stichting mathematisch centrum



AFDELING NUMERIEKE WISKUNDE

NW 14/75 AUGUST

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

2nd printing

Printed at the Mathematical Centre, 49, 2e Boerhaavestraat, Amsterdam.

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

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

P.A. Beentjes.

ABSTRACT

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.

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

Fifth order accuracy of this scheme requires

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

where 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 μ_i , λ_{ij} and θ_i , i=1(1)5, j=0(1)i-1 (see ZONNEVELD [7]).

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

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

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

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

$$\sum_{i=3}^{5} \theta_{i} \quad \mu_{i}^{k} \quad \sum_{j=1}^{i-1} \lambda_{ij} \quad \mu_{j}^{2} = \frac{1}{15},$$

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$$\sum_{i=2}^{5} \theta_{i} \quad \sum_{j=1}^{i-1} \lambda_{ij} \quad \mu_{j}^{2} = \frac{1}{20},$$

$$\sum_{i=3}^{5} \theta_{i} \quad \sum_{j=2}^{i-1} \lambda_{ij} \quad \mu_{j}^{2} = \frac{1}{20},$$

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

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

$$\sum_{i=4}^{5} \theta_{i} \quad \sum_{j=3}^{i-1} \lambda_{ij} \quad \sum_{k=2}^{i-1} \lambda_{jk} \quad \sum_{k=1}^{i-1} \lambda_{k} \quad \mu_{k} = \frac{1}{120},$$

$$\sum_{i=4}^{5} \theta_{i} \quad \sum_{j=3}^{i-3} \lambda_{ij} \quad \sum_{k=2}^{i-1} \lambda_{jk} \quad \mu_{k}^{2} = \frac{1}{120},$$

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$$\sum_{i=4}^{5} \theta_{i} \quad \sum_{j=3}^{i-1} \lambda_{ij} \quad \sum_{k=2}^{i-1} \lambda_{ij} \quad \sum_{k=$$

ENGLAND has given the following family of solutions of (2.3), μ_i , i=1,2,4,5, being free parameters

$$\mu_{3} = \frac{\mu_{2}}{10\mu_{2}^{2} - 8\mu_{2} + 2},$$

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

$$\lambda_{32} = \frac{\mu_{3}^{2}}{\mu_{2}^{2} \delta_{32}}, \quad (\delta_{ij} = \mu_{i} - \mu_{j}),$$

$$\lambda_{42} = \frac{\mu_{4}^{2} \delta_{42} [\mu_{2} + \mu_{4}^{2} - 4\mu_{2} \mu_{4}^{2} - \frac{1}{2} \mu_{3} (3 - 10\mu_{2} \mu_{4})]}{\mu_{2}^{2} \alpha_{2}^{2} \delta_{23}},$$

$$\lambda_{43} = \frac{\mu_{2}^{2} \mu_{4}^{2} \delta_{42}^{2} \delta_{34}}{2\mu_{3}^{2} \alpha_{2}^{2} \delta_{23}},$$

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

$$\theta_{2} = \frac{12 - 15(\mu_{3} + \mu_{4} + \mu_{5}) + 20(\mu_{3} \mu_{4} + \mu_{4} \mu_{5} + \mu_{5} \mu_{3}) - 30\mu_{3}^{2} \mu_{4}^{2} \mu_{5}}{60\mu_{2}^{2} \delta_{23}^{2} \delta_{24}^{2} \delta_{25}^{2}},$$

(θ , i=3,4,5 can be found by interchanging μ_2 and μ_1 , i=3,4,5 in the formula for θ_2).

The remaining parameters λ_{5i} , i=2,3,4, satisfy

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

This family has the property that, for every member, parameters θ_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

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

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

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

(θ 's and θ 's follow by interchanging μ_2 and μ_3 (μ_4) in the formula for θ 's).

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

Application of any given England scheme to this problem leads to

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

where

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

and

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

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 β should equal .725590420168 $_{10}^{-3}$ in order to make the stepsizes as large as possible (hmax $\approx \frac{6.26}{|\delta|}$). According to figure 3.1, two values of μ_2 correspond with this special value of β . The greatest value of μ_2 turns out to give the most preferable schemes. One of these schemes is given in table 3.1.

Table 3.1
Parameters for a stabilized RK56 scheme

```
\mu_1 = .2397 9755 2188 7719
\mu_2 = .3596 963 8283 1579
\mu_3 = .8641 4807 0993 4909
\mu_{\Delta} = (6+\sqrt{6})/10
\mu_5 = (6 - \sqrt{6})/10
\theta_0 = 1/9 \theta_0' = .1133 7183 4406 3626

\theta_1 = \theta_2 = \theta_3 = \theta_1' = 0 \theta_2' = .5154 2899 9323 3072

\theta_4 = (16-\sqrt{6})/36 \theta_3' = .0494 7703 5387 8394

\theta_5 = (16+\sqrt{6})/36 \theta_4' = .3217 3823 0273 4672
\lambda_{10} = \mu_1
\lambda_{20} = .0899 2403 2070 7895
\lambda_{21} = .2697722462123684
\lambda_{30} = .7628 7552 6076 9037
\lambda_{31} = -2.8102754065917028
\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
```

$$\lambda_{50} = .1562$$
 2831 0184 1035
 $\lambda_{52} = .2139$ 2740 2057 0159
 $\lambda_{53} = -.0601$ 9013 5077 9534
 $\lambda_{54} = .0450$ 8544 8558 5176

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_{ν} stands for a number of partial derivatives, depending on the differential equation under consideration. On the other hand, the coefficients T_{ν} are functions of the RK56 parameters, i.e. problem-independent (for example $T_{1} = \beta - \frac{1}{720}$, cf. FEHLBERG [3]).

