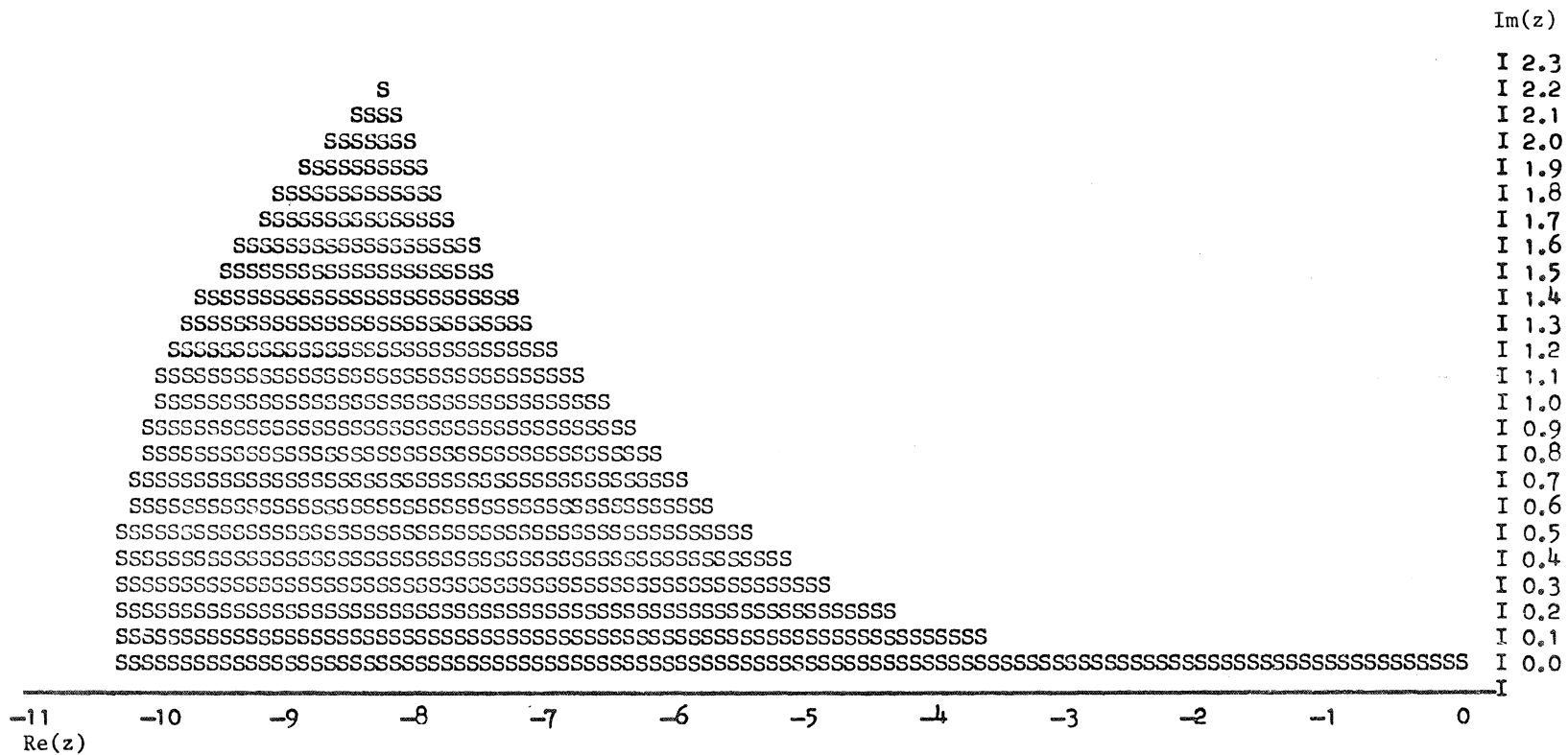


Fig. 8.3. THE STABILITY - REGION OF THE SCHEME GIVEN BY TABLE 9.2

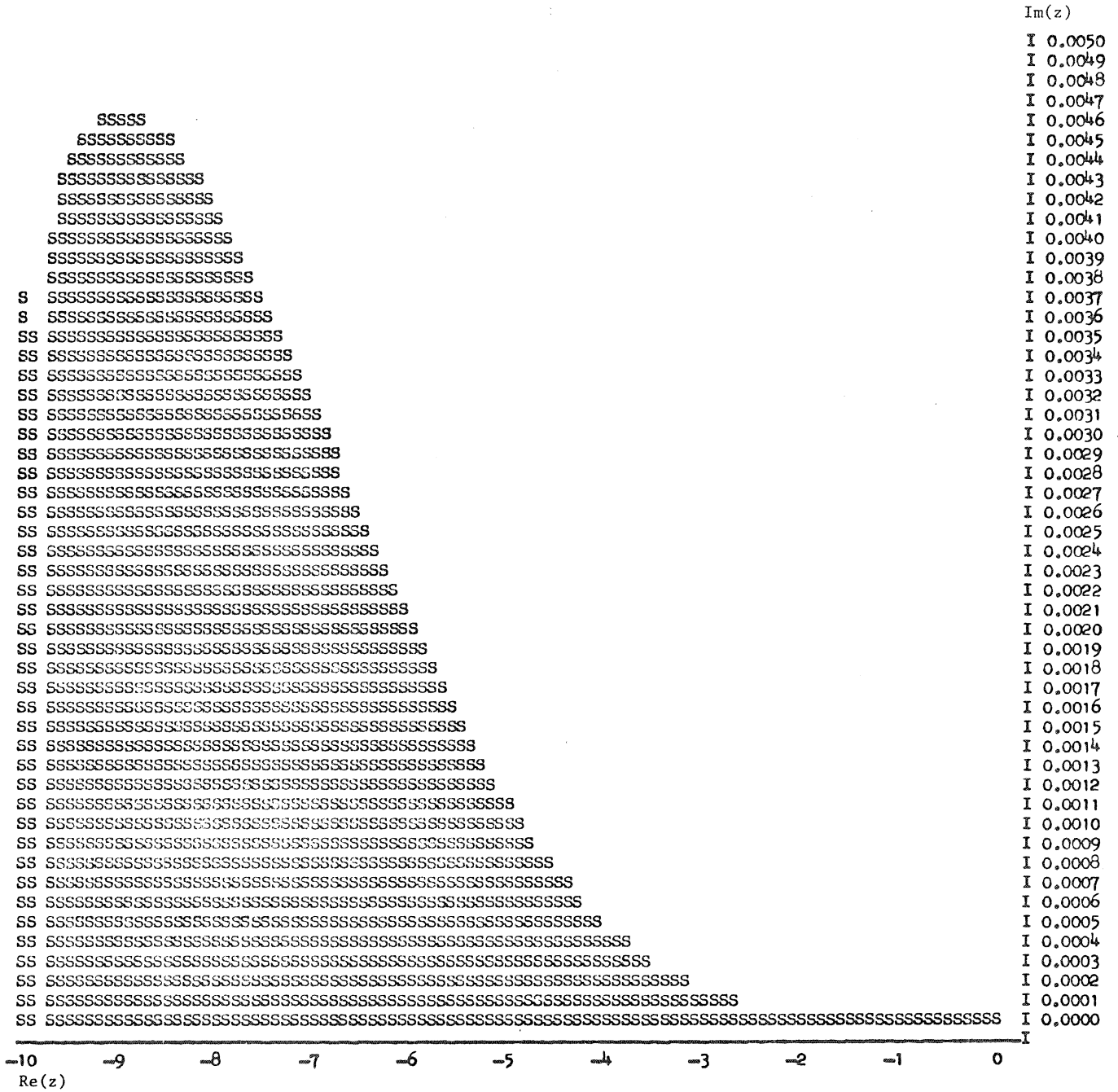


Fig. 8.4. THE STABILITY - REGION OF THE SCHEME GIVEN BY TABLE 9.3

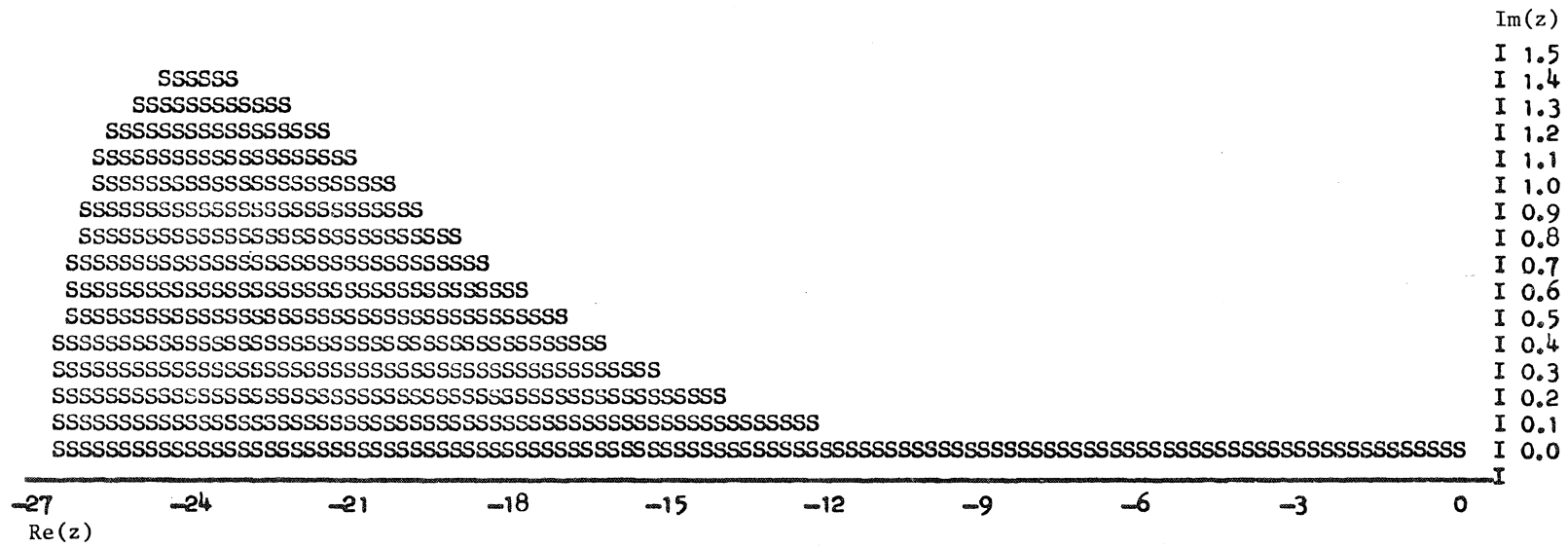


Fig. 8.5. THE STABILITY - REGION OF THE SCHEME GIVEN BY TABLE 9.4

9. SUBROUTINES AND EXAMPLES

In this section, we present four FORTRAN subroutines for the computation of the Runge-Kutta schemes given in the preceding sections. Furthermore, we give some examples obtained by these programs.

All computations were carried out in double precision on a Control Data CYBER 73-28.

