stichting mathematisch centrum

.

AFDELING NUMERIEKE WISKUNDE

NW 14/74 DECEMBER

P.A. BEENTJES SOME SPECIAL FORMULAS OF THE ENGLAND CLASS OF FIFTH ORDER RUNGA-KUTTA SCHEMES

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 nonprofit 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), by the Municipality of Amsterdam, by the University of Amsterdam, by the Free University at Amsterdam, and by industries.

AMS (MOS) subject classification scheme (1970): 65L05

Some special formulas of the England class of fifth order Runge-Kutta schemes

,

Ъy

P.A. Beentjes.

In this report two fifth order, six-point Runge-Kutta formulas will be presented. Special attention is paid to enlarge the stability regions and to minimize the truncation error of the schemes.

KEYWORDS & PHRASES: Differential equations, explicit Runge-Kutta methods.

· .

ABSTRACT

### 1. INTRODUCTION

This paper deals with some special fifth order, six-point Runge-Kutta formulas for the solution of initial value problems of the type

(1.1) 
$$y' = f(x,y), y_0 = y(x_0).$$

The formulas to be presented are members of a class of Runge-Kutta schemes given by ENGLAND [1]. The well-known schemes of SARAFYAN [6] and FEHLBERG [2] also belong to this England family.

In section 2, we give definitions and consistency conditions for fifth order, six-point Runge-Kutta formulas. Furthermore, the England class of parameters satisfying these conditions will be discussed. In section 3, schemes are derived with an extended region of stability as well as schemes characterized by a small truncation error. In section 4, test results of these formulas are compared with results of other fifth order, six-point Runge-Kutta formulas.

### 2. RK56 FORMULAS; THE ENGLAND FAMILY

A six-point Runge-Kutta scheme for the solution of (1.1) is given by

(2.1)  

$$\begin{cases}
K_{0} = hf(x_{n}, y_{n}), \\
K_{i} = hf(x_{n} + \mu_{i}h, y_{n} + \sum_{j=0}^{i-1} \lambda_{ij} K_{j}), \quad i=1(1)5, \\
x_{n+1} = x_{n} + h, \\
y_{n+1} = y_{n} + \sum_{i=0}^{5} \theta_{i} K_{i}.
\end{cases}$$

Fifth order accuracy of this scheme requires

(2.2) 
$$y_{n+1} = \tilde{y}(x_{n+1}) + O(h^6),$$

where  $\tilde{y}$ , the local analytical solution, satisfies

$$y' = f(x,y), y(x_n) = y_n$$
.

Formulas given by (2.1) and satisfying (2.2) will be called RK56 schemes.

By expanding  $y_{n+1}$  and  $\tilde{y}(x_{n+1})$  in a Taylor series about  $x_n$  and equating terms with equal powers in h, we are led to the following consistency conditions for the parameters  $\mu_i$ ,  $\lambda_{ij}$  and  $\theta_i$ , i=1(1)5, j=0(1)i-1 (see ZONNEVELD [7]).

$$\sum_{i=0}^{5} \theta_{i} \mu_{i}^{k} = \frac{1}{k+1}, \quad k=0(1)4,$$

$$\sum_{i=2}^{5} \theta_{i} \mu_{i}^{k} \sum_{j=1}^{i-1} \lambda_{ij} \mu_{j} = \frac{1}{2k+6}, \quad k=0,1,2,$$

$$\sum_{i=2}^{5} \theta_{i} \sum_{j=1}^{i-1} \lambda_{ij} \mu_{j}^{k} = \frac{1}{(k+1)(k+2)}, \quad k=2,3,$$

$$\sum_{i=3}^{5} \theta_{i} \mu_{i}^{k} \sum_{j=2}^{i-1} \lambda_{ij} \sum_{\ell=1}^{j-1} \lambda_{j\ell} \mu_{\ell} = \frac{1}{6k+24}, \quad k=0,1,$$

$$\sum_{i=2}^{5} \theta_{i} \mu_{i} \sum_{j=1}^{i-1} \lambda_{ij} \mu_{j}^{2} = \frac{1}{15},$$