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

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

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 (μ_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.

Table 3.2.

An RK56 scheme with a small truncation error

$^{\mu}$ i		${}^{\lambda}\mathtt{i}\mathtt{j}$				
5-p 15	5-p 15					$p = \sqrt{5}$
5-p 10	5-p 40	15-3p 40				
$\frac{1}{2}$	<u>3</u> 16	$-\frac{3p}{16}$	5+3 _p 16			
5+p 10	9+p 40	- 15+3p	5+3p 20	<u>2</u> 5		
1	$-\frac{3}{4}$	<u>3p</u> 4	<u>5-p</u>	-2	<u>5−p</u>	
$\theta_{i} \frac{1}{12}$	0	<u>5</u> 12	0	<u>5</u> 12	<u>1</u> 12	
θ ; Ο	0	<u>5</u>	$-\frac{2}{3}$	<u>5</u>		

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.

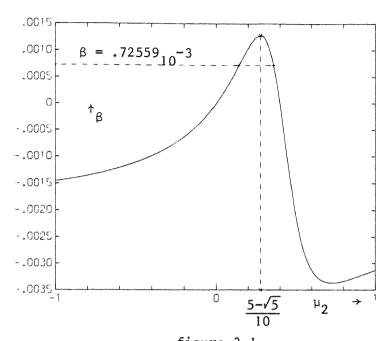


figure 3.1

The stability parameter β as a function of $\boldsymbol{\mu}_2$

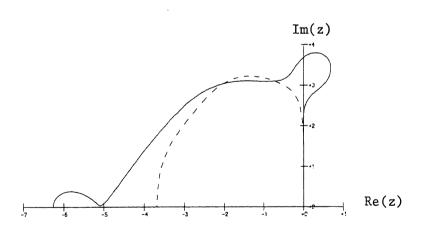


figure 3.2

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

4. TEST RESULTS

In this section, the test results of the following RK56 schemes are given $\frac{1}{2}$

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:

$$\times$$
 (RK1), + (RK2), Y (RKF), \Box (RKS) and \Diamond (RKZ).

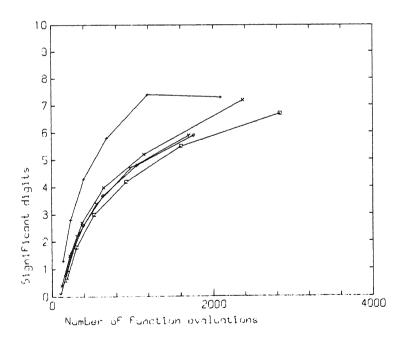


Figure 4.1
Results of problem 1

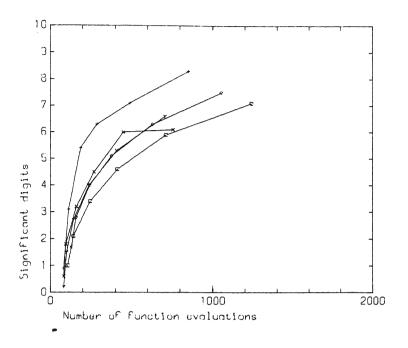


figure 4.2
Results of problem 2

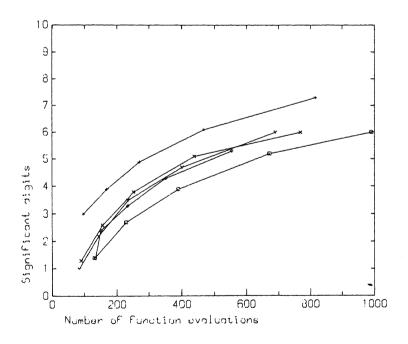


figure 4.3
Results of problem 3

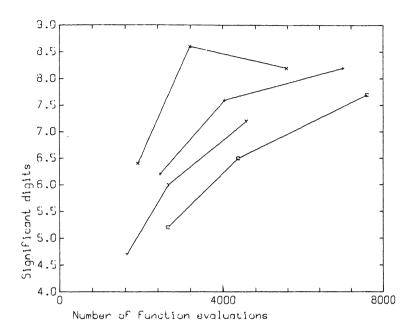


figure 4.4
Results of problem 4

Test problems

All test problems were taken from FOX [4].

Problem 1

$$\begin{cases} y_1^* = y_1^2 y_2^*, \\ y_2^* = -1/y_1^*, \quad y_1^*(0) = y_2^*(0) = 1. \end{cases}$$

Integration interval [0,5].

Solution
$$y_1 = 1/y_2 = e^x$$
.

Results for y_1 are given in figure 4.1.

Problem 2

$$y' = y - \frac{2x}{y}, \quad y(0) = 1.$$

Integration interval [0,5].

Solution
$$y = \sqrt{(2x+1)}$$
.

Results are given in figure 4.2.

Problem 3

$$y' = 10(y-x^2), y(0) = .02.$$

Integration interval [0,1].
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 y₁ 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).

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