RKPAR 45

This subroutine computes an $(n=4, p=5)$ -formula as given in section 4. The meaning of the formal parameters is

$M(i) : M_i, \quad i = 1(1)3;$
 Input : $M(2)$ and $M(3)$ should be given by the user;
 $K(i,j) : K_{ij-1}, \quad i = 1(1)3, \quad j = 1(1)i;$
 $A(i) : a_{i-1}, \quad i = 1(1)4;$
 $AA(i) : A_{i-1}, \quad i = 1(1)4;$
 $BB(i) : B_{i-1}, \quad i = 1(1)3.$

In table 9.1 we give results of RKPAR 45.

The subroutine text is given below.

```

SUBROUTINE RKPAR45(M,K,A,AA,BB)
DOUBLE K(3,3),A(4),AA(4),BB(3),M(3),H1,H2
M(1)=(M(2)*M(3)/3-(M(2)+M(3))/4+.2D0)/
$(M(2)*M(3)/2-(M(2)+M(3))/3+.25)
H1=M(1) $M(1)=M(2) $M(2)=H1
DO 1 I=2,4
A(I)=(M(2)*M(3)/2-(M(2)+M(3))/3+.25)/M(1)/(M(2)-M(1))/(M(3)-M(1))
AA(I)=(1-M(1))*A(I) $H1=M(1) $M(1)=M(2) $M(2)=M(3) $M(3)=H1
1 CONTINUE
BB(2)=(M(2)-.5)/6/M(1)/(M(2)-M(1))
BB(3)=(M(1)-.5)/6/M(2)/(M(1)-M(2))
A(1)=1-A(2)-A(3)-A(4) $AA(1)=.5-AA(2)-AA(3)-AA(4)
BB(1)=.5 -BB(2)-BB(3)
BB(1)=1-BB(2)-BB(3)
K(1,1)=M(1)*M(1)/2
K(2,2)=(M(3)*5-4)/120/M(1)/(M(3)-M(2))/A(3)
H1=(M(2)*5-4)/120/(M(2)-M(3)) $K(2,1)=M(2)*M(2)/2-K(2,2)
H2=((-M(3)*5+4)*M(1)/(M(3)-M(2))+2)/120
K(3,2)=(M(2)*H1-H2)/M(1)/(M(2)-M(1))/A(4)
K(3,3)=(M(1)*H1-H2)/M(2)/(M(1)-M(2))/A(4)
K(3,1)=M(3)*M(3)/2-K(3,2)-K(3,3)
RETURN
END