$$\sum_{i=2}^{5} \theta_{i} \sum_{j=2}^{i-1} \lambda_{ij} \mu_{j} \sum_{\ell=1}^{j-1} \lambda_{j\ell} \mu_{\ell} = \frac{1}{40},$$

$$\sum_{i=3}^{5} \theta_{i} \sum_{j=2}^{i-1} \lambda_{ij} \sum_{\ell=1}^{j-1} \lambda_{j\ell} \mu_{\ell} = \frac{1}{40},$$

$$\sum_{i=3}^{5} \theta_{i} \sum_{j=2}^{i-1} \lambda_{ij} \sum_{\ell=1}^{j-1} \lambda_{j\ell} \mu_{\ell} = \frac{1}{60},$$

$$\sum_{i=4}^{5} \theta_{i} \sum_{j=3}^{i-1} \lambda_{ij} \sum_{\ell=1}^{j-1} \lambda_{j\ell} \mu_{\ell} = \frac{1}{120},$$

$$\sum_{i=4}^{i-1} \theta_{i} \sum_{j=3}^{j-1} \lambda_{ij} \sum_{\ell=2}^{j-1} \lambda_{j\ell} \sum_{\ell=1}^{j-1} \lambda_{\ell} \mu_{\ell} = \frac{1}{120},$$

$$\sum_{i=4}^{i-1} \theta_{i} \sum_{j=3}^{j-1} \lambda_{ij} \sum_{\ell=2}^{j-1} \lambda_{j\ell} \sum_{\ell=1}^{j-1} \lambda_{\ell} \mu_{\ell} = \frac{1}{120},$$

$$\sum_{i=4}^{i-1} \theta_{i} \sum_{j=3}^{j-1} \lambda_{ij} \sum_{\ell=2}^{j-1} \lambda_{\ell} \sum_{\ell=1}^{j-1} \lambda_{\ell} \mu_{\ell} = \frac{1}{120},$$

$$\sum_{i=4}^{i-1} \theta_{i} \sum_{\ell=3}^{j-1} \lambda_{\ell} \sum_{\ell=1}^{j-1} \lambda_{\ell} \sum_{\ell=1}^{j-1} \lambda_{\ell} \mu_{\ell} = \frac{1}{120},$$

$$\sum_{i=4}^{i-1} \theta_{i} \sum_{\ell=3}^{j-1} \lambda_{\ell} \sum_{\ell=1}^{j-1} \lambda_{\ell} \sum_{\ell=1}^{j-1} \lambda_{\ell} \mu_{\ell} = \frac{1}{120},$$

ENGLAND has given the following family of solutions of (2.3),  $\mu_{\rm i},\,i=1,2,4,5,$  being free parameters

$$\mu_{3} = \frac{\mu_{2}}{10\mu_{2}^{2} - 8\mu_{2} + 2},$$
  
$$\lambda_{i1} = \frac{\alpha_{i} \mu_{i} \mu_{2}}{2\alpha_{2} \mu_{1}}, \quad i=2,3,4,5 \quad (\alpha_{i}=3-12\mu_{i}+10\mu_{i}^{2}),$$

(2.3)

$$\begin{split} \lambda_{32} &= \frac{\mu_3^2}{\mu_2^2 \delta_{32}}, \qquad (\delta_{ij} = \mu_i - \mu_j), \\ \lambda_{42} &= \frac{\mu_4 \delta_{42} [\mu_2 + \mu_4 - 4\mu_2 \mu_4 - \frac{1}{2}\mu_3 (3 - 10\mu_2 \mu_4)]}{\mu_2 \alpha_2 \delta_{23}}, \\ \lambda_{43} &= \frac{\mu_2 \mu_4 \delta_{42} \delta_{34}}{2\mu_3^2 \alpha_2 \delta_{23}}, \\ \theta_1 &= 0, \\ \theta_2 &= \frac{12 - 15(\mu_3 + \mu_4 + \mu_5) + 20(\mu_3 \mu_4 + \mu_4 \mu_5 + \mu_5 \mu_3) - 30\mu_3 \mu_4 \mu_5}{60\mu_2 \delta_{23} \delta_{24} \delta_{25}}, \end{split}$$

( $\theta_i$ , i=3,4,5 can be found by interchanging  $\mu_2$  and  $\mu_i$ , i=3,4,5 in the formula for  $\theta_2$ ).