```

TABLE 9.1 (n=4,p=5)-parameter values

M(1) =	.27767451820000000000000000d+00
M(2) =	.1030765716316241810799106d+01
M(3) =	.73665655180000000000000000d+00
K(1,0) =	.3855156902880106562000000d-01
K(2,0) =	.1035046689895335495004212d-01
K(2,1) =	.5208885140675141896374394d+00
K(3,0) =	.4043773620368925067360654d-01
K(3,1) =	.2157226811781355587552307d+00
K(3,2) =	.1517102027310823219116280d-01
A(0) =	.8299319778775747262452707d-01
A(1) =	.3049416111237371385452454d+00
A(2) =	-.1908833838070589247754553d-02
A(3) =	.1139740249265759780779821d+00
a(0) =	.8299319778775747262452707d-01
a(1) =	.4221664870022824917392322d+00
a(2) =	.6204418640702603472122545d-01
a(3) =	.4327961288029340009150153d+00
B(0) =	.5292387832180889040043506d+00
B(1) =	.4230269281599970360410908d+00
B(2) =	.4773428862191405995455855d-01

RKPAR 66

This subroutine computes an (n=6,p=6)-formula as given in section 5.

The meaning of the formal parameters is

M, K, AA, BB, : see the description of the formal parameters of
RKPAR 45;

Input : For M(3), M(4) and M(5), only permutations are
permitted of the non-zero abscissas of the 4-point
Gauss-Radau quadrature formula. These coefficients
are given in table 9.5;

B(i) : b_{i-1} , $i = 1(1)6$.

In table 9.2 we give results of RKPAR 66.

The subroutine text is given below.

The subroutines RKPAR 66, RKPAR 77 and RKPAR 98 all use the auxiliary
routine PV.

PV(n,A,b) solves the $n \times n$ - Van der Monde system $Ax = b$,
the righthand side, b, being overwritten by the solution x.

An ALGOL 60 version of PV is given by the procedure pvand of BJÖRCK and PEREYRA [1970].

```

SUBROUTINE RKPAN66(M,K,A,AA,B,BB)
DOUBLE K(5,5),A(6),AA(6),B(5),BB(5),M(5),AL(4),XB(4),H1,H2,H3
AL(1)=0DO $XB(1)=1DO
DO 1 I=2,4
AL(I)=M(I+1)
1 XB(I)=1DO/I
CALL PV(4,AL,XB)
DO 2 I=4,6
A(I)=XB(I-2)
2 AA(I)=(1-M(I-1))*A(I)
A(1)=AA(1)=B(1)=BB(1)=XB(1)
A(2)=AA(2)=B(2)=BB(2)=0DO
A(3)=A(4) $AA(3)=AA(4) $A(4)=AA(4)=0DO
BB(3)=AA(3) $BB(4)=AA(6) $BB(5)=AA(5) $B(3)=A(3)
B(4)=A(6) $B(5)=A(5)
M(2)=M(3) $M(3)=M(5)
M(1)=M(2)/2
K(2,2)=M(2)*M(2)/3 $K(2,1)=K(2,2)/2 $K(1,1)=M(1)*M(1)/2
H1=M(3)*3/M(2)/M(2)/3
K(3,2)=(M(2)*2-M(3))*H1
K(3,3)=(M(3)-M(2))*H1/2
K(3,1)=M(3)*M(3)/2-K(3,2)-K(3,3)
H1=-A(3)*M(2)*5/24 $H2=M(2)*H1+1DO/140
H1=H1+1DO/120 $H3=M(5)
K(4,2)=0DO
DO 5 I=4,5
XB(4)=(H1*H3-H2)/(H3-M(I))/A(I+1)-K(I,2)*M(1)*3
DO 3 J=1,3
AL(J+1)=M(I+J-4)
3 XB(J)=M(I)*3*(J+1)/(J+1)/J-K(I,2)*M(1)*3*(J-1)
CALL PV(4,AL,XB)
DO 4 J=2,4
4 K(I,I+J-4)=XB(J)
K(I,1)=XB(1)
K(5,2)=-(A(3)*K(2,2)+A(5)*K(4,2))/A(6)
5 H3=M(4)
RETURN
END