The remaining parameters  $\lambda_{5i}$ , i=2,3,4, satisfy

$$\begin{pmatrix} \mu_{2} & \mu_{3} & \mu_{4} \\ \mu_{2}^{2} & \mu_{3}^{2} & \mu_{4}^{2} \\ \mu_{2}^{3} & \mu_{3}^{3} & \mu_{4}^{3} \end{pmatrix} \begin{pmatrix} \lambda_{52} \\ \lambda_{53} \\ \lambda_{54} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\mu_{5} & \delta_{52}(3-10\mu_{2}\mu_{5})/\alpha_{2} \\ \mu_{5} & \delta_{52}(\mu_{2}+\mu_{5}-4\mu_{2}\mu_{5})/\alpha_{2} \\ [\frac{1}{20} - \theta_{4}(\lambda_{42}\mu_{2}^{3}+\lambda_{43}\mu_{3}^{3}) - \theta_{3}\lambda_{32}\mu_{2}^{3}]/\theta_{5} \end{pmatrix}.$$

This family has the property that, for every member, parameters  $\theta'_i$ , i=0(1)4, exist, satisfying

(2.4) 
$$y_{n+1}^{*} = y_n + \sum_{i=0}^{4} \theta_i^{*} K_i = \tilde{y}(x_{n+1}) + O(h^5),$$

i.e. in every step a fourth order approximation to  $\tilde{y}$  can also be provided. Note that this does not imply extra function evaluations.

By virtue of (2.4) we have the discrepance function

$$\rho_n = y_{n+1} - y_{n+1}^*,$$

that can be used to control the stepsize.

The parameters  $\theta_i$ , i=0(1)4, of the embedded formula (2.4) are given by

$$\theta_{0}^{\prime} = 1 - \sum_{i=1}^{4} \theta_{i}^{\prime},$$
  

$$\theta_{1}^{\prime} = 0,$$
  

$$\theta_{2}^{\prime} = \frac{3 - 4(\mu_{3} + \mu_{4}) + 6\mu_{3} \mu_{4}}{\mu_{2} \delta_{23} \delta_{24}},$$

( $\theta'_3$  and  $\theta'_4$  follow by interchanging  $\mu_2$  and  $\mu_3$  ( $\mu_4$ ) in the formula for  $\theta'_2$ ).

# 3. STABILITY AND TRUNCATION ERROR ANALYSIS

In this section, we investigate how to choose the free parameters of the England formula in order to arrive

(i) at schemes with an extended region of stability and

(ii) at schemes with a small truncation error.

Considering case (i) we restrict our investigations to the model equation

(3.1) 
$$y' = \delta y, \quad y_0 = y(x_0), \quad \delta \in \mathbb{C}.$$

Application of any given England scheme to this problem leads to

$$y_{n+1} = A^{n+1} y_0,$$

where

A = 
$$\sum_{i=0}^{5} \frac{z^{i}}{i!} + \beta z^{6}$$
, (z=h $\delta$ ),

and

$$\beta = \frac{\mu_2 (2-5\mu_2)}{480(1-4\mu_2+5\mu_2^2)} .$$

4

It is well known that stability of the computed solution is guaranteed if

$$|A(z)| \leq 1.$$

Furthermore, restricting to all  $\delta \in \mathbb{R}^-$ , it is easily verified (see VAN DER HOUWEN [5]) that  $\beta$  should equal .725590420168<sub>10</sub>-3 in order to make the stepsizes as large as possible (hmax  $\approx \frac{6.26}{|\delta|}$ ). According to figure 3.1, two values of  $\mu_2$  correspond with this special value of  $\beta$ . The greatest value of  $\mu_2$  turns out to give the most preferable schemes. One of these schemes is given in table 3.1.

 $\mu_1 = .2397 \ 9755 \ 2188 \ 7719$  $\mu_2$  = .3596 963 8283 1579  $\mu_3 = .8641 \ 4807 \ 0993 \ 4909$  $\mu_{4} = (6+\sqrt{6})/10$  $\mu_{5} = (6 - \sqrt{6}) / 10$  $\lambda_{10} = \mu_1$  $\lambda_{20} = .0899 \ 2408 \ 2070 \ 7895$  $\lambda_{21}$  = .2697 7224 6212 3684  $\lambda_{30} = .7628 7552 6076 9037$  $\lambda_{31} = -2.8102\ 7540\ 6591\ 7028$  $\lambda_{32} = 2.9115 4795 1508 2901$  $\lambda_{40} = .0863 5521 5681 8012$  $\lambda_{41} = \lambda_{51} = 0$  $\lambda_{42} = .5918 \ 6622 \ 4879 \ 5822$  $\lambda_{43} = .1667 \ 2753 \ 3716 \ 9358$ 

Next we consider case (ii). We remark that the leading term of the truncation error of an RK56 scheme consists of 20 subterms, each of the form

$$T_v \cdot P_v \cdot h^6$$
,  $v=1(1)20$ .

An expression P<sub>v</sub> stands for a number of partial derivatives, depending on the differential equation under consideration. On the other hand, the coefficients T<sub>v</sub> are functions of the RK56 parameters, i.e. problem-independent (for example T<sub>1</sub> =  $\beta - \frac{1}{720}$ , cf. FEHLBERG [3]).

Therefore, regardless of the particular equation to be solved, we might obtain small truncation errors by minimizing  $|T_{v}|$ , v=1(1)20. For this purpose, we introduce some conditions by which several  $T_{v}$  vanish

$$\sum_{j=1}^{i-1} \lambda_{ij} \mu_{j}^{2} = \frac{\mu_{i}^{3}}{3}, \quad i=2(1)5,$$

$$\sum_{i=j+1}^{5} \theta_{i} \lambda_{ij} = \theta_{j}(1-\mu_{j}), \quad j=2,3,4.$$

To satisfy these extra conditions, we must take

$$\mu_1 = \frac{2}{3}\mu_2$$
,  $\mu_5 = 1$ .

Next, we take  $\mu_2 = \frac{5-\sqrt{5}}{10}$  in order to minimize  $T_1$  (see fig. 3.1). With the last free parameter  $(\mu_4)$ , several interesting schemes are possible. In our opinion, and justified by testresults, the most promising scheme is the one given in table 3.2.

$^{\mu}$ i		$^{\lambda}$ ij				
<u>5-p</u> 15	<u>5-p</u> 15					$p = \sqrt{5}$
<u>5-p</u> 10	<u>5-p</u> 40	<u>15-3p</u> 40				
$\frac{1}{2}$	$\frac{3}{16}$	- <u>3p</u> 16	<u>5+3p</u> 16			
<u>5+p</u> 10	<u>9+p</u> 40	- <u>15+3p</u> 40	<u>5+3p</u> 20	$\frac{2}{5}$		
1	$-\frac{3}{4}$	<u>3p</u> 4	<u>5-p</u> 4	-2	<u>5-p</u> 2	
$\theta_{i} \frac{1}{12}$	0	$\frac{5}{12}$	0	5 12	$\frac{1}{12}$	
θ <b>' 0</b> i	0	<u>5</u> 6	$-\frac{2}{3}$	<u>5</u> 6		

Table 3.2.

An RK56 scheme with a small truncation error

Finally, in figure 3.2, we have illustrated the stability regions of the formulas given by tables 3.1 - 3.2.

The regions are symmetric with respect to the real z-axis. The stability area of the formula given by table 3.2 is bounded by the dashed line.