```

TABLE 9.2 (n=6,p=6)-parameter values

M(1) =	.4557060202436480263022269d+00
M(2) =	.9114120404872960526044539d+00
M(3) =	.5905331355592652891350737d+00
M(4) =	.2123405382391529439747581d+00
M(5) =	.5905331355592652891350737d+00
K(1,0) =	.1038339884431520723767253d+00
K(2,0) =	.1384453179242027631689671d+00
K(2,1) =	.2768906358484055263379342d+00
K(3,0) =	.8578857188937532666720522d-01
K(3,1) =	.1018345840159215245890866d+00
K(3,2) =	-.1325846380856805411028647d-01
K(4,0) =	.2800803003656096348645685d-01
K(4,1) =	-.8411131822307058753491315d-01
K(4,2) =	-.2031376376190042082864547d-01
K(4,3) =	.9896130403825663169358284d-01
K(5,0) =	-.2185055439822761348513357d-01
K(5,1) =	-.8599936698851550106972146d-01
K(5,2) =	.1943654655589209444882784d-01
K(5,3) =	-.5679798517591284998964446d-28
K(5,4) =	.2627780669275798172520326d+00
A(0) =	.625000000000000000000000d-01
A(1) =	0.
A(2) =	.1953029743780874450328034d-01
A(3) =	0.
A(4) =	.2590173400786056214104079d+00
A(5) =	.1589523624835856340863117d+00
a(0) =	.625000000000000000000000d-01
a(1) =	0.
a(2) =	.2204622111767683752754785d+00
a(3) =	0.
a(4) =	.3288443199800597439442892d+00
a(5) =	.3881934688431718807802323d+00
B(0) =	.625000000000000000000000d-01
B(1) =	0.
B(2) =	.1953029743780874450328034d-01
B(3) =	.1589523624835856340863117d+00
B(4) =	.2590173400786056214104079d+00
b(0) =	.625000000000000000000000d-01
b(1) =	0.
b(2) =	.2204622111767683752754785d+00
b(3) =	.3881934688431718807802323d+00
b(4) =	.3288443199800597439442892d+00

RKPAR 77

By this subroutine an $(n=7,p=7)$ -formula is computed according to section 6.

The formal parameters have the same meaning as in RKPAR 45.

Input : In $M(i)$, $i = 3(1)6$, any permutation of the non-zero abscissas of the 5-point Gauss-Radau quadrature formula is allowed.

These values are given in table 9.5.

Output is given in table 9.3

The subroutine text is given below.

```

SUBROUTINE RKPAR77(M,K,A,AA,BB)
DOUBLE K(6,6),A(7),AA(7),BB(6),M(6),AL(5),XB(5),H(4)
AL(1)=0D0 $XB(1)=1D0
DO 1 I=2,5
XB(I)=1D0/I
1  AL(I)=M(I+1)
   CALL PV(5,AL,XB)
   AA(1)=A(1)=XB(1)
DO 2 I=4,7
A(I)=XB(I-2)
2  AA(I)=(1-M(I-1))*A(I)
   A(3)=A(4) $AA(3)=AA(4)
   A(2)=AA(2)=A(4)=AA(4)=BB(2)=0D0
   M(2)=M(3) $M(1)=M(2)/2
   H(1)=M(2)*M(4)/12 $H(2)=(M(2)+M(4))/12 $H(3)=(6*M(6)-5)/30
   H(4)=(7*M(6)-6)/840
   M(3)=(H(1)*H(3)-12*H(2)*H(4)+(M(6)*8-7)/1680)/
   $( (M(6)/2-.4D0)*H(1)-H(2)*H(3)+H(4))
DO 3 I=2,5
AL(I)=M(I)
3  XB(I)=1D0/(I+1)/I
   XB(1)=.5D0
   CALL PV(5,AL,XB)
   BB(1)=XB(1)
DO 4 I=3,6
4  BB(I)=XB(I-1)
   K(2,2)=M(2)*M(2)/3 $K(2,1)=K(2,2)/2 $K(1,1)=M(1)*M(1)/2
   H(1)=M(3)*3/M(2)/M(2)/3
   K(3,3)=(M(3)-M(2))*H(1)/2
   K(3,2)=(M(2)*2-M(3))*H(1)
   K(3,1)=M(3)*M(3)/2-K(3,2)-K(3,3)
DO 5 I=1,3
AL(I)=M(I+3)
5  H(I)=.05D0/(I+5)-A(3)*M(2)*M(I+4)/24
   CALL PV(3,AL,H)
DO 6 I=2,4
AL(I)=M(I-1)