The stability parameter  $\beta$  as a function of  $\mu_2$ 



figure 3.2

Stability regions of two special RK56 methods for equations of the type y' =  $\delta y$  (z =  $h\delta$ )

4. TEST RESULTS

In this section, the test results of the following RK56 schemes are given

RK1, the formula defined by table 3.1; RK2, the formula defined by table 3.2; RKS, Sarafyan scheme; RKF, Fehlberg formula. Both RKS and RKF can be found in reference [2]; RKZ, Zonneveld formula [7].

Before testing, all methods above were implemented in a way as proposed by ZONNEVELD [7]. This design provides the formulas with automatic stepsize control.

In figures 4.1 - 4.4, test results are indicated by the following marks:



× (RK1), + (RK2),  $\gamma$  (RKF),  $\Box$  (RKS) and  $\Diamond$  (RKZ).

Figure 4.1 Results of problem 1



figure 4.2 Results of problem 2



figure 4.3 Results of problem 3



figure 4.4 Results of problem 4

Test problems

All test problems were taken from FOX [4].

Problem 1

$$\begin{cases} y_1' = y_1^2 y_2', \\ y_2' = -1/y_1, \quad y_1(0) = y_2(0) = 1. \\ \text{Integration interval [0,5].} \\ \text{Solution } y_1 = 1/y_2 = e^x. \end{cases}$$

Results for  $y_1$  are given in figure 4.1.

Problem 2

y' =  $y - \frac{2x}{y}$ , y(0) = 1. Integration interval [0,5]. Solution  $y = \sqrt{(2x+1)}$ .

Results are given in figure 4.2.

Problem 3

Solution  $y = .02 + .2x + x^{2}$ .

Results are given in figure 4.3.

Problem 4

$$\begin{cases} y_1'' = y_1 + 2y_2' - \frac{(1-\mu)(y_1+\mu)}{((y_1+\mu)^2 + y_2^2)^{3/2}} - \frac{\mu(y_1-1+\mu)}{((y_1-1+\mu)^2 + y_2^2)^{3/2}}, \\ y_2'' = y_2 - 2y_1' - \frac{(1-\mu)y_2}{((y_1+\mu)^2 + y_2^2)^{3/2}} - \frac{\mu y_2}{((y_1-1+\mu)^2 + y_2^2)^{3/2}}, \\ y_1(0) = .994, \quad y_2(0) = 0, \quad y_1'(0) = 0, \\ y_2'(0) = -2.03173263, \quad \mu = .012277471. \end{cases}$$

Integration interval: orbit closure (period = 11.124340337266). Results for y<sub>1</sub> are given in figure 4.4.

The results show that the method RK2 provides the best results for three of the four test problems. Also formula RK1 is attractive, especially in cases where the spectral radius of the Jacobian matrix of the problem can grow to relatively large values (see problem 4). Furthermore, notice that RKF and RKZ give nearly the same results (except for problem 4 where RKZ failed to give significant solutions).

## REFERENCES

- [1] ENGLAND, R., Error estimates for Runge-Kutta type solutions to systems of ordinary differential equations, The Computer Journal 12, pp. 166-170, 1969.
- [2] FEHLBERG, E., Klassische Runge-Kutta-Formeln vierter und niedriger Ordnung mit Schrittweiten-Kontrolle und ihre Anwendung auf Wärmeleitungsprobleme, Computing 6, pp. 61-71, 1970.

12

- [3] FEHLBERG, E., Classical fifth-, sixth-, seventh- and eighth-order Runge-Kutta formulas with stepsize control, NASA Technical Report 287, 1968.
- [4] FOX, P., A comparative study of computer programs for integrating differential equations, Communications of the ACM, November 1972, Volume 15, Number 11.
- [5] HOUWEN, P.J. VAN DER, One-step methods for linear initial value problems I. Polynomial methods, TW Report 119, Mathematical Centre, Amsterdam, 1970.
- [6] SARAFYAN, D., Error estimation for Runge-Kutta methods through pseudoiterative formulas, Tech. Rep. No. 14, Louisiana State University, New Orleans.
- [7] ZONNEVELD, J.A., Automatic numerical integration, MC Tract 8, Mathematical Centre, Amsterdam, 1964.