```



```

6   XB(I-1)=M(4)××I/(I-1)/I
   XB(4)=H(1)/A(5) $AL(1)=0DO
   H(1)=(3×M(1)+M(3))×XB(4)-((3×M(3)+M(2))×XB(3)-M(2)×M(3)×XB(2))×
   $M(1)
   CALL PV(4,AL,XB)
   DO 7 I=1,4
7   K(4,I)=XB(I)
   DO 8 I=1,2
   AL(I)=M(I+4)
8   XB(I)=1D0/3D1/(I+6)-A(3)×M(2)××(I+5)/48-A(5)×H(1)×M(4)××(I-1)
   CALL PV(2,AL,XB)
   H(1)=XB(2)/A(7) $XB(5)=XB(1)/A(6) $AL(1)=0DO
   DO 9 I=2,4
   AL(I)=M(I-1)
9   XB(I-1)=M(5)××I/(I-1)/I
   XB(4)=H(2)/A(6) $AL(5)=M(4)
   CALL PV(5,AL,XB)
   K(6,2)=(-A(3)×K(2,2)-A(5)×K(4,2)-A(6)×XB(2))/A(7)
   DO 10 I=1,4
   AL(I+1)=M(I+1) $K(5,I)=XB(I)
10  XB(I)=M(6)××(I+1)/(I+1)/I-K(6,2)×M(1)××(I-1)
   AL(5)=M(5) $XB(4)=H(3)/A(7)-K(6,2)×M(1)××3
   K(5,5)=XB(5) $XB(5)=H(1)-K(6,2)×M(1)××4
   CALL PV(5,AL,XB)
   K(6,1)=XB(1)
   DO 11 I=3,6
11  K(6,I)=XB(I-1)
   RETURN
   END

```

TABLE 9.3 (n=7,p=7)-parameter values

M(1) =	.6987993217189027607604354d-01
M(2) =	.1397598643437805521520871d+00
M(3) =	.4000411928274101291618510d+00
M(4) =	.7231569863618761723199540d+00
M(5) =	.9428958038854823178068788d+00
M(6) =	.4164095676310831799433023d+00
K(1,0) =	.2441602460173992818428283d-02
K(2,0) =	.3255469946898657091237711d-02
K(2,1) =	.6510939893797314182475421d-02
K(3,0) =	.6950734459359684445905069d-01
K(3,1) =	-.1316716701046432993328298d+00
K(3,2) =	.1421808034904350215588637d+00
K(4,0) =	-.2233386086311725713815682d+00
K(4,1) =	.6879702203440521524685621d+00
K(4,2) =	-.3696937466464573380016170d+00
K(4,3) =	.1665401483955731370602149d+00
K(5,0) =	.3287948790198381550170291d+00
K(5,1) =	-.7794218868929814567876664d+00
K(5,2) =	.7279190336246760330633300d+00
K(5,3) =	.8817438134280918967577427d-01
K(5,4) =	.7905984139808304501439068d-01
K(6,0) =	.1150566255049276410603826d+00
K(6,1) =	-.2661854428270603663693784d+00
K(6,2) =	.2518203160924605777305588d+00
K(6,3) =	-.1743744160125838100650920d-01
K(6,4) =	.3783359937791662092222736d-02
K(6,5) =	-.3389530995083151069699423d-03
A(0) =	.400000000000000000000000d-01
A(1) =	0.
A(2) =	.1919229301335626622286851d+00
A(3) =	0.
A(4) =	.7789144713919069940076817d-01
A(5) =	.8206647359737825115148046d-02
A(6) =	.1819789753675088132553987d+00
a(0) =	.400000000000000000000000d-01
a(1) =	0.
a(2) =	.2231039010835707444025602d+00
a(3) =	0.
a(4) =	.2813560151494620601921726d+00
a(5) =	.1437135607912259413234122d+00
a(6) =	.3118265229757412540818549d+00
B(0) =	.4349093249446002288355192d-01
B(1) =	0.
B(2) =	.1801702589208266253846778d+00
B(3) =	.1853747664252665626739922d+00
B(4) =	.8392263517292045860892212d-01
B(5) =	.7041406986526330448855974d-02

RKPAR 98

This subroutine computes an $(n=9, p=8)$ -scheme according to section 7.

The formal parameters have the same meaning as in RKPAR 45.

Input : In $M(i)$, $i = 5(1)8$, any permutation of the non-zero abscissas
of the 5-point Gauss-Radau quadrature formula is permitted.

The subroutine text is given below and output is given in table 9.4.

```

SUBROUTINE RKPAR98(M,K,A,AA,BB)
DOUBLE K(8,8),A(9),AA(9),BB(8),M(8),AL(5),XB(5),H1,H2,H3,H4
DO 1 I=1,64
1  K(I)=0DO
   M(4)=M(8) $H1=M(4)/M(5)
   H2=DSQRT((((36×H1-156)×H1+309)×H1-356)×H1+247.2DO)×H1
   $      -96)×H1+16)
   H3=((6×H1-3)×H1-6)×H1+4 $H4=(20×H1-30)×H1+12
   M(2)=(H3-H2)×M(5)/H4 $M(1)=M(2)/2
   M(3)=(-.6DO×M(4)+M(2))×M(4)/(2×M(2)-M(4))
   AL(1)=K(4,2)=0DO $XB(1)=1DO
   DO 2 I=5,8
2  K(I,2)=0DO $XB(I-3)=1DO/(I-3)
   AL(I-3)=M(I)
   CALL PV(5,AL,XB)
   AA(1)=A(1)=BB(1)=XB(1)
   DO 3 I=6,9
3  A(I)=XB(I-4) $A(I-4)=AA(I-4)=BB(I-4)=0DO
   AA(I)=(1-M(I-1))×A(I)
   BB(5)=AA(9) $BB(6)=AA(6) $BB(7)=AA(7) $BB(8)=AA(8)
   K(2,2)=M(2)×M(2)/3 $K(2,1)=K(2,2)/2 $K(1,1)=M(2)×M(2)/8
   H1=M(3)××3/M(2)/M(2)/3
   K(3,3)=(M(3)-M(2))×H1/2
   K(3,2)=(M(2)×2-M(3))×H1
   K(3,1)=M(3)×M(3)/2-K(3,2)-K(3,3)
   DO 4 I=2,5
4  AL(I)=M(I)
   DO 6 I=4,6
   I1=I-1
   DO 5 J=1,I1
5  XB(J)=M(I)××(J+1)/(J+1)/J
   CALL PV(I1,AL,XB)
   K(I,1)=XB(1)
   DO 6 J=3,I
6  K(I,J)=XB(J-1)
   H1=(M(4)-.4DO)/24 $H2=(-M(4)+.5DO)/60 $H3=(7×M(4)-4)/840
   H1=H1×M(5)+H2 $H2=H2×M(5)+H3
   K(8,8)=(H1×M(6)+H2)/M(7)/(M(4)-M(7))/(M(5)-M(7))/(M(6)-M(7))/A(9)
   K(8,3)=(-A(6)×K(5,3)-A(7)×K(6,3))/A(9)
   K(7,3)=0DO
   DO 7 I=2,5

```

```

7  AL(I)=M(I+1)
   DO 9 I=7,8
   DO 8 J=1,5
8  XB(J)=M(I)××(J+1)/(J+1)/J-M(2)××(J-1)×K(I,3)-M(7)××(J-1)×K(I,8)
   CALL PV(5,AL,XB)
   K(I,1)=XB(1)
   DO 9 J=2,5
9  K(I,J+2)=XB(J)
   RETURN
   END

```

TABLE 9.4 (n=9,p=8)-parameter values

```

M(1) = .8818229058097346629799006d-01
M(2) = .1763645811619469325959801d+00
M(3) = .6220922173571816799625451d+00
M(4) = .9428958038854823178068788d+00
M(5) = .4164095676310831799433023d+00
M(6) = .1397598643437805521520871d+00
M(7) = .7231569863618761723199540d+00
M(8) = .9428958038854823178068788d+00

K(1,0) = .3888058186053620856159670d-02
K(2,0) = .5184077581404827808212893d-02
K(2,1) = .1036815516280965561642579d-01
K(3,0) = .3134675608043437668474804d+00
K(3,1) = -.6949576439586949831692579d+00
K(3,2) = .5749894466025387040452510d+00
K(4,0) = .2810461118860262102526799d-01
K(4,1) = 0.
K(4,2) = .2677390223867939117083915d+00
K(4,3) = .1486826149170284332491982d+00
K(5,0) = .2248149984228374125063083d-01
K(5,1) = 0.
K(5,2) = .6245918460927543984770666d-01
K(5,3) = .1991771986403440151571168d-02
K(5,4) = -.2339924306098028496020526d-03
K(6,0) = .5924114075638131713906331d-02
K(6,1) = 0.
K(6,2) = .5309291308653655691200868d-02
K(6,3) = .8333008496983745026004293d-03
K(6,4) = -.7960596809014396389028383d-04
K(6,5) = -.2220690425204046670104212d-02
K(7,0) = .2771602104885062624174655d-01
K(7,1) = 0.
K(7,2) = 0.

```

$K(7,3) = .1198123112201063571813080d-01$
 $K(7,4) = .3562959533375963104928727d-03$
 $K(7,5) = .8781592732724059424652266d-01$
 $K(7,6) = .1336085380105559276286989d+00$
 $K(8,0) = .2692793813438841381260518d-01$
 $K(8,1) = 0.$
 $K(8,2) = -.1437648183915948208072228d+00$
 $K(8,3) = -.2907165771619611066932433d-01$
 $K(8,4) = .1564197820471100178394809d-02$
 $K(8,5) = .2010144318800217964285312d+00$
 $K(8,6) = .3128329549048853539632465d+00$
 $K(8,7) = .7502320186044923307662709d-01$

$A(0) = .400000000000000000000000d-01$
 $A(1) = 0.$
 $A(2) = 0.$
 $A(3) = 0.$
 $A(4) = 0.$
 $A(5) = .1819789753675088132553987d+00$
 $A(6) = .1919229301335626622286851d+00$
 $A(7) = .7789144713919069940076817d-01$
 $A(8) = .8206647359737825115148046d-02$

$a(0) = .400000000000000000000000d-01$
 $a(1) = 0.$
 $a(2) = 0.$
 $a(3) = 0.$
 $a(4) = 0.$
 $a(5) = .3118265229757412540818549d+00$
 $a(6) = .2231039010835707444025602d+00$
 $a(7) = .2813560151494620601921726d+00$
 $a(8) = .1437135607912259413234122d+00$

$B(0) = .400000000000000000000000d-01$
 $B(1) = 0.$
 $B(2) = 0.$
 $B(3) = 0.$
 $B(4) = .8206647359737825115148046d-02$
 $B(5) = .1819789753675088132553987d+00$
 $B(6) = .1919229301335626622286851d+00$
 $B(7) = .7789144713919069940076817d-01$

TABLE 9.5 Non-zero abscissas of the Gauss-Radau quadrature formula

$$\int_0^1 f(x) dx \simeq w_1 f(0) + \sum_{i=2}^{n_r} w_i f(x_i)$$

n_r	x_i
4	.212340538239152943974758110 .590533135559265289135073748 .911412040487296052604453856
5	.139759864343780552152087081 .410409567631083179943302331 .723156986361876172319954003 .942895803885482317806878807

10. CONCLUSIONS

In our opinion, a Runge-Kutta formula given by (1.2) should conform to the following three conditions:

- (i) for a given order of accuracy p , the number of function evaluations should be as small as possible for reasons of efficiency.
- (ii) the interval of stability as defined in section 8 should be as long as possible.
- (iii) the formula should make a more or less reliable error estimate for stepsize control at the cost of little computational effort.

In fact, with any formula a suitable error estimate can be established by a comparison of the results obtained by taking a step h and the results obtained by performing twice a step $h/2$.

This procedure of error estimation is rather expensive. As far as we know, the only low-cost error estimates can be made by the formulas of Fehlberg, Zonneveld and our schemes.

It is true that according to our schemes a more conservative error estimate is obtained than by those of Fehlberg and Zonneveld. On the other hand, our formulas are more favourable considering condition (i).

Furthermore, we see from table 8.2 that our fourth, fifth, sixth, and eighth formulas are considerable improvements of the existing schemes, because of their extended interval of stability. Moreover, our formulas satisfy property (i) as well as property (iii).

Only the Fehlberg ($n=9, p=7$) formula is competitive with respect to (ii).

ACKNOWLEDGEMENTS

The authors wish to thank Prof. dr. P.J. van der Houwen for his useful criticism. They are also grateful to ms. M. Jellema and ir. D. Weingarten for their careful reading of the manuscript.

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